# ITE (Information Theoretical Estimators) Matlab/Octave Toolbox Release 0.41

Zoltán Szabó

July 12, 2013

## Contents

# List of Figures



# List of Tables



# List of Examples

# List of Templates

# 1 Introduction

Since the pioneering work of Shannon [112], *entropy, mutual information, divergence* measures and their extensions have found a broad range of applications in many areas of machine learning. Entropies provide a natural notion to quantify the *uncertainty* of random variables, mutual information type indices measure the *dependence* among its arguments, divergences offer efficient tools to define the 'distance' of probability measures. Particularly, in the classical Shannon case, these three concepts form a gradually widening chain: entropy is equal to the self mutual information of a random variable, mutual information is identical to the divergence of the joint distribution and the product of the marginals [21]. Applications of Shannon entropy, -mutual information, -divergence and their generalizations cover, for example, (i) feature selection, (ii) clustering, (iii) independent component/subspace analysis, (iii) image registration, (iv) boosting, (v) optimal experiment design, (vi) causality detection, (vii) hypothesis testing, (viii) Bayesian active learning, (ix) structure learning in graphical models, (x) region-of-interest tracking, among many others. For an excellent review on the topic, the reader is referred to [7, 151, 148, 6, 88].

Independent component analysis (ICA) [54, 15, 17] a central problem of signal processing and its generalizations can be formulated as optimization problems of information theoretical objectives. One can think of ICA as a cocktail party problem: we have some speakers (sources) and some microphones (sensors), which measure the mixed signals emitted by the sources. The task is to estimate the original sources from the mixed recordings (observations). Traditional ICA algorithms are one-dimensional in the sense that all sources are assumed to be *independent* real valued random variables. However, many important applications underpin the relevance of considering extensions of ICA, such as the independent subspace analysis (ISA) problem [13, 24]. In ISA, the independent sources can be multidimensional: we have a cocktail-party, where more than one *group* of musicians are playing at the party. Successful applications of ISA include (i) the processing of EEG-fMRI, ECG data and natural images, (ii) gene expression analysis, (iii) learning of face view-subspaces, (iv) motion segmentation, (v) single-channel source separation, (vi) texture classification, (vii) action recognition in movies.

One of the most relevant and fundamental hypotheses of the ICA research is the ISA separation principle [13]: the ISA task can be solved by ICA followed by clustering of the ICA elements. This principle (i) forms the basis of the state-of-the-art ISA algorithms, (ii) can be used to design algorithms that scale well and efficiently estimate the dimensions of the hidden sources, (iii) has been recently proved [129][1], and (iv) can be extended to different linear-, controlled-, post nonlinear-, complex valued-, partially observed models, as well as to systems with nonparametric source dynamics. For a recent review on the topic, see [132].

Although there exist many exciting applications of information theoretical measures, to the best of our knowledge, available packages in this domain focus on (i) discrete variables, or (ii) quite specialized applications and information theoretical estimation methods. Our **goal** is to fill this serious gap by coming up with a (i) highly modular, (ii) free and open source, (iii) multi-platform toolbox, the ITE (information theoretical estimators) package, which

1. is capable of estimating *many* different variants of entropy, mutual information, divergence, association measures, cross quantities and kernels on distributions:
   - entropy: Shannon entropy, Rényi entropy, Tsallis entropy (Havrda and Charvát entropy), complex entropy,
   - mutual information: generalized variance (GV), kernel canonical correlation analysis (KCCA), kernel generalized variance (KGV), Hilbert-Schmidt independence criterion (HSIC), Shannon mutual information, $L_2$ mutual information, Rényi mutual information, Tsallis mutual information, copula-based kernel dependency, multivariate version of Hoeffding's $\Phi$, Schweizer-Wolff's $\sigma$ and $\kappa$, complex mutual information, Cauchy-Schwartz quadratic mutual information (QMI), Euclidean distance based QMI, distance covariance, distance correlation, approximate correntropy independence measure,
   - divergence: Kullback-Leibler divergence (relative entropy, I directed divergence), $L_2$ divergence, Rényi divergence, Tsallis divergence Hellinger distance, Bhattacharyya distance, maximum mean discrepancy (MMD, kernel distance), J-distance (symmetrised Kullback-Leibler divergence, J divergence), Cauchy-Schwartz divergence, Euclidean distance based divergence, energy distance (specially the Cramer-Von Mises distance), Jensen-Shannon divergence, Jensen-Rényi divergence, K divergence, L divergence, certain f-divergences (Csiszár-Morimoto divergence, Ali-Silvey distance), non-symmetric Bregman distance (Bregman divergence), Jensen-Tsallis divergence, symmetric Bregman distance,
   - association measures: multivariate extensions of Spearman's $\rho$ (Spearman's rank correlation coefficient, grade correlation coefficient), correntropy, centered correntropy, correntropy coefficient, correntropy induced metric, centered correntropy induced metric, multivariate extension of Blomqvist's $\beta$ (medial correlation coefficient), multivariate conditional version of Spearman's $\rho$, lower/upper tail dependence via conditional Spearman's $\rho$,

[1] Note: an alternative, exciting proof idea for deflation type methods has just now appeared in [85].

- cross quantities: cross-entropy,
- kernels on distributions: expected kernel, Bhattacharyya kernel, probability product kernel, Jensen-Shannon kernel,

based on

- nonparametric methods[2]: k-nearest neighbors, generalized k-nearest neighbors, weighted k-nearest neighbors, minimum spanning trees, geodesic spanning forests, random projection, kernel techniques, ensemble methods, sample spacing,
- kernel density estimation (KDE), adaptive partitioning, maximum entropy distribution: in plug-in scheme.

2. offers a *simple and unified framework* to
   (a) easily construct new estimators from existing ones or from scratch, and
   (b) transparently use the obtained estimators in information theoretical optimization problems.
3. with a *prototype application* in ISA and its extensions including
   - 6 different ISA objectives,
   - 4 optimization methods: (i) handling known and unknown subspace dimensions as well, with (ii) further objective-specific accelerations,
   - 5 extended problem directions: (i) different linear-, (ii) controlled-, (iii) post nonlinear-, (iv) complex valued-, (v) partially observed models, (vi) as well as systems with nonparametric source dynamics; which can be used in combinations as well.

The technical details of the ITE package are as follows:

- **Author**: Zoltán Szabó.
  - Homepage: `http://nipg.inf.elte.hu/szzoli`
  - Email: `szzoli@cs.elte.hu`
  - Affiliation: Eötvös Loránd University, Faculty of Informatics (Computer Science), Pázmány Péter sétány 1/C, Budapest, H-1117, Hungary.
- **Documentation of the source**: the source code of ITE has been enriched with numerous comments, examples, and pointers where the interested user can find further mathematical details about the embodied techniques.
- **License** (GNU GPLv3 or later): ITE is free software: you can redistribute it and/or modify it under the terms of the GNU General Public License as published by the Free Software Foundation, either version 3 of the License, or (at your option) any later version. This software is distributed in the hope that it will be useful, but WITHOUT ANY WARRANTY; without even the implied warranty of MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE. See the GNU General Public License for more details. You should have received a copy of the GNU General Public License along with ITE. If not, see <http://www.gnu.org/licenses/>.
- **Citing**: If you use the ITE toolbox in your work, please cite the papers [129, 132] (.bib in Appendix A).
- **Platforms**: The ITE package has been extensively tested on Windows and Linux. However, since it is made of standard Matlab/Octave and C/C++ files, it is expected to work on alternative platforms as well.
- **Environments**: Matlab[3], Octave[4].
- **Requirements**: The ITE package is self-contained, it only needs
  - a Matlab or an Octave environment with standard toolboxes:
    - Matlab: Image Processing, Optimization, Statistics.

[2] It is highly advantageous to apply nonparametric approaches to estimate information theoretical quantities. The bottleneck of the 'opposite' plug-in type methods, which estimate the underlying density and then plug it in into the appropriate integral formula, is that the unknown densities are nuisance parameters. As a result, plug-in type estimators scale poorly as the dimension is increasing.

[3] `http://www.mathworks.com/products/matlab/`

[4] `http://www.gnu.org/software/octave/`

    - Octave[5]: Image Processing (image), Statistics (statistics), Input/Output (io, required by statistics), Ordinary Differential Equations (odepkg), Bindings to the GNU Scientific Library (gsl), ANN wrapper (ann).
  - a C/C++ compiler – if you would like to further speed up the computations.

- **Comments, feedbacks**: are welcome.
- **Homepage of the ITE toolbox**: `https://bitbucket.org/szzoli/ite/`
- **Follower**: become a follower to be always up-to-date with ITE (`https://bitbucket.org/szzoli/ite/follow`).

The remainder of this document is organized as follows:

- Section 2 is about the installation of the ITE package. Section 3 focuses on the estimation of information theoretical quantities (entropy, mutual information, divergence, association and cross measures, kernels on distributions) and their realization in ITE. In Section 4, we present an application of Section 3 included in the ITE toolbox. The application considers the extension of independent subspace analysis (ISA, independent component analysis with multidimensional sources) to different linear-, controlled-, post nonlinear-, complex valued-, partially observed problems, as well as problems dealing with nonparametric source dynamics, i.e., the independent process analysis (IPA) problem family. Section 5 is about the organization of the directories of the ITE toolbox.
- Citing information of the ITE package is provided in Appendix A. Abbreviations of the paper are listed in Appendix B (Table 26). Functions with Octave-specific adaptations are summarized in Appendix C (Table 27). Some further formal definitions (concordance ordering, measure of concordance and -dependence, semimetric space of negative type, (covariant) Hilbertian metric, f-divergence) are given in Appendix D to make the documentation self-contained. A brief summary (lookup table) of the computations related to entropy, mutual information, divergence, association and cross measures, and kernels on distributions can be found in Appendix E.

# 2 Installation

This section is about (i) the installation of the ITE toolbox, and (ii) the external packages, dedicated solvers embedded in the ITE package. The purpose of this inclusion is twofold:

- to further increase the efficiency of certain subtasks to be solved (e.g., k-nearest neighbor search, finding minimum spanning trees, some subtasks revived by the IPA separation principles (see Section 4.1)),
- to provide both purely Matlab/Octave implementations, and specialized (often faster) non-Matlab/-Octave solutions that can be called from Matlab/Octave.

The core of the ITE toolbox has been written in Matlab, as far it was possible in an Octave compatible way. The particularities of Octave has been taken into account by adapting the code to the *actual* environment (Matlab/Octave). The working environment can be queried (e.g., in case of extending the package it is also useful) by the `working_environment_Matlab.m` function included in ITE. Adaptations has been carried out in the functions listed in Appendix C (Table 27). The functionalities extended by the external packages are also available in both environments (Table 1).

Here, a short description of the embedded/downloaded packages (directory 'shared/embedded', 'shared/downloaded') is given:

1. **fastICA** (directory 'shared/embedded/FastICA'; version 2.5):
   - **URL**: `http://research.ics.tkk.fi/ica/fastica/`
   - **License**: GNU GPLv2 or later.
   - **Solver**: ICA (independent component analysis).
   - **Installation**: Add it with subfolders to your Matlab/Octave PATH.
   - **Environment**: Matlab, Octave.
   - **Note**: By commenting out the `g_FastICA_interrupt` variable in `fpica.m`, the `fastica.m` function can be used in Octave, too. The provided fastICA code in the ITE toolbox contains this modification.
2. **Complex fastICA** (directory 'shared/embedded/CFastICA')

[5] See `http://octave.sourceforge.net/packages.php`.

- **URL**: `http://www.cs.helsinki.fi/u/ebingham/software.html`, `http://users.ics.aalto.fi/ella/publications/cfastica_public.m`
- **License**: GNU GPLv2 or later.
- **Solver**: complex ICA.
- **Installation**: Add it with subfolders to your Matlab/Octave PATH.
- **Environment**: Matlab, Octave.

3. **ANN (approximate nearest neighbor) Matlab wrapper** (directory 'shared/embedded/ann_wrapperM'; version 'Mar2012'):
   - **URL**: `http://www.wisdom.weizmann.ac.il/~bagon/matlab.html`, `http://www.wisdom.weizmann.ac.il/~bagon/matlab_code/ann_wrapper_Mar2012.tar.gz`
   - **License**: GNU LGPLv3.
   - **Solver**: approximate nearest neighbor computation.
   - **Installation**: Follow the instructions in the ANN wrapper package (README.txt: INSTALLATION) till 'ann_class_compile'. Note: If you use a more recent C++ compiler (e.g., g++ on Linux), you have to include the following 2 lines into the original code to be able to compile the source:
     (a) '#include <cstdlib>' to 'ANNx.h'
     (b) '#include <cstring>' to 'kd_tree.h'
     The provided ANN code in the ITE package contains these modifications.
   - **Environment**: Matlab, Octave[6].
   - **Note**: fast nearest neighbor alternative of `knnsearch` ∈ Matlab: Statistics Toolbox.

4. **MatlabBGL** (directory 'shared/embedded/MatlabBGL', version 4.0)
   - **URL**: `https://github.com/dgleich/matlab-bgl`, `http://www.mathworks.com/matlabcentral/fileexchange/10922`
   - **License**: 2-clause BSD, and GNU GPLv2 or later.
   - **Solver**: minimum spanning trees: Prim and Kruskal algorithm.
   - **Installation**: Add it with subfolders to your Matlab/Octave PATH. Note:
     - The package includes precompiled MEX files for Windows (32-bit and 64-bit), and Linux (32-bit and 64-bit for Matlab 2006b+), and MacOSX (32-bit Intel and 32-bit PPC).
     - The package includes source code to compile on other platforms as well.
   - **Environment**: Matlab, Octave[7].
   - **Note**: alternative of '14) = pmtk3' in finding minimum spanning trees.

5. **FastKICA** (directory 'shared/embedded/FastKICA', version 1.0):
   - **URL**: `http://people.kyb.tuebingen.mpg.de/arthur/fastkica.htm`
   - **License**: GNU GPL v2 or later.
   - **Solver**: HSIC (Hilbert-Schmidt independence criterion) mutual information estimator.
   - **Installation**: Add it with subfolders to your Matlab/Octave PATH.
   - **Environment**: Matlab, Octave.
   - **Note**: one can extend the implementation of HSIC to measure the dependence of $d_m$-dimensional variables, too. The ITE toolbox contains this modification.

6. **NCut** (Normalized Cut, directory 'shared/embedded/NCut'; version 9):
   - **URL**: `http://www.seas.upenn.edu/~timothee/software/ncut/ncut.html`, `http://www.seas.upenn.edu/~timothee/software/ncut/Ncut_9.zip`
   - **License**: GNU GPLv3.
   - **Solver**: spectral clustering, fixed number of groups.
   - **Installation**: Run `compileDir_simple.m` from Matlab to the provided directory of functions.
   - **Environment**: Matlab.

[6] At the time of writing this paper, the Octave ANN wrapper (`http://octave.sourceforge.net/ann/index.html`, version 1.0.2) supports 2.9.12 ≤ Octave < 3.4.0. According to our experiences, however the ann wrapper can also be used for higher versions of Octave provided that (i) a new swig package (`www.swig.org/`) is used (>=2.0.5), (ii) a new 'SWIG=swig' line is inserted in src/ann/bindings/Makefile (the ITE package contains the modified makefile), and (iii) the row containing 'typedef OCTAVE_IDX_TYPE octave_idx_type;' (in '.../octave/config.h') is commented out for the time of 'make'-ing.

[7] With some trick, the MatlabBGL works on Octave, see `https://answers.launchpad.net/matlab-bgl/+question/48686`.

- **Note**: the package is a fast alternative of '11) = spectral clustering'.

7. **sqdistance** (directory 'shared/embedded/sqdistance')
   - **URL**: `http://www.mathworks.com/matlabcentral/fileexchange/24599-pairwise-distance-matrix/`, `http://www.mathworks.com/matlabcentral/fileexchange/24599-pairwise-distance-matrix?download=true`
   - **License**: 2-clause BSD.
   - **Solver**: fast pairwise distance computation.
   - **Installation**: Add it with subfolders to your Matlab/Octave PATH.
   - **Environment**: Matlab, Octave.
   - **Note**: compares favourably to the Matlab/Octave function `pdist`.

8. **TCA** (directory 'shared/embedded/TCA'; version 1.0):
   - **URL**: `http://www.di.ens.fr/~fbach/tca/index.htm`, `http://www.di.ens.fr/~fbach/tca/tca1_0.tar.gz`
   - **License**: GNU GPLv2 or later.
   - **Solver**: KCCA (kernel canonical correlation analysis) / KGV (kernel generalized variance) estimator, incomplete Cholesky decomposition.
   - **Installation**: Add it with subfolders to your Matlab/Octave PATH.
   - **Environment**: Matlab, Octave.
   - **Note**: Incomplete Cholesky factorization can be carried out by the Matlab/Octave function `chol_gauss.m`. One can also compile the included `chol_gauss.c` to attain improved performance. Functions provided in the ITE toolbox contain extensions of the KCCA and KGV indices to measure the dependence of $d_m$-dimensional variables. The computations have also been accelerated in ITE by '7) = sqdistance'.

9. **Weighted kNN** (kNN: k-nearest neighbor; directory 'shared/embedded/weightedkNN' and the core of `HRenyi_weightedkNN_estimation.m`):
   - **URL**: `http://www-personal.umich.edu/~kksreddy/`
   - **License**: GNU GPLv3 or later.
   - **Solver**: Rényi entropy estimator based on the weighted k-nearest neighbor method.
   - **Installation**: Add it with subfolders to your Matlab/Octave PATH.
   - **Environment**: Matlab, Octave.
   - **Note**: in the weighted kNN technique the weights are optimized. Since Matlab and Octave rely on different optimization engines, one has to adapt the weight estimation procedure to Octave. The `calculateweight.m` function in ITE contains this modification.

10. **E4** (directory 'shared/embedded/E4'):
    - **URL**: `http://www.ucm.es/info/icae/e4/`, `http://www.ucm.es/info/icae/e4/downfiles/E4.zip`
    - **License**: GNU GPLv2 or later.
    - **Solver**: AR (autoregressive) fit.
    - **Installation**: Add it with subfolders to your Matlab/Octave PATH[8].
    - **Environment**: Matlab, Octave.
    - **Note**: alternative of '13) = ARfit' in AR identification.

11. **spectral clustering** (directory 'shared/embedded/sp_clustering'):
    - **URL**: `http://www.mathworks.com/matlabcentral/fileexchange/34412-fast-and-efficient-spectral-clustering`
    - **License**: 2-clause BSD.
    - **Solver**: spectral clustering.
    - **Installation**: Add it with subfolders to your Matlab/Octave PATH.
    - **Environment**: Matlab, Octave.
    - **Note**: the package is a purely Matlab/Octave alternative of '6)=NCut'. It is advisable to alter the eigensystem computation in the `SpectralClustering.m` function to work stably in Octave; the modification is included in the ITE toolbox and is activated in case of Octave environment.

[8] In Octave, this step results in a 'warning: function `.../shared/embedded/E4/vech.m` shadows a core library function'; it is OK, the two functions compute the same quantity.

12. **clinep** (directory 'shared/embedded/clinep'):
    - **URL**: `http://www.mathworks.com/matlabcentral/fileexchange/8597-plot-3d-color-line/content/clinep.m`
    - **License**: 2-clause BSD.
    - **Solver**: Plots a 3D line with color encoding along the length using the patch function.
    - **Installation**: Add it with subfolders to your Matlab/Octave PATH.
    - **Environment**: Matlab, Octave.
    - **Note**: (i) calling of the cylinder function (in `clinep.m`) has to modified somewhat to work in Octave, and (ii) since 'gnuplot (as of v4.2) only supports 3D filled triangular patches' one has to use the fltk graphics toolkit in Octave for drawing. The included `cline.m` code in the ITE package contains these modifications.

13. **ARfit** (directory 'shared/downloaded/ARfit', version 'March 20, 2011')
    - **URL**: `http://www.gps.caltech.edu/~tapio/arfit/`, `http://www.gps.caltech.edu/~tapio/arfit/arfit.zip`. Note: temporarily this website seems to be unavailable. The download link (at the moment) is `http://www.mathworks.com/matlabcentral/fileexchange/174-arfit?download=true`.
    - **License**: ACM.
    - **Solver**: AR identification.
    - **Installation**: Download, extract and add it with subfolders to your Matlab/Octave PATH.
    - **Environment**: Matlab, Octave.
    - **Note**: alternative of '10) = E4' in AR identification.

14. **pmtk3** (directory 'shared/embedded/pmtk3', version 'Jan 2012')
    - **URL**: `http://code.google.com/p/pmtk3`, `http://code.google.com/p/pmtk3/downloads/detail?name=pmtk3-3jan11.zip&can=2&q=`.
    - **License**: MIT.
    - **Solver**: minimum spanning trees: Prim algorithm.
    - **Installation**: Add it with subfolders to your Matlab/Octave PATH.
    - **Environment**: Matlab, Octave.
    - **Note**: purely Matlab/Octave alternative of '4) = MatlabBGL' in finding minimum spanning trees.

15. **knn** (directory 'shared/embedded/knn', version 'Nov 02, 2010')
    - **URL**: `http://www.mathworks.com/matlabcentral/fileexchange/28897-k-nearest-neighbor-search`, `http://www.mathworks.com/matlabcentral/fileexchange/28897-k-nearest-neighbor-search?download=true`
    - **License**: 2-clause BSD.
    - **Solver**: kNN search.
    - **Installation**: Run the included `build` command to compile the partial sorting function `top.cpp`. Add it with subfolders to your Matlab/Octave PATH.
    - **Environment**: Matlab, Octave.
    - **Note**: Alternative of '3)=ANN' in finding k-nearest neighbors.

16. **SWICA** (directory 'shared/embedded/SWICA')
    - **URL**: `http://www.stat.purdue.edu/~skirshne/SWICA`, `http://www.stat.purdue.edu/~skirshne/SWICA/swica.tar.gz`
    - **License**: 3-clause BSD.
    - **Solver**: Schweizer-Wolff's $\sigma$ and $\kappa$ estimation.
    - **Installation**: Add it with subfolders to your Matlab/Octave PATH.
    - **Environment**: Matlab, Octave.
    - **Note**: one can also compile the included `SW_kappa.cpp` and `SW_sigma.cpp` functions to further accelerate computations (see '`build_SWICA.m`').

17. **ITL** (directory 'shared/embedded/ITL'; version '14.11.2012'):
    - **URL**: `http://www.sohanseth.com/ITL%20Toolbox.zip?attredirects=0`, `http://www.sohanseth.com/Home/codes`.
    - **License**: GNU GPLv3.

- **Solver**: KDE based estimation of Cauchy-Schwartz quadratic mutual information, Euclidean distance based quadratic mutual information; and associated divergences; correntropy, centered correntropy, correntropy coefficient.
- **Installation**: Add it with subfolders to your Matlab/Octave PATH.
- **Environment**: Matlab, Octave.

18. **KDP** (directory 'shared/embedded/KDP'; version '1.1.1')
    - **URL**: `https://github.com/danstowell/kdpee`
    - **License**: GNU GPLv3 or later.
    - **Solver**: adaptive partitioning based Shannon entropy estimation.
    - **Installation**: Run the included `mexme` command from the `mat_oct` subfolder. Add it with subfolders to your Matlab/Octave PATH.
    - **Environment**: Matlab, Octave.

A short summary of the packages can be found in Table 1. To ease installation, the ITE package contains an installation script, `ITE_install.m`. A typical usage is to cd to the directory 'code' and call `ITE_install(pwd)`. Running the script from Matlab/Octave, it (i) adds the main ITE directory with subfolders to the Matlab/Octave PATH, (ii) downloads and extracts the ARfit package, and (iii) compiles the embedded ANN, NCut, TCA, SWICA, knn, KDP packages, .cpp accelerations of the Hoeffding's $\Phi$ [see Eq. (21)], Edgeworth expansion based entropy [see Eq.(220)] computation, and the continuously differentiable sample spacing (CDSS) based estimator [see Eq. (249)].[9] The `ITE_install.m` script automatically detects the working environment (Matlab/Octave) and performs the installation accordingly, for example, it deletes the ann wrapper not suitable for the current working environment. The output of a successful installation in Matlab is given below (the Octave output is similar):

**Example 1 (ITE installation (output; with compilation))**

```
>> ITE_install(pwd); %after cd-ing to the code directory
Installation: started.
We are working in Matlab environment. => ann_wrapper for Octave: deleted.
ARfit package: downloading, extraction: started.
ARfit package: downloading, extraction: ready.
ITE directory: added with subfolders to the Matlab PATH.
ANN compilation: started.
ANN compilation: ready.
NCut compilation: started.
NCut compilation: ready.
TCA (chol_gauss.c) compilation: started.
TCA (chol_gauss.c) compilation: ready.
SWICA (SW_kappa.cpp, SW_sigma.cpp) compilation: started.
SWICA (SW_kappa.cpp, SW_sigma.cpp) compilation: ready.
Hoeffding_term1.cpp compilation: started.
Hoeffding_term1.cpp compilation: ready.
Edgeworth_t1_t2_t3.cpp compilation: started.
Edgeworth_t1_t2_t3.cpp compilation: ready.
compute_CDSS.cpp compilation: started.
compute_CDSS.cpp compilation: ready.
knn (top.cpp) compilation: started.
knn (top.cpp) compilation: ready.
KDP (kdpee.c, kdpeemex.c) compilation: started.
KDP (kdpee.c, kdpeemex.c) compilation: ready.
------------------
Installation tests:
ANN quick test: successful.
NCut quick test: successful.
```

[9] The ITE package also offers purely Matlab/Octave implementations for the computation of Hoeffding's $\Phi$, Edgeworth expansion based entropy approximation and CDSS. Without compilation, these Matlab/Octave implementations are evoked.

| Task | Package | Written in | Environment | Directory |
|---|---|---|---|---|
| ICA | fastICA | Matlab | Matlab, Octave | shared/embedded/FastICA |
| complex ICA | complex fastICA | Matlab | Matlab, Octave | shared/embedded/CFastICA |
| kNN search | ANN | C++ | Matlab | shared/embedded/ann_wrapperM[a] |
| kNN search | ANN | C++ | Octave[b] | shared/embedded/ann_wrapperO[a] |
| Prim-, Kruskal algorithm | MatlabBGL | C++ | Matlab, Octave[c] | shared/embedded/MatlabBGL |
| HSIC estimation | FastKICA | Matlab | Matlab, Octave | shared/embedded/FastKICA |
| spectral clustering | NCut | C++ | Matlab | shared/embedded/NCut |
| fast pairwise distance computation | sqdistance | Matlab | Matlab, Octave | shared/embedded/sqdistance |
| KCCA, KGV | TCA | Matlab, C | Matlab, Octave | shared/embedded/TCA |
| Rényi entropy via weighted kNNs | weighted kNN | Matlab | Matlab, Octave | shared/embedded/weightedkNN |
| AR fit | E4 | Matlab | Matlab, Octave | shared/embedded/E4 |
| spectral clustering | spectral clustering | Matlab | Matlab, Octave | shared/embedded/sp_clustering |
| trajectory plot | clinep | Matlab | Matlab, Octave | shared/embedded/clinep |
| AR fit | ARfit | Matlab | Matlab, Octave | shared/downloaded/ARfit |
| Prim algorithm | pmtk3 | Matlab | Matlab, Octave | shared/embedded/pmtk3 |
| kNN search | knn | Matlab, C++ | Matlab, Octave | shared/embedded/knn |
| Schweizer-Wolff's $\sigma$ and $\kappa$ | SWICA | Matlab, C++ | Matlab, Octave | shared/embedded/SWICA |
| KDE based estimation[d] | ITL | Matlab | Matlab, Octave | shared/embedded/ITL |
| adaptive (k-d) partitioning | kdpee | Matlab, C | Matlab, Octave | shared/embedded/KDP |

Table 1: External, dedicated packages increasing the efficiency of ITE.

[a] In 'ann_wrapperM' 'M' stands for Matlab, in 'ann_wrapperO' 'O' denotes Octave.
[b] See footnote 6.
[c] See footnote 7.
[d] KDE based estimation of Cauchy-Schwartz quadratic mutual information, Euclidean distance based quadratic mutual information; and associated divergences; correntropy, centered correntropy, correntropy coefficient.

```
ARfit quick test: successful.
knn quick test: successful.
KDP quick test: successful.
```

# 3 Estimation of Information Theoretical Quantities

In this section we focus on the estimation of information theoretical quantities. Particularly, in the sequel, the underlying idea how the estimators are implemented in ITE are detailed, accompanied with definitions, numerous examples and extension possibilities/instructions.

The ITE package supports the estimation of many different variants of entropy, mutual information, divergence, association and cross measures, kernels on distributions:

1. From construction point of view, we distinguish two types of estimators in ITE: *base* (Section 3.1) and *meta* (Section 3.2) ones. Meta estimators are *derived* from existing base/meta ones by taking into account information theoretical identities. For example, by considering the well-known

$$I\left(\mathbf{y}^1,\ldots,\mathbf{y}^M\right) = \sum_{m=1}^{M} H\left(\mathbf{y}^m\right) - H\left(\left[\mathbf{y}^1;\ldots;\mathbf{y}^M\right]\right) \tag{1}$$

   relation [21], one can estimate mutual information ($I$) by making use of existing entropy estimators ($H$).

2. From calling point of view, base and meta estimations follow exactly the same syntax (Section 3.3).

This modular implementation of the ITE package, makes it possible to

1. construct new estimators from existing ones, and
2. transparently use *any* of these estimators in information theoretical optimization problems (see Section 4) – provided that they follow a simple template described in Section 3.3.

## 3.1 Base Estimators

This section is about the *base* information theoretical estimators of the ITE package. Entropy estimation is in the focus of Section 3.1.1; in Section 3.1.2, Section 3.1.3, Section 3.1.4, Section 3.1.5, Section 3.1.6 we consider the estimation of mutual information, divergence, association-, cross measures and kernels on distributions, respectively.

### 3.1.1 Entropy Estimators

Let us start with a simple example: our goal is to estimate the **Shannon entropy** [112]

$$H(\mathbf{y}) = -\int_{\mathbb{R}^d} f(\mathbf{u}) \log f(\mathbf{u}) \mathrm{d}\mathbf{u} \tag{2}$$

of a random variable $\mathbf{y} \in \mathbb{R}^d$ from which we have i.i.d. (independent identically distributed) samples $\{\mathbf{y}_t\}_{t=1}^T$, and $f$ denotes the density function of $\mathbf{y}$; shortly $\mathbf{y} \sim f$. The estimation of Shannon entropy can be carried out, e.g., by k-nearest neighbor techniques. Let us also assume that multiplicative contants are also important for us – in many applications, it is completely irrelevant whether we estimate, for example, $H(\mathbf{y})$ or $cH(\mathbf{y})$, where $c = c(d)$ is a constant depending only on the *dimension* of $\mathbf{y}$ ($d$), but *not on the distribution* of $\mathbf{y}$. By using the ITE package, the estimation can be carried out as simply as follows:

**Example 2 (Entropy estimation (base-1: usage))**

```
>Y = rand(5,1000);                          %generate the data of interest (d=5, T=1000)
>mult = 1;                                  %multiplicative constant is important
>co = HShannon_kNN_k_initialization(mult); %initialize the entropy ('H') estimator
                                            %('Shannon_kNN_k'), including the value of k
>H = HShannon_kNN_k_estimation(Y,co);       %perform entropy estimation
```

Alternative entropy measures of interest include the:

1. **Rényi entropy** [102]: defined as

$$H_{\mathrm{R},\alpha}(\mathbf{y}) = \frac{1}{1-\alpha} \log \int_{\mathbb{R}^d} f^\alpha(\mathbf{u}) \mathrm{d}\mathbf{u}, (\quad \alpha \neq 1) \tag{3}$$

   where the random variable $\mathbf{y} \in \mathbb{R}^d$ have density function $f$. The Shannon entropy [Eq. (2)] is a special case of the Rényi entropy family, in limit:

$$\lim_{\alpha \to 1} H_{\mathrm{R},\alpha} = H. \tag{4}$$

2. **Tsallis entropy** (also called the Havrda and Charvát entropy) [144, 40]: is closely related to the Rényi entropy. It is defined as

$$H_{\mathrm{T},\alpha}(\mathbf{y}) = \frac{1}{\alpha - 1} \left( 1 - \int_{\mathbb{R}^d} f^\alpha(\mathbf{u}) \mathrm{d}\mathbf{u} \right), \quad \alpha \neq 1. \tag{5}$$

   The Shannon entropy is a special case of the Tsallis entropy family, in limit:

$$\lim_{\alpha \to 1} H_{\mathrm{T},\alpha} = H. \tag{6}$$

In the ITE toolbox, $H_{\mathrm{R},\alpha}$ and $H_{\mathrm{T},\alpha}$ can be estimated similarly to the Shannon entropy $H$ (see Example 2):

**Example 3 (Entropy estimation (base-2: usage))**

```
>Y = rand(5,1000);                          %generate the data of interest (d=5, T=1000)
>mult = 1;                                  %multiplicative constant is important
>co = HRenyi_kNN_k_initialization(mult);    %initialize the entropy ('H') estimator ('Renyi_kNN_k'),
                                            %including the value of k and α
>H = HRenyi_kNN_k_estimation(Y,co);         %perform entropy estimation
```

Beyond k-nearest neighbor based $H$ (see [59] ($S=\{1\}$), [115, 34] $S=\{k\}$; in ITE 'Shannon_kNN_k') and $H_{\mathrm{R},\alpha}$ estimation methods [155, 64] ($S=\{k\}$; 'Renyi_kNN_k'), the ITE package also provide functions for the estimation of $H_{\mathrm{R},\alpha}(\mathbf{y})$ ($\mathbf{y}\in\mathbb{R}^d$) using (i) k-nearest neighbors ($S=\{1,\ldots,k\}$; 'Renyi_kNN_1tok') [95], (ii) generalized nearest neighbor graphs ($S\subseteq\{1,\ldots,k\}$; 'Renyi_kNN_S') [93], (iii) weighted k-nearest neighbors ('Renyi_weightedkNN') [118], (iv) minimum spanning trees ('Renyi_MST') [155], and (v) geodesic spanning forests ('Renyi_GSF') [19]. The Tsallis entropy of a d-dimensional random variable $\mathbf{y}$ ($H_{\mathrm{T},\alpha}(\mathbf{y})$) can be estimated in ITE using the k-nearest neighbors method ($S=\{k\}$; 'Tsallis_kNN_k') [64]. The multivariate Edgeworth expansion [45], the Voronoi region [73], and the k-d partitioning [120] based Shannon entropy estimators are also available in ITE ('Shannon_Edgeworth', 'Shannon_Voronoi', 'Shannon_KDP').

For the one-dimensional case ($d=1$), beside the previous techniques, ITE offers

- sample spacing based estimators:
  - Shannon entropy: by approximating the slope of the inverse distribution function [147] ('Shannon_spacing_V') and its bias corrected variant [29] ('Shannon_spacing_Vb'). The method described in [18] applies locally linear regression ('Shannon_spacing_LL'). Piecewise constant/linear correction has been applied in [83] ('Shannon_spacing_Vpconst')/[26] ('Shannon_spacing_Vplin').
  - Rényi entropy: The idea of [147] and the empiric entropy estimator of order $m$ has been recently generalized to Rényi entropies [150] ('Renyi_spacing_V', 'Renyi_spacing_E'). A continuously differentiable sample spacing (CDSS) based quadratic Rényi entropy estimator was presented in [84] ('qRenyi_CDSS').
- maximum entropy distribution based estimators for the Shannon entropy [21, 46] with different function sets, see 'Shannon_MaxEnt1', 'Shannon_MaxEnt2'.

The base entropy estimators of the ITE package are summarized in Table 2; the calling syntax of these methods is the same as in Example 2 and Example 3, one only has to change 'Shannon_kNN_k' (see Example 2) and 'Renyi_kNN_k' (see Example 3) to the cost_name given in the last column of the table.

Note: the Renyi_kNN_1tok, Renyi_kNN_S, Renyi_MST, Renyi_GSF methods (see Table 2) estimate the $H_\alpha$ Rényi entropy up to an additive constant which depends on the dimension $d$ and $\alpha$, but *not* on the distribution. In certain cases, such additive constants can also be relevant. They can be approximated via Monte-Carlo simulations, the computations are available in ITE. Let us take the example of Renyi_kNN_1tok, the estimation instructions are as follows:

1. Set co.alpha ($\alpha$) and co.k ($k$) in 'HRenyi_kNN_1tok_initialization.m'.
2. Estimate the additive constant $\beta=\beta(d,k,\alpha)$ using 'estimate_HRenyi_constant.m'.
3. Set the relevance of additive constants in the initialization function 'HRenyi_kNN_1tok_initialization.m': 'co.additive_constant_is_relevant = 1'.
4. Estimate the Rényi entropy (after initialization): 'HRenyi_kNN_1tok_estimation.m'.

### 3.1.2 Mutual Information Estimators

In our next example, we consider the estimation of the **mutual information** of the $d_m$-dimensional components of the random variable $\mathbf{y}=\left[\mathbf{y}^1;\ldots;\mathbf{y}^M\right]\in\mathbb{R}^d$ ($d=\sum_{m=1}^M d_m$):

$$I\left(\mathbf{y}^1,\ldots,\mathbf{y}^M\right)=\int_{\mathbb{R}^{d_1}}\cdots\int_{\mathbb{R}^{d_M}} f\left(\mathbf{u}^1,\ldots,\mathbf{u}^M\right)\log\left[\frac{f\left(\mathbf{u}^1,\ldots,\mathbf{u}^M\right)}{\prod_{m=1}^M f_m(\mathbf{u}^m)}\right]\mathrm{d}\mathbf{u}^1\cdots\mathrm{d}\mathbf{u}^M \tag{7}$$

using an i.i.d. sample set $\{\mathbf{y}_t\}_{t=1}^T$ from $\mathbf{y}$, where $f$ is the joint density function of $\mathbf{y}$ and $f_m$ is its $m^{th}$ marginal density, the density function of $\mathbf{y}^m$. As it is known, $I\left(\mathbf{y}^1,\ldots,\mathbf{y}^M\right)$ is non-negative and is zero, if and only if the $\{\mathbf{y}^m\}_{m=1}^M$ variables are jointly independent [21]. Mutual information can be efficiently estimated, e.g., on the basis of entropy [Eq. (1)] or Kullback-Leibler divergence; we will return to these *derived* approaches while presenting *meta* estimators in Section 3.2.

There also exist other mutual information-like quantities measuring the independence of $\mathbf{y}^m$s:

1. **Kernel canonical correlation analysis (KCCA)**: The KCCA measure is defined as

$$I_{\mathrm{KCCA}}(\mathbf{y}^1,\mathbf{y}^2)=\sup_{g_1\in\mathcal{F}^1,g_2\in\mathcal{F}^2}\frac{\mathrm{cov}[g_1(\mathbf{y}^1),g_2(\mathbf{y}^2)]}{\sqrt{\mathrm{var}\left[g_1(\mathbf{y}^1)\right]+\kappa\left\|g_1\right\|_{\mathcal{F}^1}^2}\sqrt{\mathrm{var}\left[g_2(\mathbf{y}^2)\right]+\kappa\left\|g_2\right\|_{\mathcal{F}^2}^2}},\quad(\kappa>0) \tag{8}$$

| Estimated quantity | Principle | $d$ | cost_name |
|---|---|---|---|
| Shannon entropy ($H$) | k-nearest neighbors ($S = \{k\}$) | $d \geq 1$ | 'Shannon_kNN_k' |
| Rényi entropy ($H_{\mathrm{R},\alpha}$) | k-nearest neighbors ($S = \{k\}$) | $d \geq 1$ | 'Renyi_kNN_k' |
| Rényi entropy ($H_{\mathrm{R},\alpha}$) | k-nearest neighbors ($S = \{1, \ldots, k\}$) | $d \geq 1$ | 'Renyi_kNN_1tok' |
| Rényi entropy ($H_{\mathrm{R},\alpha}$) | generalized nearest neighbor graphs ($S \subseteq \{1, \ldots, k\}$) | $d \geq 1$ | 'Renyi_kNN_S' |
| Rényi entropy ($H_{\mathrm{R},\alpha}$) | weighted k-nearest neighbors | $d \geq 1$ | 'Renyi_weightedkNN' |
| Rényi entropy ($H_{\mathrm{R},\alpha}$) | minimum spanning trees | $d \geq 1$ | 'Renyi_MST' |
| Rényi entropy ($H_{\mathrm{R},\alpha}$) | geodesic spanning forests | $d \geq 1$ | 'Renyi_GSF' |
| Tsallis entropy ($H_{\mathrm{T},\alpha}$) | k-nearest neighbors ($S = \{k\}$) | $d \geq 1$ | 'Tsallis_kNN_k' |
| Shannon entropy ($H$) | multivariate Edgeworth expansion | $d \geq 1$ | 'Shannon_Edgeworth' |
| Shannon entropy ($H$) | Voronoi regions | $d \geq 2$ | 'Shannon_Voronoi' |
| Shannon entropy ($H$) | approximate slope of the inverse distribution function | $d = 1$ | 'Shannon_spacing_V' |
| Shannon entropy ($H$) | a bias corrected version of 'Shannon_spacing_V' | $d = 1$ | 'Shannon_spacing_Vb' |
| Shannon entropy ($H$) | 'Shannon_spacing_V' with piecewise constant correction | $d = 1$ | 'Shannon_spacing_Vpconst' |
| Shannon entropy ($H$) | 'Shannon_spacing_V' with piecewise linear correction | $d = 1$ | 'Shannon_spacing_Vplin' |
| Shannon entropy ($H$) | locally linear regression | $d = 1$ | 'Shannon_spacing_LL' |
| Rényi entropy ($H_{\mathrm{R},\alpha}$) | extension of 'Shannon_spacing_V' to $H_{\mathrm{R},\alpha}$ | $d = 1$ | 'Renyi_spacing_V' |
| Rényi entropy ($H_{\mathrm{R},\alpha}$) | empiric entropy estimator of order $m$ | $d = 1$ | 'Renyi_spacing_E' |
| quadratic Rényi entropy ($H_{\mathrm{R},2}$) | continuously differentiable sample spacing | $d = 1$ | 'qRenyi_CDSS' |
| Shannon entropy ($H$) | adaptive (k-d) partitioning, plug-in | $d \geq 1$ | 'Shannon_KDP' |
| Shannon entropy ($H$) | maximum entropy distribution, function set1, plug-in | $d = 1$ | 'Shannon_MaxEnt1' |
| Shannon entropy ($H$) | maximum entropy distribution, function set2, plug-in | $d = 1$ | 'Shannon_MaxEnt2' |

Table 2: Entropy estimators (base). Third column: dimension ($d$) constraint.

for $M = 2$ components, where 'cov' denotes covariance and 'var' stands for variance. In words, $I_{\mathrm{KCCA}}$ is the regularized form of the supremum correlation of $\mathbf{y}^1 \in \mathbb{R}^{d_1}$ and $\mathbf{y}^2 \in \mathbb{R}^{d_2}$ over two 'rich enough' reproducing kernel Hilbert spaces (RKHSs), $\mathcal{F}^1$ and $\mathcal{F}^2$. The computation of $I_{\mathrm{KCCA}}$ can be reduced to a generalized eigenvalue problem and the measure can be extended to $M \geq 2$ components to measure pairwise independence [5, 129]. The cost is called 'KCCA' in ITE.

2. **Kernel generalized variance (KGV)**: Let $\mathbf{y} = \left[\mathbf{y}^1; \ldots; \mathbf{y}^M\right]$ be a multidimensional Gaussian random variable with covariance matrix $\mathbf{C}$ and let $\mathbf{C}^{i,j} \in \mathbb{R}^{d_i \times d_j}$ denote the cross-covariance between components of $\mathbf{y}^m \in \mathbb{R}^{d_m}$. In the Gaussian case, the mutual information between components $\mathbf{y}^1, \ldots, \mathbf{y}^M$ is [21]:

$$I\left(\mathbf{y}^1, \ldots, \mathbf{y}^M\right) = -\frac{1}{2} \log \left( \frac{\det \mathbf{C}}{\prod_{m=1}^M \det \mathbf{C}^{m,m}} \right). \tag{9}$$

If $\mathbf{y}$ is *not normal* then one can transform $\mathbf{y}^m$s using feature mapping $\boldsymbol{\varphi}$ associated with an RKHS and apply Gaussian approximation to obtain

$$I_{\mathrm{KGV}}\left(\mathbf{y}^1, \ldots, \mathbf{y}^M\right) = -\frac{1}{2} \log \left[ \frac{\det(\boldsymbol{\mathcal{K}})}{\prod_{m=1}^M \det(\boldsymbol{\mathcal{K}}^{m,m})} \right], \tag{10}$$

where $\boldsymbol{\phi}(\mathbf{y}) := [\boldsymbol{\varphi}(\mathbf{y}^1); \ldots; \boldsymbol{\varphi}(\mathbf{y}^M)]$, $\boldsymbol{\mathcal{K}} := cov[\boldsymbol{\phi}(\mathbf{y})]$, and the sub-matrices are $\boldsymbol{\mathcal{K}}^{i,j} = cov[\boldsymbol{\varphi}(\mathbf{y}^i), \boldsymbol{\varphi}(\mathbf{y}^j)]$. For further details on the KGV method, see [5, 129]. The objective is called 'KGV' in ITE.

3. **Hilbert-Schmidt independence criterion (HSIC)**: Let us given two separable RKHSs $\mathcal{F}^1$ and $\mathcal{F}^2$ with associated feature maps $\boldsymbol{\varphi}_1$ and $\boldsymbol{\varphi}_2$. Let the corresponding cross-covariance operator be

$$\mathbf{C}_{\mathbf{y}^1,\mathbf{y}^2} = \mathbb{E}\left( \left[\boldsymbol{\varphi}_1(\mathbf{y}^1) - \boldsymbol{\mu}_1\right] \otimes \left[\boldsymbol{\varphi}_2(\mathbf{y}^2) - \boldsymbol{\mu}_2\right] \right), \tag{11}$$

where $\otimes$ denotes tensor product, $\mathbb{E}$ is the expectation and the mean embeddings are

$$\boldsymbol{\mu}_m = \mathbb{E}[\boldsymbol{\varphi}_m(\mathbf{y}^m)] \quad (m = 1, 2). \tag{12}$$

HSIC [37] is defined as the Hilbert-Schmidt norm of the cross-covariance operator

$$I_{\mathrm{HSIC}}\left(\mathbf{y}^1,\mathbf{y}^2\right)=\left\|\mathbf{C}_{\mathbf{y}^1,\mathbf{y}^2}\right\|_{\mathrm{HS}}^2. \tag{13}$$

The HSIC measure can also be extended to the $M\geq 2$ case to measure pairwise independence; the objective is called '`HSIC`' in ITE.

Note: one can express HSIC in terms of pairwise similarities as

$$\begin{aligned}\left[I_{\mathrm{HSIC}}\left(\mathbf{y}^1,\mathbf{y}^2\right)\right]^2=&\mathbb{E}_{\mathbf{y}^1,\mathbf{y}^2}\mathbb{E}_{\mathbf{y}^{1'},\mathbf{y}^{2'}}k_1\left(\mathbf{y}^1,\mathbf{y}^{1'}\right)k_2\left(\mathbf{y}^2,\mathbf{y}^{2'}\right)+\mathbb{E}_{\mathbf{y}^1}\mathbb{E}_{\mathbf{y}^{1'}}k_1\left(\mathbf{y}^1,\mathbf{y}^{1'}\right)\mathbb{E}_{\mathbf{y}^2}\mathbb{E}_{\mathbf{y}^{2'}}k_1\left(\mathbf{y}^2,\mathbf{y}^{2'}\right)\\&-2\mathbb{E}_{\mathbf{y}^{1'}\mathbf{y}^{2'}}\left[\mathbb{E}_{\mathbf{y}^1}k_1\left(\mathbf{y}^1,\mathbf{y}^{1'}\right)\mathbb{E}_{\mathbf{y}^1}k_2\left(\mathbf{y}^2,\mathbf{y}^{2'}\right)\right],\end{aligned} \tag{14}$$

where (i) $k_i$-s are the reproducing kernels corresponding to $\mathcal{F}_i$-s, (ii) $\mathbf{y}^{i'}$ is an identical copy (in distribution) of $\mathbf{y}^i$ $(i=1,2)$.

4. **Generalized variance (GV)**: The GV measure [134] considers the decorrelation of two one-dimensional random variables $y^1\in\mathbb{R}$ and $y^2\in\mathbb{R}$ $(M=2)$ over a finite function set $\mathcal{F}$:

$$I_{\mathrm{GV}}\left(y^1,y^2\right)=\sum_{g\in\mathcal{F}}\left(corr\left[g\left(y^1\right),g\left(y^2\right)\right]\right)^2. \tag{15}$$

The name of the cost is '`GV`' in ITE.

5. **Hoeffding's $\Phi$, Schweizer-Wolff's $\sigma$ and $\kappa$**: Let $C$ be the copula of the random variable $\mathbf{y}=\left[y^1;\ldots;y^d\right]\in\mathbb{R}^d$. One may think of $C$ as the distribution function on $[0,1]^d$, which links the joint distribution function $(F)$ and the marginals $(F_i,\ i=1,\ldots,d)$ [116]:

$$F(\mathbf{y})=C\left(F_1\left(y^1\right),\ldots,F_d\left(y^d\right)\right), \tag{16}$$

or in other words

$$C(\mathbf{u})=\mathbb{P}(\mathbf{U}\leq\mathbf{u}),\quad(\mathbf{u}=[u_1;\ldots;u_d]\in[0,1]^d), \tag{17}$$

where

$$\mathbf{U}=\left[F_1\left(y^1\right);\ldots;F_d\left(y^d\right)\right]\in[0,1]^d. \tag{18}$$

It can be shown that the $y^i\in\mathbb{R}$ variables are independent if and only if $C$, the copula of $\mathbf{y}$ equals to the product copula $\Pi$ defined as

$$\Pi(u_1,\ldots,u_d)=\prod_{i=1}^d u_i. \tag{19}$$

Using this result, the independence of $y^i$s can be measured by the (normalized) $L^p$ distance of $C$ and $\Pi$:

$$\left(h_p(d)\int_{[0,1]^d}|C(\mathbf{u})-\Pi(\mathbf{u})|^p\,\mathrm{d}\mathbf{u}\right)^{\frac{1}{p}}, \tag{20}$$

where (i) $1\leq p\leq\infty$, and (ii) by an appropriate choice of the normalization constant $h_p(d)$, the value of (20) belongs to the interval $[0,1]$ for any $C$.

- For $p=2$, the special

$$I_\Phi\left(y^1,\ldots,y^d\right)=I_\Phi(C)=\left(h_2(d)\int_{[0,1]^d}[C(\mathbf{u})-\Pi(\mathbf{u})]^2\mathrm{d}\mathbf{u}\right)^{\frac{1}{2}} \tag{21}$$

quantity

  - is a generalization of Hoeffding's $\Phi$ defined for $d=2$ [43],
  - whose empirical estimation can be analytically computed [33].

The name of the objective is '`Hoeffding`' in ITE.

- For $p = 1$ and $p = \infty$, one obtains Schweizer-Wolff's $\sigma$ and $\kappa$ [108, 153]. The first measure ($I_{\text{SW1}}$) satisfies all the properties of a multivariate measure of dependence in the sense of Def. 5 (see Section D); the second index ($I_{\text{SWinf}}$) fullfills D1, D2, D5, D6 and D8 of Def. 5 [153].
  For $p \in \{1, \infty\}$ no explicit expressions for the integrals in Eq.(20) are available. For small dimensional problems, however, the quantities can be efficiently estimated numerically. ITE contains methods for the $M = 2$ case:

$$I_{\text{SW1}}\left(y^1, y^2\right) = I_{\text{SW1}}(C) = \sigma = 12 \int_{[0,1]^2} |C(\mathbf{u}) - \Pi(\mathbf{u})| \mathrm{d}\mathbf{u}, \tag{22}$$

$$I_{\text{SWinf}}\left(y^1, y^2\right) = I_{\text{SWinf}}(C) = \kappa = 4 \sup_{\mathbf{u} \in [0,1]^2} |C(\mathbf{u}) - \Pi(\mathbf{u})|. \tag{23}$$

  The two measures are called '`SW1`' and '`SWinf`'.

For an excellent introduction on copulas, see [80].

6. **Cauchy-Schwartz quadratic mutual information (QMI), Euclidean distance based QMI**: These measures are defined for the $\mathbf{y}^m \in \mathbb{R}^{d_m}$ $(m = 1, 2)$ variables as [111]:

$$I_{\text{QMI-CS}}\left(\mathbf{y}^1, \mathbf{y}^2\right) = \log \left[ \frac{\left( \int_{\mathbb{R}^{d_1}} \int_{\mathbb{R}^{d_2}} \left[ f\left(\mathbf{u}^1, \mathbf{u}^2\right) \right]^2 \mathrm{d}\mathbf{u}^1 \mathrm{d}\mathbf{u}^2 \right) \left( \int_{\mathbb{R}^{d_1}} \int_{\mathbb{R}^{d_2}} \left[ f_1\left(\mathbf{u}^1\right) \right]^2 \left[ f_2\left(\mathbf{u}^2\right) \right]^2 \mathrm{d}\mathbf{u}^1 \mathrm{d}\mathbf{u}^2 \right)}{\left[ \int_{\mathbb{R}^{d_1}} \int_{\mathbb{R}^{d_2}} f\left(\mathbf{u}^1, \mathbf{u}^2\right) f_1\left(\mathbf{u}^1\right) f_2\left(\mathbf{u}^2\right) \mathrm{d}\mathbf{u}^1 \mathrm{d}\mathbf{u}^2 \right]^2} \right], \tag{24}$$

$$\begin{aligned} I_{\text{QMI-ED}}\left(\mathbf{y}^1, \mathbf{y}^2\right) = & \left( \int_{\mathbb{R}^{d_1}} \int_{\mathbb{R}^{d_2}} \left[ f\left(\mathbf{u}^1, \mathbf{u}^2\right) \right]^2 \mathrm{d}\mathbf{u}^1 \mathrm{d}\mathbf{u}^2 \right) + \left( \int_{\mathbb{R}^{d_1}} \int_{\mathbb{R}^{d_2}} \left[ f_1\left(\mathbf{u}^1\right) \right]^2 \left[ f_2\left(\mathbf{u}^2\right) \right]^2 \mathrm{d}\mathbf{u}^1 \mathrm{d}\mathbf{u}^2 \right) \\ & - 2 \int_{\mathbb{R}^{d_1}} \int_{\mathbb{R}^{d_2}} f\left(\mathbf{u}^1, \mathbf{u}^2\right) f_1\left(\mathbf{u}^1\right) f_2\left(\mathbf{u}^2\right) \mathrm{d}\mathbf{u}^1 \mathrm{d}\mathbf{u}^2. \end{aligned} \tag{25}$$

   The measures can

   (a) be approximated in ITE via

$$\hat{f}_m(\mathbf{u}) = \frac{1}{T} \sum_{t=1}^{T} k\left(\mathbf{u} - \mathbf{y}_t^m\right) \tag{26}$$

   KDE (kernel density estimation; also termed the Parzen or the Parzen-Rosenblatt window method) in a plug-in scheme, directly or applying incomplete Cholesky decomposition ('`QMI_CS_KDE_direct`', '`QMI_CS_KDE_iChol`', '`QMI_ED_KDE_iChol`').

   (b) also be expressed in terms of the Cauchy-Schwartz and the Euclidean distance based divergences [see Eq. (51), (52)]:

$$I_{\text{QMI-CS}}\left(\mathbf{y}^1, \mathbf{y}^2\right) = D_{\text{CS}}\left(f, f_1 f_2\right), \tag{27}$$

$$I_{\text{QMI-ED}}\left(\mathbf{y}^1, \mathbf{y}^2\right) = D_{\text{ED}}\left(f, f_1 f_2\right). \tag{28}$$

7. **Distance covariance, distance correlation**: Two random variables are independent, if and only if their joint characteristic function can be factorized. This is the guiding principle behind the definition of distance covariance and distance correlation [138, 135]. Namely, let us given $\mathbf{y}^1 \in \mathbb{R}^{d_1}$, $\mathbf{y}^2 \in \mathbb{R}^{d_2}$ random variables ($M = 2$), and let $\varphi_j$ ($\varphi_{12}$) stand for the characteristic function of $\mathbf{y}^j$ ($\left[\mathbf{y}^1; \mathbf{y}^2\right]$):

$$\varphi_{12}\left(\mathbf{u}^1, \mathbf{u}^2\right) = \mathbb{E}\left[ e^{i\left\langle \mathbf{u}^1, \mathbf{y}^1 \right\rangle + i\left\langle \mathbf{u}^2, \mathbf{y}^2 \right\rangle} \right], \tag{29}$$

$$\varphi_j\left(\mathbf{u}^j\right) = \mathbb{E}\left[ e^{i\left\langle \mathbf{u}^j, \mathbf{y}^j \right\rangle} \right], \quad (j = 1, 2) \tag{30}$$

$$\tag{31}$$

   where $i = \sqrt{-1}$, $\langle \cdot, \cdot \rangle$ is the standard Euclidean scalar product, and $\mathbb{E}$ stands for expectation. The *distance covariance* is simply the $L_w^2$ norm of $\varphi_{12}$ and $\varphi_1 \varphi_2$:

$$I_{\text{dCov}}\left(\mathbf{y}^1, \mathbf{y}^2\right) = \left\| \varphi_{12} - \varphi_1 \varphi_2 \right\|_{L_w^2} = \sqrt{\int_{\mathbb{R}^{d_1 + d_2}} \left| \varphi_{12}\left(\mathbf{u}^1, \mathbf{u}^2\right) - \varphi_1\left(\mathbf{u}^1\right) \varphi_2\left(\mathbf{u}^2\right) \right|^2 w\left(\mathbf{u}^1, \mathbf{u}^2\right) \mathrm{d}\mathbf{u}^1 \mathrm{d}\mathbf{u}^2} \tag{32}$$

| Estimated quantity | Principle | $d_m$ | $M$ | `cost_name` |
|---|---|---|---|---|
| generalized variance ($I_{\mathrm{GV}}$) | f-covariance/-correlation ($f \in \mathcal{F}$, $\lvert\mathcal{F}\rvert < \infty$) | $d_m = 1$ | $M = 2$ | 'GV' |
| Hilbert-Schmidt indep. criterion ($I_{\mathrm{HSIC}}$) | HS norm of the cross-covariance operator | $d_m \geq 1$ | $M \geq 2$ | 'HSIC' |
| kernel canonical correlation ($I_{\mathrm{KCCA}}$) | sup correlation over RKHSs | $d_m \geq 1$ | $M \geq 2$ | 'KCCA' |
| kernel generalized variance ($I_{\mathrm{KGV}}$) | Gaussian mutual information of the features | $d_m \geq 1$ | $M \geq 2$ | 'KGV' |
| Hoeffding's $\Phi$ ($I_{\Phi}$), multivariate | $L^2$ distance of the joint- and the product copula | $d_m = 1$ | $M \geq 2$ | 'Hoeffding' |
| Schweizer-Wolff's $\sigma$ ($I_{\mathrm{SW1}}$) | $L^1$ distance of the joint- and the product copula | $d_m = 1$ | $M = 2$ | 'SW1' |
| Schweizer-Wolff's $\kappa$ ($I_{\mathrm{SWinf}}$) | $L^\infty$ distance of the joint- and the product copula | $d_m = 1$ | $M = 2$ | 'SWinf' |
| Cauchy-Schwartz QMI ($I_{\mathrm{QMI\text{-}CS}}$) | KDE, direct | $d_m = 1$ | $M = 2$ | 'QMI_CS_KDE_direct' |
| Cauchy-Schwartz QMI ($I_{\mathrm{QMI\text{-}CS}}$) | KDE, incomplete Cholesky decomposition | $d_m \geq 1$ | $M = 2$ | 'QMI_CS_KDE_iChol' |
| Euclidean dist. based QMI ($I_{\mathrm{QMI\text{-}ED}}$) | KDE, incomplete Cholesky decomposition | $d_m \geq 1$ | $M = 2$ | 'QMI_ED_KDE_iChol' |
| distance covariance ($I_{\mathrm{dCov}}$) | pairwise distances | $d_m \geq 1$ | $M = 2$ | 'dCov' |
| distance correlation ($I_{\mathrm{dCor}}$) | pairwise distances | $d_m \geq 1$ | $M = 2$ | 'dCor' |

Table 3: Mutual information estimators (base). Third column: dimension constraint ($d_m$; $\mathbf{y}^m \in \mathbb{R}^{d_m}$). Fourth column: constraint for the number of components ($M$; $\mathbf{y} = \left[\mathbf{y}^1; \ldots; \mathbf{y}^M\right]$).

with a suitable chosen $w$ weight function

$$w\left(\mathbf{u}^1, \mathbf{u}^2\right) = \frac{1}{c(d_1,\alpha)c(d_2,\alpha)\left[\|\mathbf{u}^1\|_2\right]^{d_1+\alpha}\left[\|\mathbf{u}^2\|_2\right]^{d_2+\alpha}}, \tag{33}$$

where $\alpha \in (0,2)$ and

$$c(d,\alpha) = \frac{2\pi^{\frac{d}{2}}\Gamma\left(1-\frac{\alpha}{2}\right)}{\alpha 2^{\alpha}\Gamma\left(\frac{d+\alpha}{2}\right)}. \tag{34}$$

The *distance variance* is defined analogously ($j = 1, 2$):

$$I_{\mathrm{dVar}}\left(\mathbf{y}^j, \mathbf{y}^j\right) = \left\|\varphi_{jj} - \varphi_j\varphi_j\right\|_{L^2_w}. \tag{35}$$

The *distance correlation* is the standardized version of the distance covariance:

$$I_{\mathrm{dCor}}\left(\mathbf{y}^1, \mathbf{y}^2\right) = \begin{cases} \frac{I_{\mathrm{dCov}}\left(\mathbf{y}^1,\mathbf{y}^2\right)}{\sqrt{I_{\mathrm{dVar}}\left(\mathbf{y}^1,\mathbf{y}^1\right)I_{\mathrm{dVar}}\left(\mathbf{y}^2,\mathbf{y}^2\right)}}, & \text{if } I_{\mathrm{dVar}}\left(\mathbf{y}^1,\mathbf{y}^1\right)I_{\mathrm{dVar}}\left(\mathbf{y}^2,\mathbf{y}^2\right) > 0, \\ 0, & \text{otherwise,} \end{cases} \tag{36}$$

a type of unsigned correlation. By construction $I_{\mathrm{dCor}}\left(\mathbf{y}^1, \mathbf{y}^2\right) \in [0,1]$, and is zero, if and only if $\mathbf{y}^1$ and $\mathbf{y}^2$ are independent. The distance covariance and distance correlation measures are called 'dCov' and 'dCor' in ITE.

The estimation of these quantities can be carried out easily in the ITE package. Let us take the KCCA measure as an example:

**Example 4 (Mutual information estimation (base: usage))**

```
>ds = [2;3;4]; Y = rand(sum(ds),5000); %generate the data of interest (ds(m)=dim(y^m), T=5000)
>mult = 1;                             %multiplicative constant is important
>co = IKCCA_initialization(mult);      %initialize the mutual information ('I') estimator ('KCCA')
>I = IKCCA_estimation(Y,ds,co);        %perform mutual information estimation
```

The calling syntax of the mutual information estimators are completely identical: one only has to change 'KCCA' to the `cost_name` given in the last column of the Table 3. The table summarizes the base mutual information estimators in ITE.

### 3.1.3 Divergence Estimators

Divergences measure the 'distance' between two probability densities, $f_1 : \mathbb{R}^d \mapsto \mathbb{R}$ and $f_2 : \mathbb{R}^d \mapsto \mathbb{R}$. One of the most well-known such index is the **Kullback-Leibler divergence** (also called relative entropy, or I directed divergence) [60][10]:

$$D(f_1, f_2) = \int_{\mathbb{R}^d} f_1(\mathbf{u}) \log\left[\frac{f_1(\mathbf{u})}{f_2(\mathbf{u})}\right] \mathrm{d}\mathbf{u}. \tag{37}$$

[10] $D(f_1, f_2) \geq 0$ with equality iff $f_1 = f_2$. The Kullback-Leibler divergence is a special f-divergence (with $f(t) = t\log(t)$), see Def. 8.

In practise, one has independent, i.i.d. samples from $f_1$ and $f_2$, $\{\mathbf{y}_t^1\}_{t=1}^{T_1}$ and $\{\mathbf{y}_t^2\}_{t=1}^{T_2}$, respectively. The goal is to estimate divergence $D$ using these samples. Of course, there exist many variants/extensions of the traditional Kullback-Leibler divergence [148, 6]; depending on the application addressed, different divergences can be advantageous. The ITE package is capable of estimating the following divergences, too:

1. $L_2$ **divergence**:

$$D_{\mathrm{L}}(f_1, f_2) = \sqrt{\int_{\mathbb{R}^d} \left[f_1(\mathbf{u}) - f_2(\mathbf{u})\right]^2 \mathrm{d}\mathbf{u}}. \tag{38}$$

   By definition $D_{\mathrm{L}}(f_1, f_2)$ is non-negative, and is zero if and only if $f_1 = f_2$.

2. **Tsallis divergence**:

$$D_{\mathrm{T},\alpha}(f_1, f_2) = \frac{1}{\alpha - 1}\left(\int_{\mathbb{R}^d} f_1^{\alpha}(\mathbf{u}) f_2^{1-\alpha}(\mathbf{u})\mathrm{d}\mathbf{u} - 1\right) \quad (\alpha \in \mathbb{R} \setminus \{1\}). \tag{39}$$

   Notes:

   - The Kullback-Leibler divergence [Eq. (37)] is a special of Tsallis' in limit sense:

$$\lim_{\alpha \to 1} D_{\mathrm{T},\alpha} = D. \tag{40}$$

   - As a function of $\alpha$, the sign of the Tsallis divergence is as follows:

$$\alpha < 0 \Rightarrow D_{\mathrm{T},\alpha}(f_1, f_2) \leq 0, \qquad \alpha = 0 \Rightarrow D_{\mathrm{T},\alpha}(f_1, f_2) = 0, \qquad \alpha > 0 \Rightarrow D_{\mathrm{T},\alpha}(f_1, f_2) \geq 0. \tag{41}$$

3. **Rényi divergence**:

$$D_{\mathrm{R},\alpha}(f_1, f_2) = \frac{1}{\alpha - 1}\log\int_{\mathbb{R}^d} f_1^{\alpha}(\mathbf{u}) f_2^{1-\alpha}(\mathbf{u})\mathrm{d}\mathbf{u} \quad (\alpha \in \mathbb{R} \setminus \{1\}). \tag{42}$$

   Notes:

   - The Kullback-Leibler divergence [Eq. (37)] is a special of Rényi's in limit sense:

$$\lim_{\alpha \to 1} D_{\mathrm{R},\alpha} = D. \tag{43}$$

   - As a function of $\alpha$, the sign of the Rényi divergence is as follows:

$$\alpha < 0 \Rightarrow D_{\mathrm{R},\alpha}(f_1, f_2) \leq 0, \qquad \alpha = 0 \Rightarrow D_{\mathrm{R},\alpha}(f_1, f_2) = 0, \qquad \alpha > 0 \Rightarrow D_{\mathrm{R},\alpha}(f_1, f_2) \geq 0. \tag{44}$$

4. **Maximum mean discrepancy** (MMD, also called the kernel distance) [36]:

$$D_{\mathrm{MMD}}(f_1, f_2) = \left\|\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2\right\|_{\mathcal{F}}, \tag{45}$$

   where $\boldsymbol{\mu}_m$ is the mean embedding of $f_m$ $(m = 1, 2)$ and $\mathcal{F} = \mathcal{F}^1 = \mathcal{F}^2$, see the definition of HSIC [Eq. (12)]. Notes:

   - $D_{\mathrm{MMD}}(f_1, f_2)$ is a Hilbertian metric [41, 35]; see Def. 7.
   - In the statistics literature, MMD is known as an integral probability metric (IPM) [157, 77, 119]:

$$D_{\mathrm{MMD}}(f_1, f_2) = \sup_{g \in \mathcal{B}} \left(\mathbb{E}\left[g\left(\mathbf{y}^1\right)\right] - \mathbb{E}[g\left(\mathbf{y}^2\right)]\right), \tag{46}$$

     where $f_i$ is the density of $\mathbf{y}^i$ $(i = 1, 2)$ and $\mathcal{B}$ is the unit ball in the RKHS $\mathcal{F}$.

   - One can easily see that the MMD measure acts as a 'divergence' on the joint and the product of the marginals in HSIC (similarly to the well-known Kullback-Leibler divergence and its extensions, see Eqs. (104)-(105)):

$$I_{\mathrm{HSIC}}\left(\mathbf{y}^1, \mathbf{y}^2\right) = D_{\mathrm{MMD}}(f, f_1 f_2), \tag{47}$$

     where $f$ is the joint density of $\left[\mathbf{y}^1; \mathbf{y}^2\right]$.

- In terms of pairwise similarities MMD satisfies the relation:

$$[D_{\mathrm{MMD}}(f_1,f_2)]^2 = \mathbb{E}_{\mathbf{y}^1,\mathbf{y}^{1'}}\left[k\left(\mathbf{y}^1,\mathbf{y}^{1'}\right)\right] + \mathbb{E}_{\mathbf{y}^2,\mathbf{y}^{2'}}\left[k\left(\mathbf{y}^2,\mathbf{y}^{2'}\right)\right] - 2\mathbb{E}_{\mathbf{y}^1,\mathbf{y}^2}\left[k\left(\mathbf{y}^1,\mathbf{y}^2\right)\right], \tag{48}$$

  where $\mathbf{y}^{i'}$ is an identical copy (in distribution) of $\mathbf{y}^i$ $(i=1,2)$.

5. **Hellinger distance**:

$$D_{\mathrm{H}}(f_1,f_2) = \sqrt{\frac{1}{2}\int_{\mathbb{R}^d}\left[\sqrt{f_1(\mathbf{u})}-\sqrt{f_2(\mathbf{u})}\right]^2 \mathrm{d}\mathbf{u}} = \sqrt{1-\int_{\mathbb{R}^d}\sqrt{f_1(\mathbf{u})}\sqrt{f_2(\mathbf{u})}\mathrm{d}\mathbf{u}}. \tag{49}$$

   Notes:

   - As it is known $D_{\mathrm{H}}(f_1,f_2)$ is a (covariant) Hilbertian metric [41]; see Def. 7.
   - $D_{\mathrm{H}}^2$ is a special f-divergence [with $f(t)=\frac{1}{2}(\sqrt{t}-1)^2$], see Def. 8.

6. **Bhattacharyya distance**:

$$D_{\mathrm{B}}(f_1,f_2) = -\log\left(\int_{\mathbb{R}^d}\sqrt{f_1(\mathbf{u})}\sqrt{f_2(\mathbf{u})}\mathrm{d}\mathbf{u}\right). \tag{50}$$

7. **Cauchy-Schwartz and Euclidean distance based divergences**:

$$D_{\mathrm{CS}}(f_1,f_2) = \log\left[\frac{\left(\int_{\mathbb{R}^d}\left[f_1(\mathbf{u})\right]^2\mathrm{d}\mathbf{u}\right)\left(\int_{\mathbb{R}^d}\left[f_2(\mathbf{u})\right]^2\mathrm{d}\mathbf{u}\right)}{\left(\int_{\mathbb{R}^d}f_1(\mathbf{u})f_2(\mathbf{u})\mathrm{d}\mathbf{u}\right)^2}\right] = \log\left[\frac{1}{\cos^2(f_1,f_2)}\right], \tag{51}$$

$$D_{\mathrm{ED}}(f_1,f_2) = \int_{\mathbb{R}^d}\left[f_1(\mathbf{u})\right]^2\mathrm{d}\mathbf{u} + \int_{\mathbb{R}^d}\left[f_2(\mathbf{u})\right]^2\mathrm{d}\mathbf{u} - 2\int_{\mathbb{R}^d}f_1(\mathbf{u})f_2(\mathbf{u})\mathrm{d}\mathbf{u} = \int_{\mathbb{R}^d}\left[f_1(\mathbf{u})-f_2(\mathbf{u})\right]^2\mathrm{d}\mathbf{u} \tag{52}$$

$$= [D_{\mathrm{L}}(f_1,f_2)]^2. \tag{53}$$

8. **Energy distance**: Let $(\mathcal{Z},\rho)$ be a semimetric space of negative type (see Def. 6, Section D), and let $\mathbf{y}^1$ and $\mathbf{y}^2$ be $\mathcal{Z}$-valued random variables with (i) densities $f_1$ and $f_2$, and (ii) let $\mathbf{y}^{1'}$ and $\mathbf{y}^{2'}$ be an identically distributed copy of $\mathbf{y}^1$ and $\mathbf{y}^2$, respectively. The energy distance of $\mathbf{y}^1$ and $\mathbf{y}^2$ is defined as [136, 137]:

$$D_{\mathrm{EnDist}}(f_1,f_2) = 2\mathbb{E}\left[\rho\left(\mathbf{y}^1,\mathbf{y}^2\right)\right] - \mathbb{E}\left[\rho\left(\mathbf{y}^1,\mathbf{y}^{1'}\right)\right] - \mathbb{E}\left[\rho\left(\mathbf{y}^2,\mathbf{y}^{2'}\right)\right]. \tag{54}$$

   An important special case is the Euclidean ($\mathcal{Z}=\mathbb{R}^d$ with $\|\cdot\|_2$), when the energy distance takes the form:

$$D_{\mathrm{EnDist}}(f_1,f_2) = 2\mathbb{E}\left\|\mathbf{y}^1-\mathbf{y}^2\right\|_2 - \mathbb{E}\left\|\mathbf{y}^1-\mathbf{y}^{1'}\right\|_2 - \mathbb{E}\left\|\mathbf{y}^2-\mathbf{y}^{2'}\right\|_2. \tag{55}$$

   In the further specialized $d=1$ case, the energy distance equals to twice the Cramer-Von Mises distance. The energy distance

   - is non-negative; and in case of *strictly* negative space $\mathcal{Z}$ (e.g., $\mathbb{R}^d$) it is zero, if and only if $\mathbf{y}^1$ and $\mathbf{y}^2$ are identically distributed,
   - in ITE it is called '`EnergyDist`'.

9. **Bregman distance**: The non-symmetric Bregman distance (also called Bregman divergence) is defined [11, 23, 64] as

$$D_{\mathrm{NB},\alpha}(f_1,f_2) = \int_{\mathbb{R}^d}\left[f_2^\alpha(\mathbf{u}) + \frac{1}{\alpha-1}f_1^\alpha(\mathbf{u}) - \frac{\alpha}{\alpha-1}f_1(\mathbf{u})f_2^{\alpha-1}(\mathbf{u})\right]\mathrm{d}\mathbf{u}, \quad (\alpha\neq 1). \tag{56}$$

10. **Symmetric Bregman distance** The symmetric Bregman distance is defined [11, 23, 64] via its non-symmetric counterpart:

$$D_{\mathrm{SB},\alpha}(f_1,f_2) = \frac{1}{\alpha}\left[D_{\mathrm{NB},\alpha}(f_1,f_2)+D_{\mathrm{NB},\alpha}(f_2,f_1)\right], \quad (\alpha\neq 1) \tag{57}$$

$$= \frac{1}{\alpha-1}\int_{\mathbb{R}^d}\left[f_1(\mathbf{u})-f_2(\mathbf{u})\right]\left[f_1^{\alpha-1}(\mathbf{u})-f_2^{\alpha-1}(\mathbf{u})\right]\mathrm{d}\mathbf{u} \tag{58}$$

$$= \frac{1}{\alpha-1}\int_{\mathbb{R}^d} f_1^{\alpha}(\mathbf{u})+f_2^{\alpha}(\mathbf{u})-f_1(\mathbf{u})f_2^{\alpha-1}(\mathbf{u})-f_2(\mathbf{u})f_1^{\alpha-1}(\mathbf{u})\mathrm{d}\mathbf{u}. \tag{59}$$

Specially, for $\alpha=2$ we obtain the square of the $L_2$-divergence [see Eq. (38)]:

$$\left[D_{\mathrm{L}}(f_1,f_2)\right]^2 = D_{\mathrm{NB},2}(f_1,f_2) = D_{\mathrm{SB},2}(f_1,f_2). \tag{60}$$

Let us note that for (39), (42), (49) and (50), it is sufficient to estimate the

$$D_{\mathrm{temp1}}(\alpha) = \int_{\mathbb{R}^d}[f_1(\mathbf{u})]^{\alpha}[f_2(\mathbf{u})]^{1-\alpha}\mathrm{d}\mathbf{u} \tag{61}$$

quantity, which is called the Bhattacharyya coefficient [8] for $\alpha=\frac{1}{2}$ (it is also known as the Bhattacharyya kernel, or the Hellinger affinity; see (49), (50) and (90)):

$$BC = \int_{\mathbb{R}^d}\sqrt{f_1(\mathbf{u})}\sqrt{f_2(\mathbf{u})}\mathrm{d}\mathbf{u}\in[0,1]. \tag{62}$$

(61) can also be further generalized to

$$D_{\mathrm{temp2}}(a,b) = \int_{\mathbb{R}^d}\left[f_1(\mathbf{u})\right]^a\left[f_2(\mathbf{u})\right]^b f_1(\mathbf{u})\mathrm{d}\mathbf{u}, \quad (a,b\in\mathbb{R}). \tag{63}$$

The calling syntax of the divergence estimators in the ITE package are again uniform. In the following example, the estimation of the Rényi divergence is illustrated using the k-nearest neighbor method:

**Example 5 (Divergence estimation (base: usage))**

```
>Y1 = randn(3,2000); Y2 = randn(3,3000); %generate the data of interest (d=3, T1=2000, T2=3000)
>mult = 1;                               %multiplicative constant is important
>co = DRenyi_kNN_k_initialization(mult); %initialize the divergence ('D') estimator ('Renyi_kNN_k')
>D = DRenyi_kNN_k_estimation(Y1,Y2,co);  %perform divergence estimation
```

Beyond the Rényi divergence $D_{\mathrm{R},\alpha}$ [97, 96, 98] ('`Renyi_kNN_k`'), the k-nearest neighbor technique can also be used to estimate the $L_2$- ($D_{\mathrm{L}}$) [97, 96, 98] ('`L2_kNN_k`'), the Tsallis ($D_{\mathrm{T},\alpha}$) divergence [97, 96] ('`Tsallis_kNN_k`'), and of course, specially to the Kullback-Leibler divergence ($D$) [64, 87, 151] ('`KL_kNN_k`', '`KL_kNN_kiTi`'). A similar approach can be applied to the estimation of the (63) quantity [92], specially to the Hellinger- and the Bhattacharyya distance ('`Hellinger_kNN_k`', '`Bhattacharyya_kNN_k`'). For the MMD measure [36], (i) an U-statistic based ('`MMD_Ustat`'), (ii) a V-statistic based ('`MMD_Vstat`'), and (iii) a linearly scaling, online method ('`MMD_online`') have been implemented in ITE. The Cauchy-Schwartz and the Euclidean distance based divergences ($D_{\mathrm{CS}}$, $D_{\mathrm{ED}}$) can be estimated using KDE based plug-in methods, applying incomplete Cholesky decomposition ('`CS_KDE_iChol`', '`'ED_KDE_iChol`'). The energy distance ($D_{\mathrm{EnDist}}$) can be approximated using pairwise distances of sample points ('`EnergyDist`'). The Bregman distance and its symmetric variant can be estimated via k-nearest neighbors ('`Bregman_kNN_k`', '`symBregman_kNN_k`'). Table 4 contains the base divergence estimators of the ITE package. The estimations can be carried out by changing the name '`Renyi_kNN_k`' in Example 5 to the `cost_name` given in the last column of the table.

### 3.1.4 Association Measure Estimators

There exist many exciting association quantities measuring certain dependency relations of random variables, for a recent excellent review on the topic, see [106]. In ITE we think of mutual information (Section 3.1.2) as a special case of association that (i) is non-negative, (ii) being zero, if its arguments are independent.

| Estimated quantity | Principle | $d$ | `cost_name` |
|---|---|---|---|
| $L_2$ divergence ($D_{\mathrm{L}}$) | k-nearest neighbors ($S=\{k\}$) | $d\geq 1$ | `'L2_kNN_k'` |
| Tsallis divergence ($D_{\mathrm{T},\alpha}$) | k-nearest neighbors ($S=\{k\}$) | $d\geq 1$ | `'Tsallis_kNN_k'` |
| Rényi divergence ($D_{\mathrm{R},\alpha}$) | k-nearest neighbors ($S=\{k\}$) | $d\geq 1$ | `'Renyi_kNN_k'` |
| maximum mean discrepancy ($D_{\mathrm{MMD}}$) | U-statistics, unbiased | $d\geq 1$ | `'MMD_Ustat'` |
| maximum mean discrepancy ($D_{\mathrm{MMD}}$) | V-statistics, biased | $d\geq 1$ | `'MMD_Vstat'` |
| maximum mean discrepancy ($D_{\mathrm{MMD}}$) | online | $d\geq 1$ | `'MMD_online'` |
| Hellinger distance ($D_{\mathrm{H}}$) | k-nearest neighbors ($S=\{k\}$) | $d\geq 1$ | `'Hellinger_kNN_k'` |
| Bhattacharyya distance ($D_{\mathrm{B}}$) | k-nearest neighbors ($S=\{k\}$) | $d\geq 1$ | `'Bhattacharyya_kNN_k'` |
| Kullback-Leibler divergence ($D$) | k-nearest neighbors ($S=\{k\}$) | $d\geq 1$ | `'KL_kNN_k'` |
| Kullback-Leibler divergence ($D$) | k-nearest neighbors ($S_i=\{k_i(T_i)\}$) | $d\geq 1$ | `'KL_kNN_kiTi'` |
| Cauchy-Schwartz divergence ($D_{\mathrm{CS}}$) | KDE, incomplete Cholesky decomposition | $d\geq 1$ | `'CS_KDE_iChol'` |
| Euclidean distance based divergence ($D_{\mathrm{ED}}$) | KDE, incomplete Cholesky decomposition | $d\geq 1$ | `'ED_KDE_iChol'` |
| energy distance ($D_{\mathrm{EnDist}}$) | pairwise distances | $d\geq 1$ | `'EnergyDist'` |
| Bregman distance ($D_{\mathrm{NB},\alpha}$) | k-nearest neighbors ($S=\{k\}$) | $d\geq 1$ | `'Bregman_kNN_k'` |
| Symmetric Bregman distance ($D_{\mathrm{SB},\alpha}$) | k-nearest neighbors ($S=\{k\}$) | $d\geq 1$ | `'symBregman_kNN_k'` |

Table 4: Divergence estimators (base). Third column: dimension ($d$) constraint.

Our goal is to estimate the dependence/association of the $d_m$-dimensional components of the random variable $\mathbf{y}=\left[\mathbf{y}^1;\ldots;\mathbf{y}^M\right]\in\mathbb{R}^d$ ($d=\sum_{m=1}^M d_m$), from which we have i.i.d. samples $\{\mathbf{y}_t\}_{t=1}^T$. One of the most well-known example of associations is that of the **Spearman's $\rho$** (also called the Spearman's rank correlation coefficient, or the grade correlation coefficient) [117]. For $d=2$, it is defined as

$$A_\rho\left(y^1,y^2\right)=corr\left(F_1\left(y^1\right),F_2\left(y^2\right)\right), \tag{64}$$

where 'corr' stands for correlation and $F_i$ denotes the (cumulative) distribution function (cdf) of $y^i$. Spearman's $\rho$ is a special association, a *measure of concordance*: if large (small) values of $y^1$ tend to be associated with large (small) values of $y^2$, it is reflected in $A_\rho$. For a formal definition of measures of concordance, see Def. 2 (Section D).

Let us now define for $d_m=1$ ($\forall m$) the comonotonicy copula (also called the Fréchet-Hoeffding upper bound) as

$$M(\mathbf{u})=\min_{i=1,\ldots,d} u_i. \tag{65}$$

The name originates from the fact that for any $C$ copula

$$W(\mathbf{u}):=\max(u_1+\ldots+u_d-d+1,0)\leq C(\mathbf{u})\leq M(\mathbf{u}),\quad(\forall\mathbf{u}\in[0,1]^d) \tag{66}$$

Here, $W$ is called the Fréchet-Hoeffding lower bound.[11]

It is known that $A_\rho$ can be interpreted as the normalized average difference of the copula of $\mathbf{y}$ ($C$) and the independence copula ($\Pi$) [see Eq. (19)]:

$$A_\rho\left(y^1,y^2\right)=A_\rho(C)=\frac{\int_{[0,1]^2}u_1u_2\mathrm{d}C(\mathbf{u})-\left(\frac{1}{2}\right)^2}{\frac{1}{12}}=12\int_{[0,1]^2}C(\mathbf{u})\mathrm{d}\mathbf{u}-3=\frac{\int_{[0,1]^2}C(\mathbf{u})\mathrm{d}\mathbf{u}-\int_{[0,1]^2}\Pi(\mathbf{u})\mathrm{d}\mathbf{u}}{\int_{[0,1]^2}M(\mathbf{u})\mathrm{d}\mathbf{u}-\int_{[0,1]^2}\Pi(\mathbf{u})\mathrm{d}\mathbf{u}}, \tag{67}$$

where the

$$\int_{[0,1]^2}M(\mathbf{u})\mathrm{d}\mathbf{u}=\frac{1}{3},\qquad\qquad\int_{[0,1]^2}\Pi(\mathbf{u})\mathrm{d}\mathbf{u}=\frac{1}{4} \tag{68}$$

properties were exploited. The association measures included in ITE are the following:

1. **Spearman's $\rho$, multivariate-1**: One can extend [153, 52, 78, 105] the Spearman's $\rho$ to the multivariate case using (67) as

$$A_{\rho_1}\left(y^1,\ldots,y^d\right)=A_{\rho_1}(C)=\frac{\int_{[0,1]^d}C(\mathbf{u})\mathrm{d}\mathbf{u}-\int_{[0,1]^d}\Pi(\mathbf{u})\mathrm{d}\mathbf{u}}{\int_{[0,1]^d}M(\mathbf{u})\mathrm{d}\mathbf{u}-\int_{[0,1]^d}\Pi(\mathbf{u})\mathrm{d}\mathbf{u}}=h_\rho(d)\left[2^d\int_{[0,1]^d}C(\mathbf{u})\mathrm{d}\mathbf{u}-1\right], \tag{69}$$

[11] $W$ is a copula only in two dimensions ($d=2$).

where

$$h_\rho(d) = \frac{d+1}{2^d - (d+1)}. \tag{70}$$

The name of the association measure is '`Spearman1`' in ITE.

Note:

- $A_{\rho_1}$ satisfies all the axioms of multivariate measure of concordance (see Def. 3 in Section D) except for Duality [140].
- $A_{\rho_1}$ can also be derived from average *lower orthant dependence* ideas [78].

2. **Spearman's $\rho$, multivariate-2**: An other multivariate extension [52, 78, 105] of Spearman's $\rho$ is using (67)

$$A_{\rho_2}\left(y^1,\ldots,y^d\right) = A_{\rho_2}(C) = \frac{\int_{[0,1]^d}\Pi(\mathbf{u})\mathrm{d}C(\mathbf{u}) - \int_{[0,1]^d}\Pi(\mathbf{u})\mathrm{d}\mathbf{u}}{\int_{[0,1]^d}M(\mathbf{u})\mathrm{d}\mathbf{u} - \int_{[0,1]^d}\Pi(\mathbf{u})\mathrm{d}\mathbf{u}} = h_\rho(d)\left[2^d\int_{[0,1]^d}\Pi(\mathbf{u})\mathrm{d}C(\mathbf{u}) - 1\right]. \tag{71}$$

The association measure is called '`Spearman2`' in ITE.

Note:

- $A_{\rho_2}$ satisfies all the axioms of multivariate measure of concordance (see Def. 3 in Section D) except for Duality [140].
- $A_{\rho_2}$ can also be derived using an average *upper orthant dependence* approach [78].

3. **Spearman's $\rho$, multivariate-3**: [79, 80] further considers the average of $A_{\rho_1}$ and $A_{\rho_2}$, i.e.

$$A_{\rho_3}\left(y^1,\ldots,y^d\right) = A_{\rho_3}(C) = \frac{A_{\rho_1}\left(y^1,\ldots,y^d\right) + A_{\rho_2}\left(y^1,\ldots,y^d\right)}{2}. \tag{72}$$

The name of this association measure is '`Spearman3`' in ITE.[12]

Note:

- For the special case of $d = 2$, the defined extensions of Spearman's $\rho$ coincide:

$$A_\rho = A_{\rho_1} = A_{\rho_2} = A_{\rho_3}. \tag{73}$$

- $A_{\rho_3}$ is a multivariate measure of concordance (see Def. 3 in Section D).

4. **Spearman's $\rho$, multivariate-4**: The average pairwise Spearman's $\rho$ is defined [57, 105] as

$$A_{\rho_4}\left(y^1,\ldots,y^d\right) = A_{\rho_4}(C) = h(2)\left[2^2\binom{d}{2}^{-1}\sum_{k,l=1;k<l}^{d}\int_{[0,1]^2}C_{kl}(u,v)\mathrm{d}u\mathrm{d}v - 1\right] = \binom{d}{2}^{-1}\sum_{k,l=1;k<l}^{d}A_\rho\left(y^k,y^l\right), \tag{74}$$

where $C_{kl}$ denotes the bivariate marginal copula of $C$ corresponding to the $k^{th}$ and $l^{th}$ margin. The name of the association measure is '`Spearman4`' in ITE. $A_{\rho_4}$ is a multivariate measure of concordance (see Def. 3 in Section D).

5. **Correntropy**, **centered correntropy**, **correntropy coefficient** [100]: These association measures are defined as

$$A_{\mathrm{CorrEntr}}\left(y^1,y^2\right) = \mathbb{E}_{y^1,y^2}\left[k\left(y^1,y^2\right)\right] = \int_{\mathbb{R}^2}k(u,v)\mathrm{d}F_{y^1,y^2}(u,v), \tag{75}$$

$$A_{\mathrm{CCorrEntr}}\left(y^1,y^2\right) = \mathbb{E}_{y^1,y^2}\left[k\left(y^1,y^2\right)\right] - \mathbb{E}_{y^1}\mathbb{E}_{y^2}\left[k\left(y^1,y^2\right)\right] = \int_{\mathbb{R}^2}k(u,v)\left[\mathrm{d}F_{y^1,y^2}(u,v) - \mathrm{d}F_{y^1}\mathrm{d}F_{y^2}(u,v)\right], \tag{76}$$

$$A_{\mathrm{CorrEntrCoeff}}\left(y^1,y^2\right) = \frac{A_{\mathrm{CCorrEntr}}\left(y^1,y^2\right)}{\sqrt{A_{\mathrm{CCorrEntr}}\left(y^1,y^1\right)}\sqrt{A_{\mathrm{CCorrEntr}}\left(y^2,y^2\right)}} \in [-1,1], \tag{77}$$

[12] Although (72) would make it possibile to implement $A_{\rho_3}$ as a meta estimator (see Section 3.2.4), for computational reasons (to not compute the same rank statistics twice), it became a base method.

where $F_{y^1,y^2}$ ($F_{y^i}$) stands for the distribution function of $\mathbf{y} = \left[y^1; y^2\right]$ ($y^i$) and $k$ is a kernel. Specially, for $k(u,v) = uv$ the centered correntropy reduces to the covariance, and the correntropy coefficient to the traditional correlation coefficient. The name of the estimators in ITE are '`CorrEntr_KDE_direct`', '`CCorrEntr_KDE_iChol`', '`CCorrEntr_KDE_Lapl`', '`CorrEntrCoeff_KDE_direct`', and '`CorrEntrCoeff_KDE_iChol`'.

6. **Multivariate extension of Blomqvist's $\beta$ (medial correlation coefficient)**: Let $\mathbf{y} \in \mathbb{R}^2$, and let $\tilde{y}^i$ be the median of $y^i$. Blomqvist's $\beta$ is defined [75, 10] as

$$A_\beta\left(y^1, y^2\right) = \mathbb{P}\left(\left(y^1 - \tilde{y}^1\right)\left(y^2 - \tilde{y}^2\right) > 0\right) - \mathbb{P}\left(\left(y^1 - \tilde{y}^1\right)\left(y^2 - \tilde{y}^2\right) < 0\right). \tag{78}$$

It can be expressed in terms of the $C$, the copula of $\mathbf{y}$:

$$A_\beta\left(y^1, y^2\right) = A_\beta(C) = 4C\left(\frac{1}{2}, \frac{1}{2}\right) - 1 = \frac{C\left(\frac{1}{2}, \frac{1}{2}\right) - \Pi\left(\frac{1}{2}, \frac{1}{2}\right) + \bar{C}\left(\frac{1}{2}, \frac{1}{2}\right) - \bar{\Pi}\left(\frac{1}{2}, \frac{1}{2}\right)}{M\left(\frac{1}{2}, \frac{1}{2}\right) - \Pi\left(\frac{1}{2}, \frac{1}{2}\right) + \bar{M}\left(\frac{1}{2}, \frac{1}{2}\right) - \bar{\Pi}\left(\frac{1}{2}, \frac{1}{2}\right)}. \tag{79}$$

where $\bar{C}(\mathbf{u})$ denotes the *survival function*[13]:

$$\bar{C}(\mathbf{u}) := \mathbb{P}(\mathbf{U} > \mathbf{u}), \quad (\mathbf{u} = [u_1; \ldots; u_d] \in [0,1]^d). \tag{80}$$

$A_\beta$ [Eq. (78)] is a measure of concordance (see Def. 2 in Section D). A natural multivariate ($\mathbf{y} \in \mathbb{R}^d$, $d_m = 1$) generalization [145, 106] of Blomqvist's $\beta$ motivated by (79) is

$$A_\beta\left(y^1, \ldots, y^d\right) = A_\beta(C) = \frac{C\left(\mathbf{1/2}\right) - \Pi\left(\mathbf{1/2}\right) + \bar{C}\left(\mathbf{1/2}\right) - \bar{\Pi}\left(\mathbf{1/2}\right)}{M\left(\mathbf{1/2}\right) - \Pi\left(\mathbf{1/2}\right) + \bar{M}\left(\mathbf{1/2}\right) - \bar{\Pi}\left(\mathbf{1/2}\right)} = h_\beta(d)\left[C(\mathbf{1/2}) + \bar{C}(\mathbf{1/2}) - 2^{1-d}\right], \tag{81}$$

where $\mathbf{1/2} = \left[\frac{1}{2}; \ldots; \frac{1}{2}\right] \in \mathbb{R}^d$ and

$$h_\beta(d) = \frac{2^{d-1}}{2^{d-1} - 1}. \tag{82}$$

The objective [Eq. (81)] is called '`Blomqvist`' in ITE.[14] $A_\beta$ [Eq. (81)] satisfies all the axioms of multivariate measure of concordance (see Def. 3 in Section D) except for Duality [140].

7. **Multivariate conditional version of Spearman's $\rho$ (lower/upper tail)**: Let $g$ be a non-negative function, for which the following integral exists [104]:

$$A_{\rho_g}\left(y^1, \ldots, y^d\right) = A_{\rho_g}(C) = \frac{\int_{[0,1]^d} C(\mathbf{u}) g(\mathbf{u}) \mathrm{d}\mathbf{u} - \int_{[0,1]^d} \Pi(\mathbf{u}) g(\mathbf{u}) \mathrm{d}\mathbf{u}}{\int_{[0,1]^d} M(\mathbf{u}) g(\mathbf{u}) \mathrm{d}\mathbf{u} - \int_{[0,1]^d} \Pi(\mathbf{u}) g(\mathbf{u}) \mathrm{d}\mathbf{u}}. \tag{83}$$

Here, $g$ is a weighting function, emphasizing specific parts of the copula.

(a) **Lower tail**: Specially, let $g(\mathbf{u}) = \mathbb{I}_{[0,p]^d}(\mathbf{u})$ ($0 < p \leq 1$), where $\mathbb{I}$ stands for the indicator function. This $g$ choice refers to the weighting of the lower part of the copula, i.e., we measure the amount of depedence in the lower tail of the multivariate distributions.

The resulting conditional version of Spearman's $\rho$ is

$$A_{\rho_{\mathrm{lt}}}\left(y^1, \ldots, y^d\right) = A_{\rho_{\mathrm{lt}}}(C) = \frac{\int_{[0,p]^d} C(\mathbf{u}) \mathrm{d}\mathbf{u} - \int_{[0,p]^d} \Pi(\mathbf{u}) \mathrm{d}\mathbf{u}}{\int_{[0,p]^d} M(\mathbf{u}) \mathrm{d}\mathbf{u} - \int_{[0,p]^d} \Pi(\mathbf{u}) \mathrm{d}\mathbf{u}} = \frac{\int_{[0,p]^d} C(\mathbf{u}) \mathrm{d}\mathbf{u} - \left(\frac{p^2}{2}\right)^d}{\frac{p^{d+1}}{d+1} - \left(\frac{p^2}{2}\right)^d}. \tag{84}$$

The name of the association measure is '`Spearman_lt`' in ITE.

Note:

- Specially, for $p = 1$ the association $A_{\rho_{\mathrm{lt}}}$ reduces to $A_{\rho_1}$ [Eq. (69)].
- One can show that $A_{\rho_{lt}}$ preserves the concordance ordering [see Eq. (167)], i.e., $C_1 \prec C_2 \Rightarrow A_{\rho_{lt}}(C_1) \leq A_{\rho_{lt}}(C_2)$, for $\forall p \in (0,1]$. Specially, from $C \prec M$ [see Eq. (66)] one obtains that $A_{\rho_{lt}} \leq 1$.

[13] $\bar{C}$ is not in general a copula.

[14] Despite Eq. (81), '`Blomqvist`' is implemented as a base association measure estimator to avoid the computation of the same rank statistics multiple times.

| Estimated quantity | Principle | $d_m$ | $M$ | cost_name |
|---|---|---|---|---|
| Spearman's $\rho$: multivariate1 ($A_{\rho_1}$) | empirical copula, explicit formula | $d_m = 1$ | $M \geq 2$ | 'Spearman1' |
| Spearman's $\rho$: multivariate2 ($A_{\rho_2}$) | empirical copula, explicit formula | $d_m = 1$ | $M \geq 2$ | 'Spearman2' |
| Spearman's $\rho$: multivariate3 ($A_{\rho_3}$) | $\rho_3$ is the average of $\rho_1$ and $\rho_2$ | $d_m = 1$ | $M \geq 2$ | 'Spearman3' |
| Spearman's $\rho$: multivariate4 ($A_{\rho_4}$) | average pairwise Spearman's $\rho$ | $d_m = 1$ | $M \geq 2$ | 'Spearman4' |
| correntropy ($A_{\text{CorrEntr}}$) | KDE, direct | $d_m = 1$ | $M = 2$ | 'CorrEntr_KDE_direct' |
| centered correntropy ($A_{\text{CCorrEntr}}$) | KDE, incomplete Cholesky decomp. | $d_m = 1$ | $M = 2$ | 'CCorrEntr_KDE_iChol' |
| centered correntropy ($A_{\text{CCorrEntr}}$) | KDE, Laplacian kernel, sorting | $d_m = 1$ | $M = 2$ | 'CCorrEntr_KDE_Lapl' |
| correntropy coefficient ($A_{\text{CorrEntrCoeff}}$) | KDE, direct | $d_m = 1$ | $M = 2$ | 'CorrEntrCoeff_KDE_direct' |
| correntropy coefficient ($A_{\text{CorrEntrCoeff}}$) | KDE, incomplete Cholesky decomp. | $d_m = 1$ | $M = 2$ | 'CorrEntrCoeff_KDE_iChol' |
| Blomqvist's $\beta$ ($A_\beta$) | empirical copula, explicit formula | $d_m = 1$ | $M \geq 2$ | 'Blomqvist' |
| conditional Spearman's $\rho$, lower tail ($A_{\rho_{\text{lt}}}$) | empirical copula, explicit formula | $d_m = 1$ | $M \geq 2$ | 'Spearman_lt' |
| conditional Spearman's $\rho$, upper tail ($A_{\rho_{\text{ut}}}$) | empirical copula, explicit formula | $d_m = 1$ | $M \geq 2$ | 'Spearman_ut' |

Table 5: Association measure estimators (base). Third column: dimension constraint ($d_m$; $\mathbf{y}^m \in \mathbb{R}^{d_m}$). Fourth column: constraint for the number of components ($M$; $\mathbf{y} = \left[\mathbf{y}^1; \ldots; \mathbf{y}^M\right]$).

(b) **Upper tail:** In this case, in Eq. (83) our choice is $g(\mathbf{u}) = \mathbb{I}_{[1-p,1]^d}(\mathbf{u})$ $(0 < p \leq 1)$, i.e., the upper tail of the copula is weighted:

$$A_{\rho_{\text{ut}}}\left(y^1, \ldots, y^d\right) = A_{\rho_{\text{ut}}}(C) = \frac{\int_{[1-p,1]^d} C(\mathbf{u})\mathrm{d}\mathbf{u} - \int_{[1-p,1]^d} \Pi(\mathbf{u})\mathrm{d}\mathbf{u}}{\int_{[1-p,1]^d} M(\mathbf{u})\mathrm{d}\mathbf{u} - \int_{[1-p,1]^d} \Pi(\mathbf{u})\mathrm{d}\mathbf{u}}. \tag{85}$$

The name of the objective is 'Spearman_ut' in ITE.

The calling syntax of the association measure estimators is uniform and very simple; as an example the $A_{\rho_1}$ measure is estimated:

**Example 6 (Association measure estimation (base: usage))**

```
>ds = ones(3,1); Y = rand(sum(ds),5000); %generate the data of interest (ds(m)=dim(y^m), T=5000)
>mult = 1;                               %multiplicative constant is important
>co = ASpearman1_initialization(mult);   %initialize the association ('A') estimator ('Spearman1')
>A = ASpearman1_estimation(Y,ds,co);     %perform association measure estimation
```

For the estimation of other association measures it is sufficient to change 'Spearman1' to the cost_name given in the last column of Table 5 summarizing the base association measure estimators.

### 3.1.5 Cross Quantity Estimators

'Cross'-type measures arise naturally in information theory – we think of divergences (see Section 3.1.3) in ITE as a special class of cross measures which (i) are non-negative, (ii) being zero, if and only if $f_1 = f_2$. Our goal is to estimate such cross quantities from independent, i.i.d. samples $\left\{\mathbf{y}_t^1\right\}_{t=1}^{T_1}$ and $\left\{\mathbf{y}_t^2\right\}_{t=1}^{T_2}$ distributed according to $f_1$ and $f_2$, respectively. One of the most well-known such quantity is **cross-entropy**. The cross-entropy of two probability densities, $f_1 : \mathbb{R}^d \mapsto \mathbb{R}$ and $f_2 : \mathbb{R}^d \mapsto \mathbb{R}$ is defined as:

$$C_{\text{CE}}(f_1, f_2) = -\int_{\mathbb{R}^d} f_1(\mathbf{u}) \log\left[f_2(\mathbf{u})\right] \mathrm{d}\mathbf{u}. \tag{86}$$

One can estimate $C_{\text{CE}}$ via the k-nearest neighbor ($S = \{k\}$) technique [64]; the method is available in ITE and is called 'CE_kNN_k'. The calling syntax of the cross quantity estimators is uniform, an example is given below:

**Example 7 (Cross quantity estimation (base: usage))**

```
>Y1 = randn(3,2000); Y2 = randn(3,3000); %generate the data of interest (d=3, T_1=2000, T_2=3000)
>mult = 1;                               %multiplicative constant is important
>co = CCE_kNN_k_initialization(mult);    %initialize the cross ('C') estimator ('CE_kNN_k')
>C = CCE_kNN_k_estimation(Y1,Y2,co);     %perform cross-entropy estimation
```

The base cross quantity estimators of ITE are summarized in Table 6.

| Estimated quantity | Principle | $d$ | `cost_name` |
|---|---|---|---|
| cross-entropy ($C_{\mathrm{CE}}$) | k-nearest neighbors ($S = \{k\}$) | $d \geq 1$ | `'CE_kNN_k'` |

Table 6: Cross quantity estimators (base). Third column: dimension ($d$) constraint.

#### 3.1.6 Estimators of Kernels on Distributions

Kernels on distributions quantify the 'similarity' of $\nu_1$ and $\nu_2$, two distributions (probability measures) on a given $\mathcal{X}$ space ($\nu_1, \nu_2 \in \mathcal{M}_+^1(\mathcal{X})$). By definition the $K : \mathcal{M}_+^1(\mathcal{X}) \times \mathcal{M}_+^1(\mathcal{X}) \to \mathbb{R}$ kernel is symmetric and positive definite, i.e.,

1. $K(\nu_1, \nu_2) = K(\nu_2, \nu_1)$ $(\forall \nu_1, \nu_2 \in \mathcal{M}_+^1(\mathcal{X}))$, and
2. $\sum_{i,j=1}^n c_i c_j K(\nu_i, \nu_j) \geq 0$, for all $n$ positive number, $\{c_i\}_{i=1}^n \in \mathbb{R}^n$ and $\{\nu_i\}_{i=1}^n \in \left[\mathcal{M}_+^1(\mathcal{X})\right]^n$.

An alternative, equivalent view of kernels is that they compute the inner product of their arguments embedded into a suitable Hilbert space ($\mathcal{H}$). In other words, there exist a $\varphi : \mathcal{M}_+^1(\mathcal{X}) \to \mathcal{H}$ mapping, where $\mathcal{H}$ is a Hilbert space such that

$$K(\nu_1, \nu_2) = \langle \varphi(\nu_1), \varphi(\nu_2) \rangle_{\mathcal{H}}, \quad (\forall \nu_1, \nu_2 \in \mathcal{M}_+^1(\mathcal{X})). \tag{87}$$

In the simplest case $\mathcal{X} = \mathbb{R}^d$ and the $\nu_1, \nu_2$ distributions are identified with their densities $f_1 : \mathbb{R}^d \mapsto \mathbb{R}$ and $f_2 : \mathbb{R}^d \mapsto \mathbb{R}$. Our goal is to estimate the value of the kernel $[K(f_1, f_2)]$ given independent, i.i.d. samples from $f_1$ and $f_2$, $\{\mathbf{y}_t^1\}_{t=1}^{T_1}$ and $\{\mathbf{y}_t^2\}_{t=1}^{T_2}$, respectively. It is also worth noting that many widely used divergences (see Section 3.1.3 and 3.1.3) can be induced by kernels, see [41].

ITE can estimate the following kernels on distributions:

1. **Expected kernel**: The expected kernel is the inner product of $\boldsymbol{\mu}_1$ and $\boldsymbol{\mu}_2$, the mean embedding of $f_1$ and $f_2$ [see (45)]

$$K_{\exp}(f_1, f_2) = \langle \boldsymbol{\mu}_1, \boldsymbol{\mu}_2 \rangle_{\mathcal{F}} = \mathbb{E}_{\mathbf{y}^1, \mathbf{y}^2}\left[k\left(\mathbf{y}^1, \mathbf{y}^2\right)\right], \tag{88}$$

   i.e., it generates MMD

$$[D_{\mathrm{MMD}}(f_1, f_2)]^2 = K_{\exp}(f_1, f_1) - 2K_{\exp}(f_1, f_2) + K_{\exp}(f_1, f_2). \tag{89}$$

   The estimator of the expected kernel is called '`expected`' in ITE.

2. **Bhattacharyya kernel**: The Bhattacharyya kernel [8, 50] (also known as the Bhattacharyya coefficient, or the Hellinger affinity; see (62)) is defined as

$$K_{\mathrm{B}}(f_1, f_2) = \int_{\mathbb{R}^d} \sqrt{f_1(\mathbf{u})}\sqrt{f_2(\mathbf{u})}\mathrm{d}\mathbf{u}. \tag{90}$$

   It

   - is intimately related to, induces the Hellinger distance [see Eq. (49)]:

$$[D_{\mathrm{H}}(f_1, f_2)]^2 = \frac{1}{2}\left[K_{\mathrm{B}}(f_1, f_1) - 2K_{\mathrm{B}}(f_1, f_2) + K_{\mathrm{B}}(f_2, f_2)\right] = \frac{1}{2}[2 - 2K_{\mathrm{B}}(f_1, f_2)] = 1 - K_{\mathrm{B}}(f_1, f_2)]. \tag{91}$$

   - is sufficient to estimate (63), for which there exist k-nearest neighbor methods [92]. The associated estimator is called '`Bhattacharyya_kNN_k`' in ITE.

3. **Probability product kernel:** The probability product kernel [50] is the inner product of the $\rho^{th}$ power of the densities

$$K_{\mathrm{PP}}(f_1, f_2) = \int_{\mathbb{R}^d} [f_1(\mathbf{u})]^\rho [f_2(\mathbf{u})]^\rho \, \mathrm{d}\mathbf{u}, \quad (\rho > 0). \tag{92}$$

   Notes:

| Estimated quantity | Principle | $d$ | `cost_name` |
|---|---|---|---|
| expected kernel ($K_{\exp}$) | mean of pairwise kernel values | $d \geq 1$ | `'expected'` |
| Bhattacharyya kernel ($K_{\mathrm{B}}$) | k-nearest neighbors ($S = \{k\}$) | $d \geq 1$ | `'Bhattacharyya_kNN_k'` |
| probability product kernel ($K_{\mathrm{PP}}$) | k-nearest neighbors ($S = \{k\}$) | $d \geq 1$ | `'PP_kNN_k'` |

Table 7: Estimators of kernels on distributions (base). Third column: dimension ($d$) constraint.

- Specially, for $\rho = \frac{1}{2}$ we get back the Bhattacharyya kernel [see (90)].
- It is sufficient to estimate the (63) quantity, for which k-nearest neighbor techniques are available [92]. The corresponding estimator is called '`PP_kNN_k`' in ITE.

The calling syntax of kernels on distributions is uniform. In the following example the estimation of the expected kernel is illustrated:

**Example 8 (Kernel estimation on distributions (base: usage))**

```
>Y1 = randn(3,2000); Y2 = randn(3,3000); %generate the data of interest (d=3, T1=2000, T2=3000)
>mult = 1;                               %multiplicative constant is important
>co = Kexpected_initialization(mult); %initialize the kernel ('K') estimator on
                                       %distributions ('expected')
>K = Kexpected_estimation(Y1,Y2,co);  %perform kernel estimation on distributions
```

The available base kernel estimators on distributions are enlisted in Table 7; for the estimation of other kernels it is enough to change '`expected`' to the `cost_name` given in the last column of the table.

## 3.2 Meta Estimators

Here, we present how one can easily derive in the ITE package new information theoretical estimators from existing ones on the basis of relations between entropy, mutual information, divergence, association and cross quantities. These *meta* estimators are included in ITE. The additional goal of this section is to provide examples for meta estimator construction so that users could simply create novel ones. In Section 3.2.1, Section 3.2.2, Section 3.2.3, Section 3.2.4 and Section 3.2.5, we focus on entropy, mutual information, divergence, association measure and cross quantity estimators, respectively.

### 3.2.1 Entropy Estimators

Here, we present the idea of the meta construction in entropy estimation through examples:

1. **Ensemble**: The first example considers estimation via the ensemble approach. As it has been recently demonstrated the computational load of entropy estimation can be heavily decreased by (i) dividing the available samples into groups and then (ii) computing the averages of the group estimates [61]. Formally, let the samples be denoted by $\{\mathbf{y}_t\}_{t=1}^T$ ($\mathbf{y}_t \in \mathbb{R}^d$) and let us partition them into $N$ groups of size $g$ ($gN = T$), $\{1, \ldots, T\} = \cup_{n=1}^N I_n$ ($I_i \cap I_j = \emptyset$, $i \neq j$) and average the estimations based on the groups

$$H_{\text{ensemble}}(\mathbf{y}) = \frac{1}{N} \sum_{n=1}^{N} \hat{H}\left(\{\mathbf{y}_t\}_{t \in I_n}\right). \tag{93}$$

   As a prototype example for meta entropy estimation the implementation of the ensemble method [Eq. (93)] is provided below (see Example 9 and Example 10). In the example, the individual estimators in the ensemble are based on k-nearest neighbors ('`Shannon_kNN_k`'). However, the flexibility of the ITE package allows to change the $H$ estimator [r.h.s of (93)] to *any* other entropy estimation technique (base/meta, see Table 2 and Table 8).

   **Example 9 (Entropy estimation (meta: initialization))**

```
function [co] = Hensemble_initialization(mult)
co.name = 'ensemble';              %name of the estimator: 'ensemble'
```

```
co.mult = mult;                     %set whether multiplicative constant is important
co.group_size = 500;                %group size (g=500)
co.member_name = 'Shannon_kNN_k'; %estimator used in the ensemble ('Shannon_kNN_k')
co.member_co = H_initialization(co.member_name,mult);%initialize the member in the ensemble,
                                                     %the value of 'mult' is passed
```

The estimation part is carried out in accordance with (93):

**Example 10 (Entropy estimation (meta: estimation))**

```
function [H] = Hensemble_estimation(Y,co)
g = co.group_size;                          %initialize group size (g)
num_of_samples = size(Y,2);                 %initialize number of samples (T)
num_of_groups = floor(num_of_samples/g);    %initialize number of groups (N)

H = 0;
for k = 1 : num_of_groups                   %compute the average over the ensemble
  H = H + H_estimation(Y(:,(k-1)*g+1:k*g),co.member_co); %add the estimation
                                                         %of the initialized member
end
H = H / num_of_groups;
```

The usage of the defined method follows the syntax of base entropy estimators (Example 2, Example 3):

**Example 11 (Entropy estimation (meta: usage))**

```
>Y = rand(5,1000);                    %generate the data of interest (d=5, T=1000)
>mult = 1;                            %multiplicative constant is important
>co = Hensemble_initialization(mult); %initialize the entropy ('H') estimator ('ensemble'),
>H = Hensemble_estimation(Y,co);       %perform entropy estimation
```

2. **Random projected ensemble**: Since (i) entropy can be estimated consistently using pairwise distances of sample points[15], and (ii) random projection (RP) techniques realize approximate isometric embeddings [53, 31, 49, 1, 65, 4, 72], one can construct efficient estimation methods by the integration of the ensemble and the RP technique.

   Formally, the definition of the estimation is identical to that of the ensemble approach [Eq. (93)], except for random projections $\mathbf{R}_n \in \mathbb{R}^{d_{RP} \times d}$ $(n = 1, \ldots, N)$. The final estimation is

$$H_{\text{RPensemble}}(\mathbf{y}) = \frac{1}{N} \sum_{n=1}^{N} \hat{H}\left(\{\mathbf{R}_n \mathbf{y}_t\}_{t \in I_n}\right). \tag{94}$$

   The approach shows exciting potentials with serious computational speed-ups in independent subspace analysis [125] and image registration [126]. The technique has been implemented in the ITE toolbox under the name '`RPensemble`'.

3. **Complex**: Information theoretical quantities can be defined over the complex domain via the Hilbert transformation [28]

$$\varphi_v : \mathbb{C}^d \ni \mathbf{v} \mapsto \mathbf{v} \otimes \begin{bmatrix} \Re(\cdot) \\ \Im(\cdot) \end{bmatrix} \in \mathbb{R}^{2d}, \tag{95}$$

   as the entropy of the mapped 2d-dimensional real variable

$$H_{\mathbb{C}}(\mathbf{y}) := H(\varphi_v(\mathbf{y})). \tag{96}$$

   Relation (96) can be transformed to a meta entropy estimator, the method is available under the name '`complex`'.

[15] The construction holds for other information theoretical quantities like mutual information and divergence.

| Estimated quantity | Principle | $d$ | `cost_name` |
|---|---|---|---|
| complex entropy ($H_{\mathbb{C}}$) | entropy of a real random vector variable | $d \geq 1$ | `'complex'` |
| Shannon entropy ($H$) | average the entropy over an ensemble | $d \geq 1$ | `'ensemble'` |
| Shannon entropy ($H$) | average the entropy over a random projected ensemble | $d \geq 1$ | `'RPensemble'` |
| Tsallis entropy ($H_{\mathrm{T},\alpha}$) | function of the Rényi entropy | $d \geq 1$ | `'Tsallis_HRenyi'` |
| Shannon entropy ($H$) | -KL divergence from the normal distribution | $d \geq 1$ | `'Shannon_DKL_N'` |
| Shannon entropy ($H$) | -KL divergence from the uniform distribution | $d \geq 1$ | `'Shannon_DKL_U'` |

Table 8: Entropy estimators (meta). Third column: dimension ($d$) constraint.

4. **Rényi entropy $\rightarrow$ Tsallis entropy**: Using (3) and (5), the Tsallis entropy can be computed from the Rényi entropy:
$$H_{\mathrm{T},\alpha}(\mathbf{y}) = \frac{e^{(1-\alpha)H_{\mathrm{R},\alpha}(\mathbf{y})} - 1}{1-\alpha}. \tag{97}$$
The formula is realized in ITE by the '`Tsallis_HRenyi`' meta entropy estimator. Making use of this approach, for example, the Rényi entropy estimators of Table 2 can be instantly applied for Tsallis entropy estimation.

5. **Divergence from the Gaussian distribution**: Let $\mathbf{y}_G \in \mathbb{R}^d$ be a normal random variable with the same mean and covariance as $\mathbf{y}$:
$$\mathbf{y}_G \sim f_G = N(\mathbb{E}(\mathbf{y}), cov(\mathbf{y})). \tag{98}$$
The Shannon entropy of a normal random variable can be explicitly computed
$$H(\mathbf{y}_G) = \frac{1}{2}\log\left[(2\pi e)^d \det(cov(\mathbf{y}))\right], \tag{99}$$
moreover, $H(\mathbf{y})$ equals to $H(\mathbf{y}_G)$ minus the Kullback-Leibler divergence [see Eq. (37)] of $\mathbf{y} \sim f$ and $f_G$ [152]:
$$H(\mathbf{y}) = H(\mathbf{y}_G) - D(f, f_G). \tag{100}$$
The associated meta entropy estimator is called '`Shannon_DKL_N`'.

6. **Divergence from the uniform distribution**: If $\mathbf{y} \in [0,1]^d$ ($\sim f$), then the entropy of $\mathbf{y}$ equals to minus the Kullback-Leibler divergence [see Eq. (37)] of $f$ and $f_U$, the uniform distribution on $[0,1]^d$:
$$H(\mathbf{y}) = -D(f, f_U). \tag{101}$$
If $\mathbf{y} \in [\mathbf{a}, \mathbf{b}] = \times_{i=1}^d [a_i, b_i] \subseteq \mathbb{R}^d$ ($\sim f$), then let $\mathbf{y}' = \mathbf{A}\mathbf{y} + \mathbf{d} \sim f'$ be its linearly transformed version to $[0,1]^d$, where $\mathbf{A} = diag\left(\frac{1}{b_i - a_i}\right) \in \mathbb{R}^{d\times d}$, $\mathbf{d} = \left[\frac{a_i}{a_i - b_i}\right] \in \mathbb{R}^d$. Applying the previous result and the entropy transformation rule under linear mappings [21], one obtains that
$$H(\mathbf{y}) = -D(f', f_U) + \log\left[\prod_{i=1}^d (b_i - a_i)\right]. \tag{102}$$
This meta entropy estimation technique is called '`Shannon_DKL_U`' in ITE.

The meta entropy estimator methods in ITE are summarized in Table 8. The calling syntax of the estimators is identical to Example 11, one only has to change the name '`ensemble`' to the `cost_name` of the target estimators, see the last column of the table.

### 3.2.2 Mutual Information Estimators

In this section we are dealing with meta mutual information estimators:

1. As it has been seen in Eq. (1), **mutual information** can be expressed via entropy terms. The corresponding method is available in the ITE package under the name '`Shannon_HShannon`'. As a prototype example for meta mutual information estimator the implementation is provided below:

**Example 12 (Mutual information estimator (meta: initialization))**

```
function [co] = IShannon_HShannon_initialization(mult)
co.name = 'Shannon_HShannon';      %name of the estimator: 'Shannon_HShannon'
co.mult = mult;                     %set the importance of multiplicative factors
co.member_name = 'Shannon_kNN_k';  %method used for entropy estimation: 'Shannon_kNN_k'
co.member_co = H_initialization(co.member_name,1);%initialize entropy estimation member, mult=1
```

**Example 13 (Mutual information estimator (meta: estimation))**

```
function [I] = IShannon_HShannon_estimation(Y,ds,co) %samples(Y), component dimensions(ds),
                                                     %initialized estimator (co)
num_of_comps = length(ds);                      %number of components, M
cum_ds = cumsum([1;ds(1:end-1)]);               %starting indices of the components
I = -H_estimation(Y,co.member_co);              %minus the joint entropy, H([y^1;...;y^M]) using
                                                %the initialized H estimator
for k = 1 : num_of_comps                        %add the entropy of the y^m components, H(y^m)
  idx = [cum_ds(k) : cum_ds(k)+ds(k)-1];
  I = I + H_estimation(Y(idx,:),co.member_co);%use the initialized H estimator
end
```

The usage of the meta mutual information estimators follow the syntax of base mutual information estimators (see Example 4):

**Example 14 (Mutual information estimator (meta: usage))**

```
>ds = [1;2]; Y=rand(sum(ds),5000);            %generate the data of interest
                                              %(ds(m)=dim(y^m), T=5000)
>mult = 1;                                    %multiplicative constant is important
>co = IShannon_HShannon_initialization(mult); %initialize the mutual information ('I')
                                              %estimator ('Shannon_HShannon')
>I = IShannon_HShannon_estimation(Y,ds,co);   %perform mutual information estimation
```

2. **Complex**: The mutual information of complex random variables ($\mathbf{y} \in \mathbb{C}^{d_m}$) can be defined via the Hilbert transformation [Eq. (95)]:

$$I_{\mathbb{C}}\left(\mathbf{y}^1,\ldots,\mathbf{y}^M\right) = I\left(\varphi_v\left(\mathbf{y}^1\right),\ldots,\varphi_v\left(\mathbf{y}^M\right)\right). \tag{103}$$

The relation is realized in ITE by the '`complex`' meta estimator.

3. **Shannon-, $\mathbf{L_2}$-, Tsallis- and Rényi mutual information**: The Shannon-, $L_2$-, Tsallis- and Rényi mutual information can be expressed in terms of the corresponding divergence of the joint ($f$) and the product of marginals ($\prod_{m=1}^M f_m$)[16]:

$$I\left(\mathbf{y}^1,\ldots,\mathbf{y}^M\right) = D\left(f, \prod_{m=1}^M f_m\right), \qquad I_L\left(\mathbf{y}^1,\ldots,\mathbf{y}^M\right) = D_{\mathrm{L}}\left(f, \prod_{m=1}^M f_m\right), \tag{104}$$

$$I_{\mathrm{T},\alpha}\left(\mathbf{y}^1,\ldots,\mathbf{y}^M\right) = D_{\mathrm{T},\alpha}\left(f, \prod_{m=1}^M f_m\right), \qquad I_{\mathrm{R},\alpha}\left(\mathbf{y}^1,\ldots,\mathbf{y}^M\right) = D_{\mathrm{R},\alpha}\left(f, \prod_{m=1}^M f_m\right). \tag{105}$$

Shannon mutual information is a special case of Rényi's and Tsallis' in limit sense:

$$I_{\mathrm{R},\alpha} \xrightarrow{\alpha\to 1} I, \qquad I_{\mathrm{T},\alpha} \xrightarrow{\alpha\to 1} I. \tag{106}$$

The associated Rényi-, $L_2$- and Tsallis meta mutual information estimators are available in ITE using the names '`Renyi_DRenyi`', '`L2_DL2`' and '`Tsallis_DTsallis`'.

[16] For the definitions of $f$ and $f_m$s, see Eq. (7). The divergence definitions can be found in Eqs. (37), (38), (39) and (42).

4. **Copula based kernel dependency**: [88] has recently defined a novel, robust, copula-based mutual information measure of the random variable $y^m \in \mathbb{R}$ $(m = 1, \ldots, M)$ as the MMD divergence [Eq. (45)] of the joint copula and the M-dimensional uniform distribution on $[0,1]^M$:

$$I_{\mathrm{c}}\left(y^1, \ldots, y^M\right) = D_{\mathrm{MMD}}(\mathbb{P}_{\mathbf{Z}}, \mathbb{P}_{\mathbf{U}}), \tag{107}$$

where $\mathbf{Z} = \left[F_1\left(y^1\right); \ldots; F_M\left(y^M\right)\right] \in \mathbb{R}^M$ is the joint copula, $F_m$ is the cumulative density function of $y^m$ and $\mathbb{P}$ denotes the distribution. The associated meta estimator has the name '`MMD_DMMD`' in ITE.

5. **Distance covariance**: An alternative form of the distance covariance [Eq. (32) and $\alpha = 1$] in terms of pairwise distances is

$$\begin{aligned} I_{\mathrm{dCov}}\left(\mathbf{y}^1, \mathbf{y}^2\right) = &\mathbb{E}_{\mathbf{y}^1,\mathbf{y}^2}\mathbb{E}_{\mathbf{y}^{1'},\mathbf{y}^{2'}}\left[\left\|\mathbf{y}^1 - \mathbf{y}^{1'}\right\|_2 \left\|\mathbf{y}^2 - \mathbf{y}^{2'}\right\|_2\right] + \mathbb{E}_{\mathbf{y}^1,\mathbf{y}^{1'}}\left[\left\|\mathbf{y}^1 - \mathbf{y}^{1'}\right\|_2\right]\mathbb{E}_{\mathbf{y}^2,\mathbf{y}^{2'}}\left[\left\|\mathbf{y}^2 - \mathbf{y}^{2'}\right\|_2\right] \\ &- 2\mathbb{E}_{\mathbf{y}^1,\mathbf{y}^2}\left[\mathbb{E}_{\mathbf{y}^{1'}}\left\|\mathbf{y}^1 - \mathbf{y}^{1'}\right\|_2 \mathbb{E}_{\mathbf{y}^{2'}}\left\|\mathbf{y}^2 - \mathbf{y}^{2'}\right\|_2\right], \end{aligned} \tag{108}$$

where $(\mathbf{y}^1, \mathbf{y}^2)$ and $(\mathbf{y}^{1'}, \mathbf{y}^{2'})$ are i.i.d. variables. The concept of distance covariance and the formula above can also be extended to semimetric spaces $[(\mathcal{Y}_1, \rho_1), (\mathcal{Y}_2, \rho_2)]$ of negative type [69, 109] (see Def. 6, Section D):

$$\begin{aligned} I_{\mathrm{dCov}}\left(\mathbf{y}^1, \mathbf{y}^2\right) = &\mathbb{E}_{\mathbf{y}^1,\mathbf{y}^2}\mathbb{E}_{\mathbf{y}^{1'},\mathbf{y}^{2'}}\left[\rho_1\left(\mathbf{y}^1, \mathbf{y}^{1'}\right)\rho_2\left(\mathbf{y}^2, \mathbf{y}^{2'}\right)\right] + \mathbb{E}_{\mathbf{y}^1,\mathbf{y}^{1'}}\left[\rho_1\left(\mathbf{y}^1, \mathbf{y}^{1'}\right)\right]\mathbb{E}_{\mathbf{y}^2,\mathbf{y}^{2'}}\left[\rho_2\left(\mathbf{y}^2, \mathbf{y}^{2'}\right)\right] \\ &- 2\mathbb{E}_{\mathbf{y}^1,\mathbf{y}^2}\left(\mathbb{E}_{\mathbf{y}^{1'}}\left[\rho_1\left(\mathbf{y}^1, \mathbf{y}^{1'}\right)\right]\mathbb{E}_{\mathbf{y}^{2'}}\left[\left(\mathbf{y}^2, \mathbf{y}^{2'}\right)\right]\right). \end{aligned} \tag{109}$$

The resulting measure can be proved to be expressible in terms of HSIC [Eq. (13)]:

$$\left[I_{\mathrm{dCov}}\left(\mathbf{y}^1, \mathbf{y}^2\right)\right]^2 = 4[D_{\mathrm{MMD}}(f, f_1 f_2)]^2 = 4\left[I_{\mathrm{HSIC}}\left(\mathbf{y}^1, \mathbf{y}^2\right)\right]^2, \tag{110}$$

where the kernel $k$ (used in HSIC) is

$$k((\mathbf{u}_1, \mathbf{v}_1), (\mathbf{u}_2, \mathbf{v}_2)) = k_1(\mathbf{u}_1, \mathbf{u}_2)k_2(\mathbf{v}_1, \mathbf{v}_2) \tag{111}$$

with $k_i$ kernels generating [see Eq. (118)] $\rho_i$-s $(i = 1, 2)$. The meta estimator is called '`dCov_IHSIC`' in ITE.

6. **Approximate correntropy independence measure** [100]: This measure is defined as

$$I_{\mathrm{ACorrEntr}}\left(y^1, y^2\right) = \max\left[\left|A_{\mathrm{CCorrEntr}}\left(y^1, y^2\right)\right|, \left|A_{\mathrm{CCorrEntr}}\left(-y^1, y^2\right)\right|\right]. \tag{112}$$

The meta mutual information estimator is available in ITE under the name '`ApprCorrEntr`'.

Note: the correntropy independence measure

$$\sup_{a,b\in\mathbb{R}} |U_{a,b}\left(y^1, y^2\right)|, \tag{113}$$

where

$$U_{a,b}\left(y^1, y^2\right) = A_{\mathrm{CCorrEntr}}\left(ay^1 + b, y^2\right) \quad (a \neq 0) \tag{114}$$

is a valid independence measure in the sense, that it [Eq. (113)] is zero if and only if $y^1$ and $y^2$ are independent. $I_{\mathrm{ACorrEntr}}$ [Eq. (112)] is an approximation of this quantity in a bivariate mixture of Gaussian approach.

The calling syntax of the meta mutual information are identical (and the same as that of the base estimators, see Section 3.1.2), the possible methods are summarized in Table 9. The techniques are identified by their '`cost_name`', see the last column of the table.

### 3.2.3 Divergence Estimators

In this section we focus on meta divergence estimators (Table 10). Our prototype example is the estimation of the **symmetrised Kullback-Leibler divergence**, the so-called J-distance (or J divergence):

$$D_{\mathrm{J}}(f_1, f_2) = D(f_1, f_2) + D(f_2, f_1). \tag{115}$$

The definition of meta divergence estimators follows the idea of meta entropy and mutual information estimators (see Example 9, 10, 12 and 13). Initialization and estimation of the meta J-distance estimator can be carried out as follows:

| Estimated quantity | Principle | $d_m$ | $M$ | cost_name |
|---|---|---|---|---|
| complex mutual information ($I_{\mathbb{C}}$) | mutual information of a real random vector variable | $\geq 1$ | $\geq 2$ | 'complex' |
| $L_2$ mutual information ($I_L$) | $L_2$-divergence of the joint and the product of marginals | $\geq 1$ | $\geq 2$ | 'L2_DL2' |
| Rényi mutual information ($I_{\mathrm{R},\alpha}$) | Rényi divergence of the joint and the product of marginals | $\geq 1$ | $\geq 2$ | 'Renyi_DRenyi' |
| copula-based kernel dependency ($I_{\mathrm{c}}$) | MMD div. of the joint copula and the uniform distribution | $= 1$ | $\geq 2$ | 'MMD_DMMD' |
| Rényi mutual information ($I_{\mathrm{R},\alpha}$) | minus the Rényi entropy of the joint copula | $= 1$ | $\geq 2$ | 'Renyi_HRenyi' |
| (Shannon) mutual information ($I$) | entropy sum of the components minus the joint entropy | $\geq 1$ | $\geq 2$ | 'Shannon_HShannon' |
| Tsallis mutual information ($I_{\mathrm{T},\alpha}$) | $L_2$-divergence of the joint and the product of marginals | $\geq 1$ | $\geq 2$ | 'Tsallis_DTsallis' |
| distance covariance ($I_{\mathrm{dCov}}$) | pairwise distances, equivalence to HSIC | $\geq 1$ | $= 2$ | 'dCov_IHSIC' |
| appr. correntropy indep. ($I_{\mathrm{ACorrEntr}}$) | maximum of centered correntropies | $= 1$ | $= 2$ | 'ApprCorrEntr' |

Table 9: Mutual information estimators (meta). Third column: dimension constraint ($d_m$; $\mathbf{y}^m \in \mathbb{R}^{d_m}$). Fourth column: constraint for the number of components ($M$; $\mathbf{y} = \left[\mathbf{y}^1; \ldots; \mathbf{y}^M\right]$).

**Example 15 (Divergence estimator (meta: initialization))**

```
function [co] = DJdistance_initialization(mult)
co.name = 'Jdistance';           %name of the estimator: 'Jdistance'
co.mult = mult;                  %set whether multiplicative constant is important
co.member_name = 'Renyi_kNN_k';  %method used for Kullback-Leibler divergence estimation
co.member_co = D_initialization(co.member_name,mult); %initialize the Kullback-Leibler divergence
                                                      %estimator
```

**Example 16 (Divergence estimator (meta: estimation))**

```
function [D_J] = DJdistance_estimation(X,Y,co)
D_J = D_estimation(X,Y,co.member_co) + D_estimation(Y,X,co.member_co); %definition of J-distance
```

Having defined the J-distance estimator, the calling syntax is completely analogous to base estimators (see Example 5).

**Example 17 (Divergence estimator (meta: usage))**

```
>Y1 = rand(3,1000); Y2 = rand(3,2000); %generate the data of interest (d=3, T_1=1000, T_2=2000)
>mult = 1;                            %multiplicative constant is important
>co = DJdistance_initialization(mult); %initialize the divergence ('D') estimator ('Jdistance')
>D = DJdistance_estimation(Y1,Y2,co);  %perform divergence estimation
```

Further meta divergence estimators of ITE are the following:

1. **Cross-entropy + entropy → Kullback-Leibler divergence**: As is well-known the Kullback-Leibler divergence can be expressed in terms of cross-entropy (see Eq. (86)) and entropy:

$$D(f_1, f_2) = C_{\mathrm{CE}}(f_1, f_2) - H(f_1). \tag{116}$$

   The associated meta divergence estimator is called 'KL_CE_HShannon'.

2. **MMD → energy distance**: As it has been proved recently [69, 109], the energy distance [Eq. (54)] is closely related to MMD [Eq. (45)]:

$$D_{\mathrm{EnDist}}(f_1, f_2) = 2\left[D_{\mathrm{MMD}}(f_1, f_2)\right]^2, \tag{117}$$

   where the kernel $k$ (used in MMD) generates the semimetric $\rho$ (used in energy distance), i.e.,

$$\rho(\mathbf{u}, \mathbf{v}) = k(\mathbf{u}, \mathbf{u}) + k(\mathbf{v}, \mathbf{v}) - 2k(\mathbf{u}, \mathbf{v}). \tag{118}$$

   The name of the associated meta estimator is 'EnergyDist_DMMD'.

3. **Jensen-Shannon divergence**: This divergence is defined [66] in terms of the Shannon entropy as

$$D_{\mathrm{JS}}^{\pi}(f_1, f_2) = H\left(\pi_1 \mathbf{y}^1 + \pi_2 \mathbf{y}^2\right) - \left[\pi_1 H\left(\mathbf{y}^1\right) + \pi_2 H\left(\mathbf{y}^2\right)\right], \tag{119}$$

where $\mathbf{y}^i \sim f_i$ and $\pi_1 \mathbf{y}^1 + \pi_2 \mathbf{y}^2$ denotes the mixture distribution obtained from $\mathbf{y}^1$ and $\mathbf{y}^2$ with $\pi_1$, $\pi_2$ weights ($\pi_1, \pi_2 > 0$, $\pi_1 + \pi_2 = 1$). The meta estimator is called '`JensenShannon_HShannon`' in ITE.

Notes:

- As it is known $0 \leq D_{\mathrm{JS}}^{\pi}(f_1, f_2) \leq \log(2)$, $D_{\mathrm{JS}}^{\pi}(f_1, f_2) = 0 \Leftrightarrow f_1 = f_2$.
- Specially, for $\pi_1 = \pi_2 = \frac{1}{2}$ we obtain

$$D_{\mathrm{JS}}(f_1, f_2) = D_{\mathrm{JS}}^{\left(\frac{1}{2}, \frac{1}{2}\right)}(f_1, f_2) = H\left(\frac{\mathbf{y}^1 + \mathbf{y}^2}{2}\right) - \frac{H\left(\mathbf{y}^1\right) + H\left(\mathbf{y}^2\right)}{2} = \frac{1}{2}\left[D\left(f_1, \frac{f_1 + f_2}{2}\right) + D\left(f_2, \frac{f_1 + f_2}{2}\right)\right]. \tag{120}$$

  It is known that $\sqrt{D_{\mathrm{JS}}(f_1, f_2)}$ is a (covariant) Hilbertian metric [143, 27, 41]; see Def. 7.
- One can also generalize the Jensen-Shannon divergence [Eq. (119)] to multiple components as

$$D_{\mathrm{JS}}^{\pi}(f_1, \ldots, f_M) = H\left(\sum_{m=1}^{M} \pi_m \mathbf{y}^m\right) - \sum_{m=1}^{M} \pi_m H\left(\mathbf{y}^m\right), \tag{121}$$

  where $\pi_m > 0$ $(m = 1, \ldots, M)$, $\sum_{m=1}^{M} \pi_m = 1$, $\mathbf{y}^m \sim f_m$ $(m = 1, \ldots, M)$.

4. **Jensen-Rényi divergence**: The definition of the Jensen-Rényi divergence is analogous to (121); the difference to $D_{\mathrm{JS}}^{\pi}$ is that the Shannon entropy is changed to the Rényi entropy [38]

$$D_{\mathrm{JR},\alpha}^{\pi}(f_1, \ldots, f_M) = H_{\mathrm{R},\alpha}\left(\sum_{m=1}^{M} \pi_m \mathbf{y}^m\right) - \sum_{m=1}^{M} \pi_m H_{\mathrm{R},\alpha}\left(\mathbf{y}^m\right), \quad (\alpha \geq 0) \tag{122}$$

where $\pi_m > 0$ $(m = 1, \ldots, M)$, $\sum_{m=1}^{M} \pi_m = 1$, $\mathbf{y}^m \sim f_m$ $(m = 1, \ldots, M)$. The name of the meta estimator is '`JensenRenyi_HRenyi`' in ITE ($M = 2$).

5. **K divergence, L divergence**: The K divergence and the L divergence measures [66] are defined as

$$D_{\mathrm{K}}(f_1, f_2) = D\left(f_1, \frac{f_1 + f_2}{2}\right), \tag{123}$$

$$D_{\mathrm{L}}(f_1, f_2) = D_{\mathrm{K}}(f_1, f_2) + D_{\mathrm{K}}(f_2, f_1). \tag{124}$$

Notes: They are

- non-negative, and are zero if and only if $f_1 = f_2$.
- closely related to the Jensen-Shannon divergence in case of unifosee Eq. (120).
- available in ITE ('`K_DKL`' and '`L_DKL`').

6. **Jensen-Tsallis divergence**: The definition of the Jensen-Tsallis divergence [12] follows that of the Jensen-Shannon divergence [Eq. (120)]; only the Shannon entropy is replaced with the Tsallis entropy [Eq. (5)]

$$D_{\mathrm{JT},\alpha}(f_1, f_2) = H_{\mathrm{T},\alpha}\left(\frac{\mathbf{y}^1 + \mathbf{y}^2}{2}\right) - \frac{H_{\mathrm{T},\alpha}\left(\mathbf{y}^1\right) + H_{\mathrm{T},\alpha}\left(\mathbf{y}^2\right)}{2}, \quad (\alpha \neq 1) \tag{125}$$

where $\mathbf{y}^m \sim f_m$ $(m = 1, 2)$. Notes:

- The Jensen-Shannon divergence is special case in limit sense:

$$\lim_{\alpha \to 1} D_{\mathrm{JT},\alpha}(f_1, f_2) = D_{\mathrm{JS}}(f_1, f_2). \tag{126}$$

- The name of the associated meta estimator is '`JensenTsallis_HTsallis`' in ITE.

7. **Symmetric Bregman distance**: This measure [11, 23, 64] can be estimated using Eq. (57); its name is '`symBregman_DBregman`' in ITE.

The calling form the meta divergence estimators is uniform, one only has to change in Example 17 the `cost_name` to the value in the last column of Table 10.

| Estimated quantity | Principle | $d$ | cost_name |
|---|---|---|---|
| J-distance ($D_{\mathrm{J}}$) | symmetrised Kullback-Leibler divergence | $d \geq 1$ | 'Jdistance' |
| Kullback-Leibler divergence ($D$) | difference of cross-entropy and entropy | $d \geq 1$ | 'KL_CCE_HShannon' |
| Energy distance ($D_{\mathrm{EnDist}}$) | pairwise distances, equivalence to MMD | $d \geq 1$ | 'EnergyDist_DMMD' |
| Jensen-Shannon divergence ($D^{\pi}_{\mathrm{JS}}$) | smoothed ($\pi$), defined via the Shannon entropy | $d \geq 1$ | 'JensenShannon_HShannon' |
| Jensen-Rényi divergence ($D^{\pi}_{\mathrm{JR},\alpha}$) | smoothed ($\pi$), defined via the Rényi entropy | $d \geq 1$ | 'JensenRenyi_HRenyi' |
| K divergence ($D_{\mathrm{K}}$) | smoothed Kullback-Leibler divergence | $d \geq 1$ | 'K_DKL' |
| L divergence ($D_{\mathrm{L}}$) | symmetrised K divergence | $d \geq 1$ | 'L_DKL' |
| Jensen-Tsallis divergence ($D_{\mathrm{JT},\alpha}$) | smoothed, defined via the Tsallis entropy | $d \geq 1$ | 'JensenTsallis_HTsallis' |
| Symmetric Bregman distance ($D_{\mathrm{SB},\alpha}$) | symmetrised Bregman distance | $d \geq 1$ | 'symBregman_DBregman' |

Table 10: Divergence estimators (meta). Third column: dimension ($d$) constraint.

#### 3.2.4 Association Measure Estimators

One can define and use meta association measure estimators completely analogously to meta mutual information estimators (see Section 3.2.2). The meta association measure estimators included in ITE are the

- **Correntropy induced metric** [67, 110], **centered correntropy induced metric** [100]:

$$A_{\mathrm{CIM}}\left(y^1, y^2\right) = \sqrt{k(0,0) - A_{\mathrm{CorrEntr}}\left(y^1, y^2\right)}, \tag{127}$$

$$A_{\mathrm{CCIM}}\left(y^1, y^2\right) = \sqrt{A_{\mathrm{CCorrEntr}}\left(y^1, y^1\right) + A_{\mathrm{CCorrEntr}}\left(y^2, y^2\right) - 2A_{\mathrm{CCorrEntr}}\left(y^1, y^2\right)}, \tag{128}$$

  where $k$ is the kernel used in the correntropy estimator [Eqs. (75)-(76)]. The corresponding meta estimators are called 'CIM' and 'CCIM' in ITE.

- **Lower tail dependence via conditional Spearman's $\rho$**: This lower tail dependence measure has been defined [104] as the limit of $\hat{A}_{\rho_{\mathrm{lt}}} = \hat{A}_{\rho_{\mathrm{lt}}}(p)$ [Eq. (84)]:

$$A_{\rho_{\mathrm{L}}}\left(y^1, \ldots, y^d\right) = A_{\rho_{\mathrm{L}}}(C) = \lim_{p \to 0, p>0} A_{\rho_{\mathrm{lt}}}(C) = \lim_{p \to 0, p>0} \frac{d+1}{p^{d+1}} \int_{[0,p]^d} C(\mathbf{u}) \mathrm{d}\mathbf{u}, \tag{129}$$

  provided that the limit exists. The name of the association measure is 'Spearman_L' in ITE.

  Note:

  - Similarly to $A_{\rho_{\mathrm{lt}}}$ [Eq. (84)], $A_{\rho_{\mathrm{L}}}$ preserves concordance ordering [see Eq. (66)]: $C_1 \prec C_2 \Rightarrow A_{\rho_{\mathrm{L}}}(C_1) \leq A_{\rho_{\mathrm{L}}}(C_2)$.
  - Moreover, $0 \leq A_{\rho_{\mathrm{L}}}(C) \leq 1$; the comomonotonic copula $M$ implies $A_{\rho_{\mathrm{L}}} = 1$ and the independence copula $\Pi$ yields $A_{\rho_{\mathrm{L}}} = 0$.
  - $A_{\rho_{\mathrm{L}}}$ can be used as an alternative of the tail-dependence coefficient [114] widely spreaded in bivariate extreme value theory:

$$\lambda_L = \lambda_L(C) = \lim_{p \to 0, p>0} \frac{C(p,p)}{p}. \tag{130}$$

    An important drawback of $\lambda_L$ is that it takes into account the copula only on the diagonal ($C(p,p)$).

- **Upper tail dependence via conditional Spearman's $\rho$**: This upper tail dependence measure has been introduced in [104] as the limit of $\hat{A}_{\rho_{\mathrm{ut}}} = \hat{A}_{\rho_{\mathrm{ut}}}(p)$ [Eq. (85)]:

$$A_{\rho_{\mathrm{U}}}\left(y^1, \ldots, y^d\right) = A_{\rho_{\mathrm{U}}}(C) = \lim_{p \to 0, p>0} A_{\rho_{\mathrm{ut}}}(C), \tag{131}$$

  provided that the limit exists. The measure is an analogue of (129) in the 'upper' domain. It is called 'Spearman_U' in ITE.

The meta association measure estimators are summarized in Table 11.

| Estimated quantity | Principle | $d_m$ | $M$ | cost_name |
|---|---|---|---|---|
| correntropy induced metric ($A_{\text{CIM}}$) | metric from correntropy | $d_m = 1$ | $M = 2$ | 'CIM' |
| centered correntropy induced metric ($A_{\text{CCIM}}$) | metric from centered correntropy | $d_m = 1$ | $M = 2$ | 'CCIM' |
| lower tail dependence via conditional Spearman's $\rho$ ($A_{\rho_{\text{L}}}$) | limit of $A_{\rho_{\text{lt}}}$ | $d_m = 1$ | $M \geq 2$ | 'Spearman_L' |
| upper tail dependence via conditional Spearman's $\rho$ ($A_{\rho_{\text{U}}}$) | limit of $A_{\rho_{\text{ut}}}$ | $d_m = 1$ | $M \geq 2$ | 'Spearman_U' |

Table 11: Association measure estimators (meta). Third column: dimension constraint ($d_m$; $\mathbf{y}^m \in \mathbb{R}^{d_m}$). Fourth column: constraint for the number of components ($M$; $\mathbf{y} = \left[\mathbf{y}^1; \ldots; \mathbf{y}^M\right]$).

| Estimated quantity | Principle | $d$ | cost_name |
|---|---|---|---|
| Jensen-Shannon kernel ($K_{\text{JS}}$) | function of the Jensen-Shannon divergence | $d \geq 1$ | 'JS_DJS' |

Table 12: Estimators of kernels on distributions (meta). Third column: dimension ($d$) constraint.

#### 3.2.5 Cross Quantity Estimators

One can define and use meta cross quantity estimators completely analogously to meta divergence estimators (see Section 3.2.3).

#### 3.2.6 Estimators of Kernels on Distributions

It is possible to define and use meta estimators of kernels on distributions similarly to meta divergence estimators (see Section 3.2.3). ITE contains the following meta estimators (see Table 12):

**Jensen-Shannon kernel:** The Jensen-Shannon kernel [70, 71] is defined as

$$K_{\text{JS}}(f_1, f_2) = \log(2) - D_{\text{JS}}(f_1, f_2), \tag{132}$$

where $D_{\text{JS}}$ is the Jensen-Shannon divergence [Eq. (120)]. The corresponding meta estimator is called 'JS_DJS' in ITE.

Let us take a simple estimation example:

**Example 18 (Kernel estimation on distributions (meta: usage))**

```
>Y1 = randn(3,2000); Y2 = randn(3,3000); %generate the data of interest (d=3, T_1=2000, T_2=3000)
>mult = 1;                               %multiplicative constant is important
>co = KJS_DJS_initialization(mult); %initialize the kernel ('K') estimator on distributions ('JS_DJS')
>K = KJS_DJS_estimation(Y1,Y2,co);  %perform kernel estimation on distributions
```

### 3.3 Uniform Syntax of the Estimators

The modularity of the ITE package in terms of (i) the definition and usage of the estimators of base/meta entropy, mutual information, divergence, association measures, cross quantities, kernels on distributions, and (ii) the possibility to simple embed novel estimators can be assured by following the templates:

1. Initialization:

   **Template 1 (Entropy estimator: initialization)**

   ```
   function [co] = H<cost_name>_initialization(mult)
   co.name = <cost_name>;
   co.mult = mult;
   ...
   ```

**Template 2 (Mutual information estimator: initialization)**

```
function [co] = I<cost_name>_initialization(mult)
co.name = <cost_name>
co.mult = mult;
...
```

**Template 3 (Divergence estimator: initialization)**

```
function [co] = D<cost_name>_initialization(mult)
co.name = <cost_name>
co.mult = mult;
...
```

**Template 4 (Association measure estimator: initialization)**

```
function [co] = A<cost_name>_initialization(mult)
co.name = <cost_name>
co.mult = mult;
...
```

**Template 5 (Cross quantity estimator: initialization)**

```
function [co] = C<cost_name>_initialization(mult)
co.name = <cost_name>
co.mult = mult;
...
```

**Template 6 (Estimator of kernel on distributions: initialization)**

```
function [co] = K<cost_name>_initialization(mult)
co.name = <cost_name>
co.mult = mult;
...
```

2. Estimation:

**Template 7 (Entropy estimator: estimation)**

```
function [H] = H<cost_name>_estimation(Y,co)
...
```

**Template 8 (Mutual information estimator: estimation)**

```
function [I] = I<cost_name>_estimation(Y,ds,co)
...
```

**Template 9 (Divergence estimator: estimation)**

```
function [D] = D<cost_name>_estimation(Y1,Y2,co)
...
```

**Template 10 (Association measure estimator: estimation)**

```
function [A] = A<cost_name>_estimation(Y,ds,co)
...
```

**Template 11 (Cross quantity estimator: estimation)**

```
function [C] = C<cost_name>_estimation(Y1,Y2,co)
...
```

**Template 12 (Estimator of kernel on distributions: estimation)**

```
function [K] = K<cost_name>_estimation(Y1,Y2,co)
...
```

The unified implementation in the ITE toolbox, makes it possible to use high-level initialization and estimation of the information theoretical quantities. The corresponding functions are

- for initialization: `H_initialization.m`, `I_initialization.m`, `D_initialization.m`, `A_initialization.m`, `C_initialization.m`, `K_initialization.m`,
- for estimation: `H_estimation.m`, `I_estimation.m`, `D_estimation.m`, `A_estimation.m`, `C_estimation.m`, `K_estimation.m`

following the templates:

```
function [co] = H_initialization(cost_name,mult)
function [co] = I_initialization(cost_name,mult)
function [co] = D_initialization(cost_name,mult)
function [co] = A_initialization(cost_name,mult)
function [co] = C_initialization(cost_name,mult)
function [co] = K_initialization(cost_name,mult)

function [H] = H_estimation(Y,co)
function [I] = I_estimation(Y,ds,co)
function [D] = D_estimation(Y1,Y2,co)
function [A] = A_estimation(Y,ds,co)
function [C] = C_estimation(Y1,Y2,co)
function [K] = K_estimation(Y1,Y2,co)
```

Here, the `cost_name` of the entropy, mutual information, divergence, association measure and cross quantity estimator can be freely chosen in case of

- entropy: from the last column of Table 2 and Table 8,
- mutual information: from the last column of Table 3 and Table 9,
- divergence: from the last column of Table 4 and Table 10,
- association measures: from the last column of Table 5,
- cross quantities: from the last column of Table 6.
- kernels on distributions: from the last column of Table 7.

By the ITE construction, following for

- entropy: Template 1 (initialization) and Template 7 (estimation),

- mutual information: Template 2 (initialization) and Template 8 (estimation),
- divergence: Template 3 (initialization) and Template 9 (estimation),
- association measure: Template 4 (initialization) and Template 10 (estimation),
- cross quantity: Template 5 (initialization) and Template 11 (estimation),
- kernel on distributions: Template 6 (initialization) and Template 12 (estimation),

user-defined estimators can be immediately used. Let us demonstrate idea of the high-level initialization and estimation with a simple example, Example 2 can equivalently be written as:[17]

**Example 19 (Entropy estimation (high-level, usage))**

```
>Y = rand(5,1000);                        %generate the data of interest (d=5, T=1000)
>cost_name = 'Shannon_kNN_k';             %select the objective (Shannon entropy) and
                                          %its estimation method (k-nearest neighbor)
>mult = 1;                                %multiplicative constant is important
>co = H_initialization(cost_name,mult); %initialize the entropy estimator
>H = H_estimation(Y,co);                 %perform entropy estimation
```

A more complex example family will be presented in Section 4. There, the basic idea will be the following:

1. Independent subspace analysis and its extensions can be formulated as the optimization of information theoretical quantities. There exist many equivalent formulations (objective functions) in the literature, as well as approximate objectives.
2. Choosing a given objective function, estimators following the template syntaxes (Template 1-9) can be used simply by giving their names (`cost_name`).
3. Moreover, the selected estimator can be immediately used in different optimization algorithms of the objective.

# 4 ITE Application in Independent Process Analysis (IPA)

In this section we present an application of the presented estimators in independent subspace analysis (ISA) and its extensions (IPA, independent process analysis). Application of ITE in IPA serves as an illustrative example, how complex tasks formulated as information theoretical optimization problems can be tackled by the estimators detailed in Section 3.

Section 4.1 formulates the problem domain, the independent process analysis (IPA) problem family. In Section 4.2 the solution methods of IPA are detailed. Section 4.3 is about the Amari-index, which can be used to measure the precision of the IPA estimations. The IPA datasets included in the ITE package are introduced in Section 4.4.

## 4.1 IPA Models

In Section 4.1.1 we focus on the simplest linear model, which allows hidden, independent multidimensional sources (subspaces), the so-called independent subspace analysis (ISA) problem. Section 4.1.2 is about the extensions of ISA.

### 4.1.1 Independent Subspace Analysis (ISA)

The ISA problem is defined in the first paragraph. Then (i) the ISA ambiguities, (ii) equivalent ISA objective functions, and (iii) the ISA separation principle are detailed. Thanks to the ISA separation principle one can define many different equivalent *clustering* based ISA objectives and approximations; this is the topic of the next paragraph. ISA optimization methods are presented in the last paragraph.

[17] One can perform mutual information, divergence, association measure and cross quantity estimations similarly.

**The ISA equations** One may think of independent subspace analysis (ISA)[18] [13, 24] as a cocktail party problem, where (i) more than one group of musicians (sources) are playing at the party, and (ii) we have microphones (sensors), which measure the mixed signals emitted by the sources. The task is to estimate the original sources from the mixed recordings (observations) only.

Formally, let us assume that we have an observation ($\mathbf{x} \in \mathbb{R}^{D_x}$), which is instantaneous linear mixture ($\mathbf{A}$) of the hidden source ($\mathbf{e}$), that is,

$$\mathbf{x}_t = \mathbf{A}\mathbf{e}_t, \tag{133}$$

where

1. the unknown mixing matrix $\mathbf{A} \in \mathbb{R}^{D_x \times D_e}$ has full column rank,
2. source $\mathbf{e}_t = \left[\mathbf{e}_t^1; \ldots; \mathbf{e}_t^M\right] \in \mathbb{R}^{D_e}$ is a vector concatenated (using Matlab notation ';') of components $\mathbf{e}_t^m \in \mathbb{R}^{d_m}$ ($D_e = \sum_{m=1}^{M} d_m$), subject to the following conditions:
   (a) $\mathbf{e}_t$ is assumed to be i.i.d. (independent identically distributed) in time $t$,
   (b) there is at most one Gaussian variable among $\mathbf{e}^m$s; this assumption will be referred to as the 'non-Gaussian' assumption, and
   (c) $\mathbf{e}^m$s are independent, that is $I\left(\mathbf{e}^1, \ldots, \mathbf{e}^M\right) = 0$.

The goal of the ISA problem is to eliminate the effect of the mixing ($\mathbf{A}$) with a suitable $\mathbf{W} \in \mathbb{R}^{D_e \times D_x}$ *demixing matrix* and estimate the original source components $\mathbf{e}^m$s by using observations $\{\mathbf{x}_t\}_{t=1}^T$ only ($\hat{\mathbf{e}} = \mathbf{W}\mathbf{x}$). If all the $\mathbf{e}^m$ source components are one-dimensional ($d_m = 1, \forall m$), then the independent component analyis (ICA) task [54, 15, 17] is recovered. For $D_x > D_e$ the problem is called *undercomplete*, while the case of $D_x = D_e$ is regarded as *complete*.

**The ISA objective function** One may assume without loss of generality in case of $D_x \geq D_e$ for the full column rank matrix $\mathbf{A}$ that it is invertible – by applying principal component analysis (PCA) [44]. The estimation of the demixing matrix $\mathbf{W} = \mathbf{A}^{-1}$ in ISA is equivalent to the minimization of the mutual information between the estimated components ($\mathbf{y}^m$),

$$J_{\mathrm{I}}(\mathbf{W}) = I\left(\mathbf{y}^1, \ldots, \mathbf{y}^M\right) \rightarrow \min_{\mathbf{W} \in GL(D)}, \tag{134}$$

where $\mathbf{y} = \mathbf{W}\mathbf{x}$, $\mathbf{y} = \left[\mathbf{y}^1; \ldots; \mathbf{y}^M\right]$, $\mathbf{y}^m \in \mathbb{R}^{d_m}$, $GL(D)$ denotes the set of $D \times D$ sized invertible matrices, and $D = D_e$. The joint mutual information [Eq. (134)] can also be expressed from only *pair-wise* mutual information by recursive methods [21]

$$I\left(\mathbf{y}^1, \ldots, \mathbf{y}^M\right) = \sum_{m=1}^{M-1} I\left(\mathbf{y}^m, \left[\mathbf{y}^{m+1}, ..., \mathbf{y}^M\right]\right). \tag{135}$$

Thus, an equivalent information theoretical ISA objective to (134) is

$$J_{\mathrm{Irecursive}}(\mathbf{W}) = \sum_{m=1}^{M-1} I\left(\mathbf{y}^m, \left[\mathbf{y}^{m+1}, ..., \mathbf{y}^M\right]\right) \rightarrow \min_{\mathbf{W} \in GL(D)}. \tag{136}$$

However, since in ISA, it can be assumed without any loss of generality—applying zero mean normalization and PCA—that

- $\mathbf{x}$ and $\mathbf{e}$ are *white*, i.e., their expectation value is zero, and their covariance matrix is the identity matrix ($\mathbf{I}$),
- mixing matrix $\mathbf{A}$ is orthogonal ($\mathbf{A} \in \mathcal{O}^D$), that is $\mathbf{A}^T\mathbf{A} = \mathbf{I}$, and
- the task is complete ($D = D_x = D_e$),

[18] ISA is also called multidimensional ICA, independent feature subspace analysis, subspace ICA, or group ICA in the literature. We will use the ISA abbreviation.

one can restrict the optimization in (134) and (136) to the orthogonal group ($\mathbf{W} \in \mathcal{O}^D$). Under the whiteness assumption, well-known identities of mutual information and entropy expressions [21] show that the ISA problem is equivalent to

$$J_{\text{sumH}}(\mathbf{W}) = \sum_{m=1}^{M} H\left(\mathbf{y}^m\right) \to \min_{\mathbf{W}\in\mathcal{O}^D}, \tag{137}$$

$$J_{H,I}(\mathbf{W}) = \sum_{m=1}^{M}\sum_{i=1}^{d_m} H(y_i^m) - \sum_{m=1}^{M} I\left(y_1^m, \ldots, y_{d_m}^m\right) \to \min_{\mathbf{W}\in\mathcal{O}^D}, \tag{138}$$

$$J_{I,I}(\mathbf{W}) = I\left(y_1^1, \ldots, y_{d_M}^M\right) - \sum_{m=1}^{M} I\left(y_1^m, \ldots, y_{d_m}^m\right) \to \min_{\mathbf{W}\in\mathcal{O}^D}, \tag{139}$$

where $\mathbf{y}^m = \left[y_1^m; \ldots; y_{d_m}^m\right]$.

**The ISA ambiguities** Identification of the ISA model is ambiguous. However, the ambiguities of the model are simple: hidden components can be determined up to permutation of the subspaces and up to invertible linear transformations[19] within the subspaces [142].

**The ISA separation principle** One of the most exciting and fundamental hypotheses of the ICA research is the ISA separation principle dating back to 1998 [13]: the ISA task can be solved by ICA preprocessing and then clustering of the ICA elements into statistically independent groups. While the extent of this conjecture, is still an open issue, it has recently been rigorously proven for some distribution types [129]. This principle

- forms the basis of the state-of-the-art ISA algorithms,
- can be used to design algorithms that scale well and efficiently estimate the dimensions of the hidden sources, and
- can be extended to different linear-, controlled-, post nonlinear-, complex valued-, partially observed models, as well as to systems with nonparametric source dynamics.

For a recent review on the topic, see [132]. The addressed extension directions are (i) presented in Section 4.1.2, (ii) are covered by the ITE package. In the ITE package the solution of the ISA problem is based on the ISA separation principle, for a demonstration, see `demo_ISA.m`.

**Equivalent clustering based ISA objectives and approximations** According to the ISA separation principle, the solution of the ISA task, i.e., the *global* optimum of the ISA cost function can be found by permuting/clustering the ICA elements into statistically independent groups. Using the concept of demixing matrices, it is sufficient to explore forms

$$\mathbf{W}_{\text{ISA}} = \mathbf{P}\mathbf{W}_{\text{ICA}}, \tag{140}$$

where (i) $\mathbf{P} \in \mathbb{R}^{D\times D}$ is a permutation matrix ($\mathbf{P} \in \mathcal{P}^D$) to be determined, (ii) $\mathbf{W}_{\text{ICA}}$ and $\mathbf{W}_{\text{ISA}}$ is the ICA and ISA demixing matrix, respectively. Thus, assuming that the ISA separation principle holds, and since permuting does not alter the ICA objective [see, e.g., the first term in (138) and (139)], the ISA problem is equivalent to

$$J_{\text{I}}(\mathbf{P}) = I\left(\mathbf{y}^1, \ldots, \mathbf{y}^M\right) \to \min_{\mathbf{P}\in\mathcal{P}^D}, \tag{141}$$

$$J_{\text{Irecursive}}(\mathbf{P}) = \sum_{m=1}^{M-1} I\left(\mathbf{y}^m, \left[\mathbf{y}^{m+1}, ..., \mathbf{y}^M\right]\right) \to \min_{\mathbf{P}\in\mathcal{P}^D}, \tag{142}$$

$$J_{\text{sumH}}(\mathbf{P}) = \sum_{m=1}^{M} H\left(\mathbf{y}^m\right) \to \min_{\mathbf{P}\in\mathcal{P}^D}, \tag{143}$$

$$J_{\text{sum-I}}(\mathbf{P}) = -\sum_{m=1}^{M} I\left(y_1^m, ..., y_{d_m}^M\right) \to \min_{\mathbf{P}\in\mathcal{P}^D}. \tag{144}$$

[19] The condition of invertible linear transformations simplifies to orthogonal transformations for the 'white' case.

Let us note that if our observations are generated by an ISA model then—unlike in the ICA task when $d_m = 1$ $(\forall m)$—pairwise independence is *not* equivalent to mutual independence [17]. However, minimization of the pairwise dependence of the estimated subspaces

$$J_{\text{Ipairwise}}(\mathbf{P}) = \sum_{m_1 \neq m_2} I\left(\mathbf{y}^{m_1}, \mathbf{y}^{m_2}\right) \rightarrow \min_{\mathbf{P} \in \mathcal{P}^D} \tag{145}$$

is an efficient approximation in many situations. An alternative approximation is to consider only the pairwise dependence of the coordinates belonging to different subspaces:

$$J_{\text{Ipairwise1d}}(\mathbf{P}) = \sum_{m_1, m_2 = 1; m_1 \neq m_2}^{M} \sum_{i_1=1}^{d_{m_1}} \sum_{i_2=1}^{d_{m_2}} I\left(y_{i_1}^{m_1}, y_{i_2}^{m_2}\right) \rightarrow \min_{\mathbf{P} \in \mathcal{P}^D}. \tag{146}$$

**ISA optimization methods** Let us fix an ISA objective $J$ [Eq. (141)-(146)]. Our goal is to solve the ISA task, i.e., by the ISA separation principle to find the permutation ($\mathbf{P}$) of the ICA elements minimizing $J$. Below we list a few possibilities for finding $\mathbf{P}$; the methods are covered by ITE.

**Exhaustive way:** The possible number of all permutations, i.e., the number of $\mathbf{P}$ matrices is $D!$, where '!' denotes the factorial function. Considering that the ISA cost function is invariant to the exchange of elements *within* the subspaces (see, e.g., (144)), the number of relevant permutations decreases to $\frac{D!}{\prod_{m=1}^{M} d_m!}$. This number can still be enormous, and the related computations could be formidable justifying searches for efficient approximations that we detail below.

**Greedy way:** Two estimated ICA components belonging to different subspaces are exchanged, if it decreases the value of the ISA cost $J$, as long as such pairs exist [134].

**'Global' way:** Experiences show that greedy permutation search is often sufficient for the estimation of the ISA subspaces. However, if the greedy approach cannot find the true ISA subspaces, then global permutation search method of higher computational burden may become necessary [128]: the cross-entropy solution suggested for the traveling salesman problem [101] can be adapted to this case.

**Spectral clustering:** Now, let us assume that source dimensions ($d_m$) are not known in advance. The lack of such knowledge causes combinatorial difficulty in such a sense that one should try all possible

$$D = d_1 + \ldots + d_M \quad (d_m > 0, M \leq D) \tag{147}$$

dimension allocations to the subspace ($\mathbf{e}^m$) dimensions, where $D$ is the dimension of the hidden source $\mathbf{e}$. The number of these $f(D)$ possibilities grows quickly with the argument, its asymptotic behaviour is known [39, 146]:

$$f(D) \sim \frac{e^{\pi\sqrt{2D/3}}}{4D\sqrt{3}} \tag{148}$$

as $D \rightarrow \infty$. An efficient method with good scaling properties has been put forth in [90] for searching the permutation group for the ISA separation theorem (see Table 13). This approach builds upon the fact that the mutual information between different ISA subspaces $\mathbf{e}^m$ is zero due to the assumption of independence. The method assumes that coordinates of $\mathbf{e}^m$ that fall into the same subspace can be paired by using the *pairwise dependence of the coordinates*. The approach can be considered as objective (146) with unknown $d_m$ subspace dimensions. One may carry out the clustering by applying spectral approaches (included in ITE), which are (i) robust and (ii) scale excellently, a single general desktop computer can handle about a million observations (in our case estimated ICA elements) within several minutes [154].

### 4.1.2 Extensions of ISA

Below we list some extensions of the ISA model and the ISA separation principle. These different extensions, however, can be used in combinations, too. In all these models, (i) the dimension of the source components ($d_m$) can be different and (ii) one can apply the Amari-index as the performance measure (Section 4.3). The ITE package directly implements the estimation of the following models[20] (the relations of the different models are summarized in Fig.1):

[20] The ITE package includes demonstrations for all the touched directions. The name of the demo files are specified at the end the problem definitions, see paragraphs 'Separation principle'.

| |
|---|
| Construct an undirected graph with nodes corresponding to ICA coordinates and edge weights (similarities) defined by the *pairwise* statistical dependencies, i.e., the mutual information of the estimated ICA elements: $\mathbf{S} = [\hat{I}(\hat{e}_{\mathrm{ICA},i}, \hat{e}_{\mathrm{ICA},j})]_{i,j=1}^{D}$. Cluster the ICA elements, i.e., the nodes using similarity matrix $\mathbf{S}$. |

Table 13: Well-scaling approximation for the permutation search problem in the ISA separation theorem in case of unknown subspace dimensions [`estimate_clustering_UD1_S.m`].

**Linear systems:**

**AR-IPA:**

**Equations, assumptions:** In the AR-IPA (autoregressive-IPA) task [47] ($d_m = 1$, $\forall m$), [91] ($d_m \geq 1$), the traditional *i.i.d.* assumption for the sources is generalized to AR time series: the hidden sources ($\mathbf{s}^m \in \mathbb{R}^{d_m}$) are not necessarily independent in time, only their driving noises ($\mathbf{e}^m \in \mathbb{R}^{d_m}$) are. The observation ($\mathbf{x} \in \mathbb{R}^D$, $D = \sum_{m=1}^{M} d_m$) is an instantaneous linear mixture ($\mathbf{A}$) of the source $\mathbf{s}$:

$$\mathbf{x}_t = \mathbf{A}\mathbf{s}_t, \qquad \mathbf{s}_t = \sum_{i=1}^{L_s} \mathbf{F}_i \mathbf{s}_{t-i} + \mathbf{e}_t, \tag{149}$$

where $L_s$ is the order of the AR process, $\mathbf{s}_t = \left[\mathbf{s}_t^1; \ldots; \mathbf{s}_t^M\right]$ and $\mathbf{e}_t = \left[\mathbf{e}_t^1; \ldots; \mathbf{e}_t^M\right] \in \mathbb{R}^D$ denote the hidden sources and the hidden driving noises, respectively. (149) can be rewritten in the following concise form:

$$\mathbf{x} = \mathbf{A}\mathbf{s}, \qquad \mathbf{F}[z]\mathbf{s} = \mathbf{e} \tag{150}$$

using the polynomial of the time-shift operator $\mathbf{F}[z] := \mathbf{I} - \sum_{i=1}^{L_s} \mathbf{F}_i z^i \in \mathbb{R}[z]^{D \times D}$ [62]. We assume that

1. polynomial matrix $\mathbf{F}[z]$ is *stable*, that is $\det(\mathbf{F}[z]) \neq 0$, for all $z \in \mathbb{C}, |z| \leq 1$,
2. mixing matrix $\mathbf{A} \in \mathbb{R}^{D \times D}$ is invertible ($\mathbf{A} \in GL(D)$), and
3. $\mathbf{e}$ satisfies the ISA assumptions (see Section 4.1.1)

**Goal:** The aim of the AR-IPA task is to estimate hidden sources $\mathbf{s}^m$, dynamics $\mathbf{F}[z]$, driving noises $\mathbf{e}^m$ and mixing matrix $\mathbf{A}$ or its $\mathbf{W}$ inverse given observations $\{\mathbf{x}_t\}_{t=1}^{T}$. For the special case of $L_s = 0$, the ISA task is obtained.

**Separation principle:** The AR-IPA estimation can be carried out by (i) applying AR fit to observation $\mathbf{x}$, (ii) followed by ISA on the estimated innovation of $\mathbf{x}$ [47, 91]. Demo: `demo_AR_IPA.m`.

**MA-IPA:**

**Equations, assumptions:** Here, the assumption on *instantaneous* linear mixture of the ISA model is weakened to convolutions. This problem is called moving average independent process analysis (MA-IPA, also known as blind subspace deconvolution) [129]. We describe this task for the undercomplete case. Assume that the convolutive mixture of hidden sources $\mathbf{e}^m \in \mathbb{R}^{d_m}$ is available for observation ($\mathbf{x} \in \mathbb{R}^{D_x}$)

$$\mathbf{x}_t = \sum_{l=0}^{L_e} \mathbf{H}_l \mathbf{e}_{t-l}, \tag{151}$$

where

1. $D_x > D_e$ (undercomplete, $D_e = \sum_{m=1}^{M} d_m$),
2. the polynomial matrix $\mathbf{H}[z] = \sum_{l=0}^{L_e} \mathbf{H}_l z^l \in \mathbb{R}[z]^{D_x \times D_e}$ has a (polynomial matrix) left inverse[21], and
3. source $\mathbf{e} = [\mathbf{e}^1; \ldots; \mathbf{e}^M] \in \mathbb{R}^{D_e}$ satisfies the conditions of ISA.

**Goal:** The goal of this undercomplete MA-IPA problem (uMA-IPA problem, where 'u' stands for undercomplete) is to estimate the original $\mathbf{e}^m$ sources by using observations $\{\mathbf{x}_t\}_{t=1}^{T}$ only. The case $L_e = 0$ corresponds to the ISA task, and in the blind source deconvolution problem [86] $d_m = 1$ ($\forall m$), and $L_e$ is a non-negative integer.

[21] One can show for $D_x > D_e$ that under mild conditions $\mathbf{H}[z]$ has a left inverse with probability 1 [99]; e.g., when the matrix $[\mathbf{H}_0, \ldots, \mathbf{H}_{L_e}]$ is drawn from a continuous distribution.

**Note:** We note that in the ISA task the full column rank of matrix $\mathbf{H}_0$ was presumed, which is equivalent to the assumption that matrix $\mathbf{H}_0$ has left inverse. This left inverse assumption is extended in the uMA-IPA model for the polynomial matrix $\mathbf{H}[z]$.

**Separation principle:**

- By applying temporal concatenation (TCC) on the observation, one can reduce the uMA-IPA estimation problem to ISA [129]. Demo: `demo_uMA_IPA_TCC.m`.
- However, upon applying the TCC technique, the associated ISA problem can easily become 'high dimensional'. This dimensionality problem can be alleviated by the linear prediction approximation (LPA) approach, i.e., AR fit, followed by ISA on the estimation innovation [130]. Demo: `demo_uMA_IPA_LPA.m`.
- In the complete ($D_x = D_e$) case, the $\mathbf{H}[z]$ polynomial matrix does not have (polynomial matrix) left inverse in general. However, provided that the convolution can be represented by an infinite order autoregressive [AR($\infty$)] process, one [121] can construct an efficient estimation method for the hidden components via an asymptotically consistent LPA procedure augmented with ISA. Such AR($\infty$) representation can be guaranteed by assuming the stability of $\mathbf{H}[z]$ [32]. Demo: `demo_MA_IPA_LPA.m`.

**Post nonlinear models:**

**Equations, assumptions:** In the post nonlinear ISA (PNL-ISA) problem [133] the *linear* mixing assumption of the ISA model is alleviated. Assume that the observations ($\mathbf{x} \in \mathbb{R}^D$) are post nonlinear mixtures ($\mathbf{g}(\mathbf{A}\cdot)$) of multidimensional independent sources ($\mathbf{e} \in \mathbb{R}^D$):

$$\mathbf{x}_t = \mathbf{g}(\mathbf{A}\mathbf{e}_t), \tag{152}$$

where the

- unknown function $\mathbf{g} : \mathbb{R}^D \to \mathbb{R}^D$ is a component-wise transformation, i.e, $\mathbf{g}(\mathbf{v}) = [g_1(v_1); \ldots; g_D(v_D)]$ and $\mathbf{g}$ is invertible, and
- mixing matrix $\mathbf{A} \in \mathbb{R}^{D\times D}$ and hidden source $\mathbf{e}$ satisfy the ISA assumptions.

**Goal:** The PNL-ISA problem is to estimate the hidden source components $\mathbf{e}^m$ knowing only the observations $\{\mathbf{x}_t\}_{t=1}^T$. For $d_m = 1$, we get back the PNL-ICA problem [139] (for a review see [55]), whereas '$\mathbf{g}$=identity' leads to the ISA task.

**Separation principle:** the estimation of the PNL-ISA problem can be carried out on the basis of the mirror structure of the task, applying gaussianization followed by linear ISA [133]. Demo: `demo_PNL_ISA.m`.

**Complex models:**

**Equations, assumptions:** One can define the independence, mutual information and entropy of complex random variables via the Hilbert transformation [Eq. (95), (96), (103)]. Having these definitions at hand, the complex ISA problem can be formulated analogously to the real case, the observations ($\mathbf{x}_t \in \mathbb{C}^D$) are generated as the instantaneous linear mixture ($\mathbf{A}$) of the hidden sources ($\mathbf{e}_t$):

$$\mathbf{x}_t = \mathbf{A}\mathbf{e}_t, \tag{153}$$

where

- the unknown $\mathbf{A} \in \mathbb{C}^{D\times D}$ mixing matrix is invertible ($D = \sum_{m=1}^M d_m$),
- $\mathbf{e}_t$ is assumed to be i.i.d. in time $t$, and
- $\mathbf{e}^m \in \mathbb{C}^{d_m}$s are independent, that is $I\left(\varphi_v\left(\mathbf{e}^1\right), \ldots, \varphi_v\left(\mathbf{e}^M\right)\right) = 0$.

**Goal:** The goal is to estimate the hidden source $\mathbf{e}$ and the mixing matrix $\mathbf{A}$ (or its $\mathbf{W} = \mathbf{A}^{-1}$ inverse) using the observation $\{\mathbf{x}_t\}_{t=1}^T$. If all the components are one-dimensional ($d_m = 1$, $\forall m$), one obtains the complex ICA problem.

**Separation principle:**

- Supposing that the $\varphi_v(\mathbf{e}^m) \in \mathbb{R}^{2d_m}$ variables are 'non-Gaussian', and exploiting the operation preserving property of the Hilbert transformation, the solution of the complex ISA problem can be reduced to an ISA task over the real domain with observation $\varphi_v(\mathbf{x})$ and $M$ pieces of $2d_m$-dimensional hidden components $\varphi_v(\mathbf{e}^m)$. The consideration can be extended to *linear models* including AR, MA, ARMA (autoregressive moving average), ARIMA (integrated ARMA), ... terms [124]. Demo: `demo_complex_ISA.m`.

- Another possible solution is to apply the ISA separation theorem, which remains valid even for complex variables [129]: the solution can be accomplished by complex ICA and clustering of the complex ICA elements. Demo: `demo_complex_ISA_C.m`.

**Controlled models:**

**Equations, assumptions:** In the *ARX-IPA* (ARX – autoregressive with exogenous input) problem [123] the AR-IPA assumption holds (Eq. (149)), but the time evolution of the hidden source $\mathbf{s}$ can be influenced via *control* variable $\mathbf{u}_t \in \mathbb{R}^{D_u}$ through matrices $\mathbf{B}_j \in \mathbb{R}^{D\times D_u}$:

$$\mathbf{x}_t = \mathbf{A}\mathbf{s}_t \qquad\qquad \mathbf{s}_t = \sum_{i=1}^{L_s} \mathbf{F}_i \mathbf{s}_{t-i} + \sum_{j=1}^{L_u} \mathbf{B}_j \mathbf{u}_{t+1-j} + \mathbf{e}_t. \tag{154}$$

**Goal:** The goal is to estimate the hidden source $\mathbf{s}$, the driving noise $\mathbf{e}$, the parameters of the dynamics and control matrices ($\{\mathbf{F}_i\}_{i=1}^{L_s}$ and $\{\mathbf{B}_j\}_{j=1}^{L_u}$), as well as the mixing matrix $\mathbf{A}$ or its inverse $\mathbf{W}$ by using observations $\mathbf{x}_t$ and controls $\mathbf{u}_t$. In the special case of $L_u = 0$, the ARX-IPA task reduces to AR-IPA.

**Separation principle:** The solution can be reduced to ARX identification followed by ISA [123]. Demo: `demo_ARX_IPA.m`.

**Partially observed models:**

**Equations, assumptions:** In the *mAR-IPA* (mAR – autoregressive with missing values) problem [122], the AR-IPA assumptions (Eq. (149)) are relaxed by allowing a few coordinates of the mixed AR sources $\mathbf{x}_t \in \mathbb{R}^D$ to be *missing* at certain time instants. Formally, we observe $\mathbf{y}_t \in \mathbb{R}^D$ instead of $\mathbf{x}_t$, where 'mask mappings' $\boldsymbol{\mathcal{M}}_t : \mathbb{R}^D \mapsto \mathbb{R}^D$ represent the coordinates and the time indices of the non-missing observations:

$$\mathbf{y}_t = \boldsymbol{\mathcal{M}}_t(\mathbf{x}_t), \qquad\qquad \mathbf{x}_t = \mathbf{A}\mathbf{s}_t, \qquad\qquad \mathbf{s}_t = \sum_{i=1}^{L_s} \mathbf{F}_i \mathbf{s}_{t-i} + \mathbf{e}_t. \tag{155}$$

**Goal:** Our task is the estimation of the hidden source $\mathbf{s}$, its driving noise $\mathbf{e}$, parameters of the dynamics $\mathbf{F}[z]$, mixing matrix $\mathbf{A}$ (or its inverse $\mathbf{W}$) from observation $\{\mathbf{y}_t\}_{t=1}^T$. The special case of '$\boldsymbol{\mathcal{M}}_t$ = identity' corresponds to the AR-IPA task.

**Separation principle:** One can reduce the solution to mAR identification followed by ISA on the estimated innovation process [122]. Demo: `demo_mAR_IPA.m`.

**Models with nonparametric dynamics:**

**Equations, assumptions:** In the *fAR-IPA* (fAR – functional autoregressive) problem [127], the *parametric* assumption for the dynamics of the hidden sources is circumvented by functional AR sources:

$$\mathbf{x}_t = \mathbf{A}\mathbf{s}_t, \qquad\qquad \mathbf{s}_t = \mathbf{f}(\mathbf{s}_{t-1}, \ldots, \mathbf{s}_{t-L_s}) + \mathbf{e}_t. \tag{156}$$

**Goal:** The goal is to estimate the hidden sources $\mathbf{s}^m \in \mathbb{R}^{d_m}$ including their dynamics $\mathbf{f}$ and their driving innovations $\mathbf{e}^m \in \mathbb{R}^{d_m}$ as well as mixing matrix $\mathbf{A}$ (or its inverse $\mathbf{W}$) given observations $\{\mathbf{x}_t\}_{t=1}^T$. If we knew the parametric form of $\mathbf{f}$ and if it were linear, then the problem would be AR-IPA.

**Separation principle:** The problem can be solved by nonparametric regression followed by ISA [127]. Demo: `demo_fAR_IPA.m`.

## 4.2 Estimation via ITE

Having (i) the information theoretical estimators (Section 3), (ii) the ISA/IPA problems and separation principles (Section 4.1) at hand, we now detail the solution methods offered by the ITE package. Due to the *separation principles* of the IPA problem family, the solution methods can be implemented in a completely *modular* way; the estimation techniques can be built up from the solvers of the obtained *subproblems*. From developer point of view, this flexibility makes it possible to easily modify/extend the ITE toolbox. For example, (i) in case of ISA, one can select/replace the ICA method and clustering technique applied independently, (ii) in case of AR-IPA one has freedom in chosing/extending the AR identificator and the ISA solver, etc. This is the underlying idea of the solvers offered by the ITE toolbox.

In Section 4.2.1 the solution techniques for the ISA task are detailed. Extensions of the ISA problem are in the focus of Section 4.2.2.

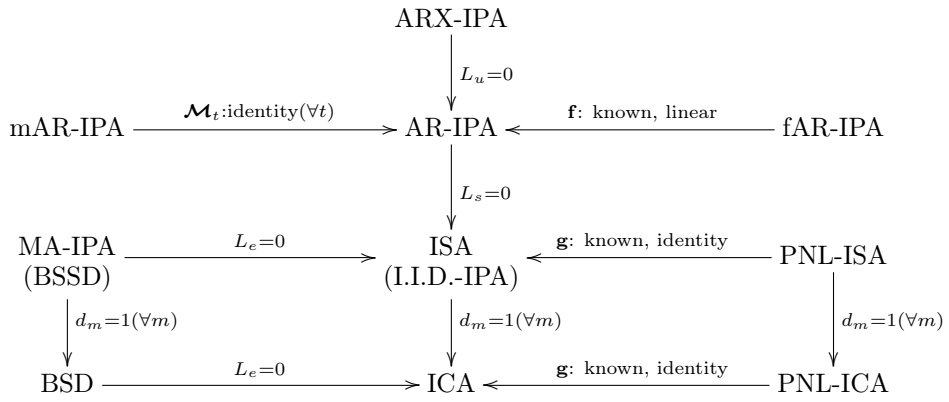



Figure 1: IPA problem family, relations. Arrows point to special cases. For example, 'ISA $\xrightarrow{d_m=1(\forall m)}$ ICA' means that ICA is a special case of ISA, when all the source components are one-dimensional.

#### 4.2.1 ISA

As it has been detailed in Section 4.1.1, the ISA problem can be formulated as the optimization of information theoretical objectives (see Eqs. (141), (142), (143), (144), (145), (146)). In the ITE package,

**All the detailed ISA formulations:**

- are available by the appropriate choice of the variable `ISA.cost_type` (see Table 14), and
- can be used by *any* entropy/mutual information estimator satisfying the ITE template construction (see Table 2, Table 3, Table 8, Table 9 and Section 3.3).

**The dimension of the subspaces can be given/unknown:** the priori knowledge about the dimension of the subspaces can be conveyed by the variable `unknown_dimensions`. `unknown_dimensions=0` (`=1`) means given $\{d_m\}_{m=1}^M$ subspace dimensions (unknown subspace dimensions, it is sufficient to give $M$, the number of subspaces). In case of

- given subspace dimensions: clustering of the ICA elements can be carried out in ITE by the exhaustive (`ISA.opt_type = 'exhaustive'`), greedy (`ISA.opt_type = 'greedy'`), or the cross-entropy (`ISA.opt_type = 'CE'`) method.
- unknown subspace dimensions: clustering of the ICA elements can be performed by applying spectral clustering. In this case, the clustering is based on the pairwise mutual information of the one-dimensional ICA elements (Table 14) and the objective is (146), i.e., `ISA.cost_type = 'Ipairwise1d'`. The ITE package supports 4 different spectral clustering methods/implementations (Table 15):
  - the unnormalized cut method (`ISA.opt_type = 'SP1'`), and two normalized cut techniques (`ISA.opt_type = 'SP2'` or `ISA.opt_type = 'SP3'`) [113, 82, 149] – the implementations are purely Matlab/Octave, and
  - a fast, normalized cut implementation [113, 20] in C++ with compilable mex files (`ISA.opt_type = 'NCut'`).

The ISA estimator capable of handling these options is called `estimate_ISA.m`, and is accompanied by the demo file `demo_ISA.m`. Let us take some examples for the parameters to set in `demo_ISA.m`:

**Example 20 (ISA-1)**

- *Goal: the subspace dimensions $\{d_m\}_{m=1}^M$ are known; apply sum of entropy based ISA formulation (Eq.* (143)*); estimate the entropy via the Rényi entropy using k-nearest neighbors ($S = \{1, \ldots, k\}$); optimize the objective in a greedy way.*
- *Parameters to set:* `unknown_dimensions = 0`; `ISA.cost_type = 'sumH'`; `ISA.cost_name = 'Renyi_kNN_1tok'`, `ISA.opt_type = 'greedy'`.

| Cost function to minimize | Name (`ISA.cost_type`) |
|---|---|
| $I\left(\mathbf{y}^1,\ldots,\mathbf{y}^M\right)$ | `'I'` |
| $\sum_{m=1}^{M} H\left(\mathbf{y}^m\right)$ | `'sumH'` |
| $-\sum_{m=1}^{M} I\left(y_1^m,...,y_{d_m}^M\right)$ | `'sum-I'` |
| $\sum_{m=1}^{M-1} I\left(\mathbf{y}^m,\left[\mathbf{y}^{m+1},...,\mathbf{y}^M\right]\right)$ | `'Irecursive'` |
| $\sum_{m1\neq m2} I\left(\mathbf{y}^{m_1},\mathbf{y}^{m_2}\right)$ | `'Ipairwise'` |
| $\sum_{m_1,m_2=1;m_1\neq m_2}^{M}\sum_{i_1=1}^{d_{m_1}}\sum_{i_2=1}^{d_{m_2}} I\left(y_{i_1}^{m_1},y_{i_2}^{m_2}\right)$ | `'Ipairwise1d'` |

Table 14: ISA formulations. $1-4^{th}$ row: equivalent, $5-6^{th}$ row: necessary conditions.

| Optimization technique (`ISA.opt_type`) | Principle | Environment |
|---|---|---|
| `'NCut'` | normalized cut | Matlab |
| `'SP1'` | unnormalized cut | Matlab, Octave |
| `'SP2'`, `'SP3'` | 2 normalized cut methods | Matlab, Octave |

Table 15: Spectral clustering optimizers for given number of subspaces ($M$) [`unknown_dimensions=1`]: `clustering_UD1.m`: `estimate_clustering_UD1_S.m`.

**Example 21 (ISA-2)**

- *Goal: the subspace dimensions $\{d_m\}_{m=1}^M$ are known; apply an ISA formulation based on the sum of mutual information within the subspaces (Eq. (144)); estimate the mutual information via the KCCA method; optimize the objective in a greedy way.*
- *Parameters to set:* `unknown_dimensions = 0; ISA.cost_type = 'sum-I'; ISA.cost_name = 'KCCA', ISA.opt_type = 'greedy'.`

**Example 22 (ISA-3)**

- *Goal: the subspace dimensions are unknown, only $M$, the number of the subspaces is given; the ISA objective is based on the pairwise mutual information of the estimated ICA elements (Eq. (146)); estimate the mutual information using the KGV method; optimize the objective via the NCut normalized cut method.*
- *Parameters to set:* `unknown_dimensions = 1; ISA.cost_type = 'Ipairwise1d'; ISA.cost_name = 'KGV', ISA.opt_type = 'NCut'.`

In case of given subspace dimensions, the special structure of the ISA objectives can be taken into account to further increase the efficiency of the **optimization**, i.e., the clustering step. The ITE package realizes this idea:

- In case of (i) one-dimensional mutual information based ISA formulation (Eq. (146)), and (ii) cross-entropy or exhaustive optimization the $\mathbf{S} = [I(\hat{e}_{\text{ICA,i}}, \hat{e}_{\text{ICA,j}})]_{i,j=1}^D$ similarity matrix can be precomputed.
- In case of greedy optimization:
  - upon applying ISA objective (146), the $\mathbf{S} = [I(\hat{e}_{\text{ICA,i}}, \hat{e}_{\text{ICA,j}})]_{i,j=1}^D$ similarity matrix can again be precomputed giving rise to more efficient optimization.
  - ISA formulations (143), (144) are both additive w.r.t. the estimated subspaces. Making use of this special structure of these objective, it is sufficient to recompute the objective only on the touched subspaces while greedily testing a new permutation candidate. Provided that the number of the subspaces ($M$) is high, the decreased computational load of the specialized method is emphasized.
  - objective (145) is pair-additive w.r.t. the subspaces. In this case, it is enough to recompute the objective on the subspaces connected the actual subspace estimates. Again the increased efficiency is striking in case of large number of subspaces.

| Cost type (`ISA.cost_type`) | Recommended/chosen optimizer |
|---|---|
| `'I'`, `'Irecursive'` | `clustering_UD0_greedy_general.m` |
| `'sumH'`, `'sum-I'` | `clustering_UD0_greedy_additive_wrt_subspaces.m` |
| `'Ipairwise'` | `clustering_UD0_greedy_pairadditive_wrt_subspaces.m` |
| `'Ipairwise1d'` | `clustering_UD0_greedy_pairadditive_wrt_coordinates.m` |

Table 16: Recommended/chosen optimizers for given subspace dimensions ($\{d_m\}_{m=1}^M$) [`unknown_dimensions=0`] applying greedy [`ISA.opt_type='greedy'`] ISA optimization: `clustering_UD0.m`.

| Cost type (`ISA.cost_type`) | Recommended/chosen optimizer |
|---|---|
| `'I'`, `'sumH'`, `'sum-I'`, `'Irecursive'`, `'Ipairwise'` | `clustering_UD0_CE_general.m` |
| `'Ipairwise1d'` | `clustering_UD0_CE_pairadditive_wrt_coordinates.m` |

Table 17: Recommended/chosen optimizers for given subspace dimensions ($\{d_m\}_{m=1}^M$) [`unknown_dimensions=0`] applying cross-entropy [`ISA.opt_type='CE'`] ISA optimization: `clustering_UD0.m`.

The general and the recommended (which are chosen by default in the toolbox) ISA optimization methods of ITE are listed Table 16 (greedy), Table 17 (cross-entropy), Table 18 (exhaustive).

**Extending the capabilities of the ITE toolbox**: In case of

- known subspaces dimensions ($\{d_m\}_{m=1}^M$): the clustering is carried out in `clustering_UD0.m`. Before clustering, first the importance of the constant multipliers must be set in `set_mult.m`.[22]
  - To add a new ISA formulation (`ISA.cost_type`):
    - to be able to carry it out general optimization: it is sufficient to add the new `cost_type` entry to `clustering_UD0.m`, and the computation of the new objective to `cost_general.m`.
    - to be able to perform an existing, specialized (not general) optimization: add the new `cost_type` entry to `clustering_UD0.m`, and the computation of the new objective to the corresponding cost procedure. For example, in case of a new objective being additive w.r.t. subspaces (similarly to (143), (144)) it is sufficient to modify `cost_additive_wrt_subspaces_one_subspace.m` in `cost_additive_wrt_subspaces.m`.
    - to be able to perform a non-existing optimization: add the new `cost_type` entry to `clustering_UD0.m` with the specialized solver.
  - To add a new optimization method (`ISA.opt_type`): please follow the 3 examples included in `clustering_UD0.m`.
- unknown subspace dimensions ($M$): `clustering_UD1.m` is responsible for the clustering step. It first computes the $\mathbf{S} = [\hat{I}(\hat{e}_{\mathrm{ICA},i}, \hat{e}_{\mathrm{ICA},j})]_{i,j=1}^D$ similarity matrix, and then performs spectral clustering (see Table 13). To include a new clustering technique, one only has to add it to a new case entry in `estimate_clustering_UD1_S.m`.

[22] For example, upon applying objective (143) multiplicative constants are irrelevant (important) in case of equal (different) $d_m$ subspace dimensions.

| Cost type (`ISA.cost_type`) | Recommended/chosen optimizer |
|---|---|
| `'I'`, `'sumH'`, `'sum-I'`, `'Irecursive'`, `'Ipairwise'` | `clustering_UD0_exhaustive_general.m` |
| `'Ipairwise1d'` | `clustering_UD0_exhaustive_pairadditive_wrt_coordinates.m` |

Table 18: Recommended/chosen optimizers for given subspace dimensions ($\{d_m\}_{m=1}^M$) [`unknown_dimensions=0`] applying exhaustive [`ISA.opt_type='exhaustive'`] ISA optimization: `clustering_UD0.m`.

#### 4.2.2 Extensions of ISA

Due to the IPA separation principles, the solution of the problem family can be carried out in a *modular* way. The solution of all the presented IPA directions are demonstrated through examples in ITE, the demo files and the actual estimators are listed in Table 19. For the obtained subtasks the ITE package provides many efficient estimators (see Table 20):

**ICA, complex ICA:**

- The fastICA method [48] and its complex variant [9] is one of the most popular ICA approach, it is available in ITE.
- The EASI (equivariant adaptive separation via independence) [14] ICA method family realizes a very exciting online, adaptive approach offering uniform performance w.r.t. the mixing matrix. It is capable of handling the real and the complex case, too.
- As we have seen the search for the demixing matrix in ISA (specially in ICA) can be restricted to the orthogonal group ($\mathbf{W} \in \mathcal{O}^D$, see Section 4.1.1). Moreover, ortogonal matrices can be written as a product of elementary Jacobi/Givens rotation matrices. The method carries out the search for $\mathbf{W}$ in the ICA problem by the sequential optimization of such elementary rotations on a gradually fined scale. ITE supports Jacobi/Givens based ICA optimization using general entropy and mutual information estimators (`ICA.cost_type = 'sumH'` or `'I'`) for the real case; the pseudo-code of the method is given in Alg. 1.[23] Let us take an example:

  **Example 23 (ISA-4)**
  - *Goal:*
    - *Task: ISA with known subspace dimensions* $\{d_m\}_{m=1}^M$.
    - *ICA subtask: minimize the mutual information of the estimated coordinate pairs using the KCCA objective; optimize the ICA cost via the Jacobi method,*
    - *ISA subtask (clustering of the ICA elements): apply entopy sum based ISA formulation (Eq.* (143)*) and estimate the entropy via the Rényi entropy using k-nearest neighbors* ($S = \{1, \ldots, k\}$*); optimize the ISA objective in a greedy way.*
  - *Parameters to set (see* `demo_ISA.m`*):* `unknown_dimensions = 0`; `ICA.cost_type = 'I'`; `ICA.cost_name = 'KCCA'`; `ICA.opt_type = 'Jacobi1'`; `ISA.cost_type = 'sumH'`; `ISA.cost_name = 'Renyi_kNN_1tok'`; `ISA.opt_type = 'greedy'`.

- An alternative Jacobi optimization method with a different fining scheme in the rotation angle search is also available in ITE, see Alg. 2. The optimization extends the idea of the RADICAL ICA method [63] to general entropy, mutual information objectives. The RADICAL approach can be obtained in ITE by setting `ICA.cost_type = 'sumH'`; `ICA.cost_name = 'Shannon_spacing_V'`; `ICA.opt_type = 'Jacobi2'` (see `demo_ISA.m`).

See `estimate_ICA.m` and `estimate_complex_ICA.m`.

**AR identification:** Identification of AR processes can be carried in the ITE toolbox in 5 different ways (see `estimate_AR.m`):

- using the online Bayesian technique with normal-inverted Wishart prior [56, 89],
- applying [51]
  - nonlinear least squares estimator based on the subspace representation of the system,
  - exact maximum likelihood optimization using the BFGS (Broyden-Fletcher-Goldfarb-Shannon; or the Newton-Raphson) technique,
  - the combination of the previous two approaches.
- making use of the stepwise least squares technique [81, 107].

**ARX identification:** Identification of ARX processes can be carried out by the D-optimal technique of [89] assuming normal-inverted Wishart prior; see `estimate_ARX_IPA.m`.

**mAR identification:** The

[23] The optimization extends the idea of the SWICA package [58].

| IPA model | Reduction | | Demo (Estimator) |
|---|---|---|---|
| | Task1 | Task2 | |
| ISA | ICA | clustering of the ICA elements | `demo_ISA.m` (`estimate_ISA.m`) |
| AR-IPA | AR fit | ISA | `demo_AR_IPA.m` (`estimate_AR_IPA.m`) |
| ARX-IPA | ARX fit | ISA | `demo_ARX_IPA.m` (`estimate_ARX_IPA.m`) |
| mAR-IPA | mAR fit | ISA | `demo_mAR_IPA.m` (`estimate_mAR_IPA.m`) |
| complex ISA | Hilbert transformation | real ISA | `demo_complex_ISA.m` (`estimate_complex_ISA.m`) |
| complex ISA | complex ICA | clustering of the ICA elements | `demo_complex_ISA_C.m` (`estimate_complex_ISA_C.m`) |
| fAR-IPA | nonparametric regression | ISA | `demo_fAR_IPA.m` (`estimate_fAR_IPA.m`) |
| (complete) MA-IPA | linear prediction (LPA) | ISA | `demo_MA_IPA_LPA.m` (`estimate_MA_IPA_LPA.m`) |
| undercomplete MA-IPA | temporal concatenation (TCC) | ISA | `demo_uMA_IPA_TCC.m` (`estimate_uMA_IPA_TCC.m`) |
| undercomplete MA-IPA | linear prediction (LPA) | ISA | `demo_uMA_IPA_LPA.m` (`estimate_uMA_IPA_LPA.m`) |
| PNL-ISA | gaussianization | ISA | `demo_PNL_ISA.m` (`estimate_PNL_ISA.m`) |

Table 19: IPA separation principles.

- online Bayesian technique with normal-inverted Wishart prior [56, 89],
- nonlinear least squares [51],
- exact maximum likelihood [51], and
- their combination [51]

are available for the identification of mAR processes; see `estimate_mAR.m`.

**fAR identification:** Identification of fAR processes in ITE can be carried out by the strongly consistent, recursive Nadaraya-Watson estimator [42]; see `estimate_fAR.m`.

**spectral clustering:** The ITE toolbox provides 4 methods to perform spectral clustering (see `estimate_clustering_UD1_S.m`):

- the unnormalized cut method, and two normalized cut techniques [113, 82, 149] – the implemetations are purely Matlab/Octave, and
- a fast, normalized cut implementation [113, 20] in C++ with compilable mex files.

**gaussianization:** Gaussianization of the observations can be carried out by the efficient rank method [156], see `estimate_gaussianization.m`.

**Extending the capabilities of the ITE toolbox**: additional methods for the obtained subtasks can be easily embedded and instantly used in IPA, by simply adding a new 'switch: case' entry to the subtask solvers listed in Table 20.

Beyond the solvers for the IPA subproblems detailed above, the ITE toolbox offers:

- 4 different alternatives for *k-nearest neighbor* estimation (Table 21):
  - exact nearest neighbors: based on fast computation of pairwise distances and C++ partial sort (knn package).
  - exact nearest neighbors: based on fast computation of pairwise distances.
  - exact nearest neighbors: carried out by the `knnsearch` function of the Statistics Toolbox in Matlab.

**Algorithm 1** Jacobi optimization - 1; see `estimate_ICA_Jacobi1.m`.

**Input:**
  whitened observation $\mathbf{X} = [\mathbf{x}_1, \dots, \mathbf{x}_T] \in \mathbb{R}^{d \times T}$,
  ICA cost function on coordinate pairs $J(z_1, z_2) = I(z_1, z_2)$ or $J(z_1, z_2) = H(z_1) + H(z_2)$,
  number of levels $L(= 3 : \text{default value})$, number of sweeps $S(= d)$, number of angles $A(= 90)$.
**Notation:**
  $\mathbf{R}(\theta) = \begin{bmatrix} \cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{bmatrix}$. // rotation with angle $\theta$
**Initialization:**
  estimated demixing matrix $\hat{\mathbf{W}} = \mathbf{I} \in \mathbb{R}^{d \times d}$, estimated source $\hat{\mathbf{E}} = \mathbf{X} \in \mathbb{R}^{d \times T}$.
**for** $l = 1$ to $L$ **do**
  $a = \left\lceil \frac{A}{2^{L-l}} \right\rceil$. // number of angles at the actual level
  **for** $s = 1$ to $S$ **do**
    **for all** $(i_1, i_2) \in \{(i, j) : 1 \le i < j \le d\}$ **do**
      $\theta^* = \arg\min_{\theta \in \left\{ \frac{k}{a} \frac{\pi}{2} : k = 0, \dots, a-1 \right\}} J\left(\mathbf{R}(\theta)\mathbf{e}([i_1, i_2], :)\right)$. // best rotation angle for the $(i_1, i_2)^{th}$ coordinate pair
      Apply the optimal rotation found ($\theta^*$):
        $\hat{\mathbf{W}}([i_1, i_2], :) = \mathbf{R}(\theta^*)\, \hat{\mathbf{W}}([i_1, i_2], :)$,
        $\hat{\mathbf{E}}([i_1, i_2], :) = \mathbf{R}(\theta^*)\, \hat{\mathbf{E}}([i_1, i_2], :)$.
**Output:** $\hat{\mathbf{W}}$, $\hat{\mathbf{E}}$.

**Algorithm 2** Jacobi optimization - 2; see `estimate_ICA_Jacobi2.m`.

**Input:**
  whitened observation $\mathbf{X} = [\mathbf{x}_1, \dots, \mathbf{x}_T] \in \mathbb{R}^{d \times T}$,
  ICA cost function on coordinate pairs $J(z_1, z_2) = I(z_1, z_2)$ or $J(z_1, z_2) = H(z_1) + H(z_2)$,
  number of sweeps $S(= d - 1 : \text{default})$, number of angles $A(= 150)$.
**Notation:**
  $\mathbf{R}(\theta) = \begin{bmatrix} \cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{bmatrix}$. // rotation with angle $\theta$
**Initialization:**
  estimated demixing matrix $\hat{\mathbf{W}} = \mathbf{I} \in \mathbb{R}^{d \times d}$, estimated source $\hat{\mathbf{E}} = \mathbf{X} \in \mathbb{R}^{d \times T}$,
  minimum number of angles $a_{min} = \frac{A}{1.3^{\left\lceil \frac{S}{2} \right\rceil}}$.
**for** $s = 1$ to $S$ **do**
  **if** $s > \frac{S}{2}$ **then**
    $a = \left\lfloor a_{min} 1.3^{\left\lceil s - \frac{S}{2} \right\rceil} \right\rfloor$. // number of angles at the actual sweep
  **else**
    $a = \max\left(30, \lfloor a_{min} \rfloor\right)$. // number of angles at the actual sweep
  **for all** $(i_1, i_2) \in \{(i, j) : 1 \le i < j \le d\}$ **do**
    $\theta^* = \arg\min_{\theta \in \left\{ \frac{k}{a} \frac{\pi}{2} : k = 0, \dots, a-1 \right\}} J\left(\mathbf{R}(\theta)\mathbf{e}([i_1, i_2], :)\right)$. // best rotation angle for the $(i_1, i_2)^{th}$ coordinate pair
    Apply the optimal rotation found ($\theta^*$):
      $\hat{\mathbf{W}}([i_1, i_2], :) = \mathbf{R}(\theta^*)\, \hat{\mathbf{W}}([i_1, i_2], :)$,
      $\hat{\mathbf{E}}([i_1, i_2], :) = \mathbf{R}(\theta^*)\, \hat{\mathbf{E}}([i_1, i_2], :)$.
**Output:** $\hat{\mathbf{W}}$, $\hat{\mathbf{E}}$.

| Subtask | Estimator | Method |
|---|---|---|
| ICA | `estimate_ICA.m` | `'fastICA'`, `'EASI'`, `'Jacobi1'`, `'Jacobi2'` |
| complex ICA | `estimate_complex_ICA.m` | `'fastICA'`, `'EASI'` |
| AR fit (LPA) | `estimate_AR.m` | `'NIW'`, `'subspace'`, `'subspace-LL'`, `'LL'`, `'stepwiseLS'` |
| ARX fit | `estimate_ARX.m` | `'NIW'` |
| mAR fit | `estimate_mAR.m` | `'NIW'`, `'subspace'`, `'subspace-LL'`, `'LL'` |
| fAR fit | `estimate_fAR.m` | `'recursiveNW'` |
| spectral clustering | `estimate_clustering_UD1_S.m` | `'NCut'`, `'SP1'`, `'SP2'`, `'SP3'` |
| gaussianization | `estimate_gaussianization.m` | `'rank'` |

Table 20: IPA subtasks and estimators.

| `co.kNNmethod` | Principle | Environment |
|---|---|---|
| `'knnFP1'` | exact NNs, fast pairwise distance computation and C++ partial sort | Matlab, Octave |
| `'knnFP2'` | exact NNs, fast pairwise distance computation | Matlab, Octave |
| `'knnsearch'` | exact NNs, Statistics Toolbox $\in$ Matlab | Matlab |
| `'ANN'` | approximate NNs, ANN library | Matlab, Octave[a] |

Table 21: k-nearest neighbor (kNN) methods. The main kNN function is `kNN_squared_distances.m`.

[a] See Table 1.

  - approximate nearest neighbors: implemented by the ANN library.

  The method applied for the estimation can be chosen by setting `co.method` to `'knnFP1'`, `'knnFP2'`, `'knnsearch'`, or `'ANN'`. For examples, please see:

  - `HRenyi_GSF_initialization.m`, `HShannon_kNN_k_initialization.m`, `HRenyi_kNN_1tok_initialization.m`, `HRenyi_kNN_k_initialization.m`, `HRenyi_kNN_S_initialization.m`, `HRenyi_weightedkNN_initialization.m`, `HTsallis_kNN_k_initialization.m`,
  - `DL2_kNN_k_initialization.m`, `DRenyi_kNN_k_initialization.m`, `DTsallis_kNN_k_initialization.m`, `DKL_kNN_kiTi_initialization.m`, `DHellinger_kNN_k_initialization.m`, `DKL_kNN_k_initialization.m`, `DBhattacharyya_kNN_k_initialization.m`, `DBregman_kNN_k_initialization.m`,
  - `CCE_kNN_k_initialization.m`.

  The central function of kNN computations is `kNN_squared_distances.m`.

- 4 techniques for *minimum spanning tree* computation (Table 22):

  - the two functions of the MatlabBGL library can be envoked by setting `co.STmethod` to `'MatlabBGL_Prim'` or `'MatlabBGL_Kruskal'`.
  - the purely Matlab/Octave implementations based on the pmtk3 toolbox can be called by setting `co.STmethod` to `'pmtk3_Prim'` or `'pmtk3_Kruskal'`.

  For an example, please see `H_Renyi_MST_initialization.m`. The central function for MST computation is `compute_MST.m`.

To **extend** the capabilities of ITE in k-nearest neighbor or minimum spanning tree computation (which is also immediately inherited to entropy, mutual information, divergence, association measure and cross quantity estimation), it sufficient to the add the new method to `kNN_squared_distances.m` or `compute_MST.m`.

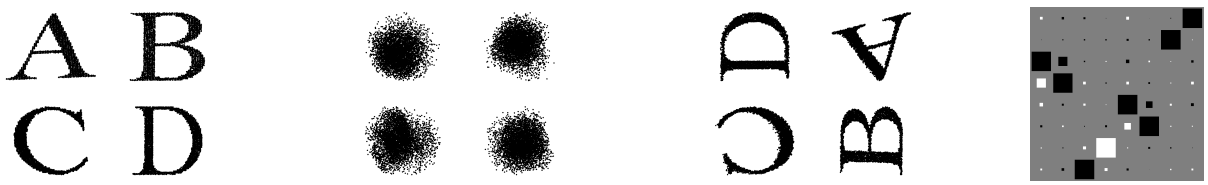
## 4.3 Performance Measure, the Amari-index

Here, we introduce the Amari-index, which can be used to measure the efficiency of the estimators in the ISA problem and its extensions.

| co.MSTmethod | Method | Environment |
|---|---|---|
| 'MatlabBGL_Prim' | Prim algorithm (MatlabBGL) | Matlab, Octave[a] |
| 'MatlabBGL_Kruskal' | Kruskal algorithm (MatlabBGL) | Matlab, Octave |
| 'pmtk3_Prim' | Prim algorithm (pmtk3) | Matlab, Octave |
| 'pmtk3_Kruskal' | Kruskal algorithm (pmtk3) | Matlab, Octave |

Table 22: Minimum spanning tree (MST) methods. The main MST function is compute_MST.m.

[a]See Table 1.



(a) (b) (c) (d)

Figure 2: ISA demonstration (demo_ISA.m). (a): hidden components ($\{\mathbf{e}^m\}_{m=1}^M$). (b): observed, mixed signal ($\mathbf{x}$). (c): estimated components ($\{\hat{\mathbf{e}}^m\}_{m=1}^M$). (d): Hinton-diagram: the product of the mixing matrix and the estimated demixing matrix; approximately block-permutation matrix with $2 \times 2$ blocks.

Identification of the ISA model is ambiguous. However, the ambiguities of the model are simple: hidden components can be determined up to permutation of the subspaces and up to invertible linear transformations within the subspaces [142]. Thus, in the ideal case, the product of the estimated ISA demixing matrix $\hat{\mathbf{W}}_{\mathrm{ISA}}$ and the ISA mixing matrix $\mathbf{A}$, i.e., matrix

$$\mathbf{G} = \hat{\mathbf{W}}_{\mathrm{ISA}}\mathbf{A} \tag{157}$$

is a block-permutation matrix (also called block-scaling matrix [141]). This property can also be measured for source components with different dimensions by a simple extension [127] of the Amari-index [3], that we present below. Namely, assume that we have a weight matrix $\mathbf{V} \in \mathbb{R}^{M\times M}$ made of positive matrix elements, and a $q \geq 1$ real number. Loosely speaking, we shrink the $d_i \times d_j$ blocks of matrix $\mathbf{G}$ according to the weights of matrix $\mathbf{V}$ and apply the traditional Amari-index for the matrix we obtain. Formally, one can (i) assume without loss of generality that the component dimensions and their estimations are ordered in increasing order ($d_1 \leq \ldots \leq d_M$, $\hat{d}_1 \leq \ldots \leq \hat{d}_M$), (ii) decompose $\mathbf{G}$ into $d_i \times d_j$ blocks ($\mathbf{G} = \left[\mathbf{G}^{ij}\right]_{i,j=1,\ldots,M}$) and define $g^{ij}$ as the $\ell_q$ norm[24] of the elements of the matrix $\mathbf{G}^{ij} \in \mathbb{R}^{d_i\times d_j}$, weighted with $V_{ij}$:

$$g^{ij} = V_{ij}\left(\sum_{k=1}^{d_i}\sum_{l=1}^{d_j} |\left(\mathbf{G}^{ij}\right)_{k,l}|^q\right)^{\frac{1}{q}}. \tag{158}$$

Then the Amari-index with parameters $\mathbf{V}$ can be adapted to the ISA task of possibly different component dimensions as follows

$$r_{\mathbf{V},q}(\mathbf{G}) := \frac{1}{2M(M-1)}\left[\sum_{i=1}^M\left(\frac{\sum_{j=1}^M g^{ij}}{\max_j g^{ij}} - 1\right) + \sum_{j=1}^M\left(\frac{\sum_{i=1}^M g^{ij}}{\max_i g^{ij}} - 1\right)\right]. \tag{159}$$

One can see that $0 \leq r_{\mathbf{V},q}(\mathbf{G}) \leq 1$ for any matrix $\mathbf{G}$, and $r_{\mathbf{V},q}(\mathbf{G}) = 0$ if and only if $\mathbf{G}$ is block-permutation matrix with $d_i \times d_j$ sized blocks. $r_{\mathbf{V},q}(\mathbf{G}) = 1$ is in the worst case, i.e, when all the $g^{ij}$ elements are equal. Let us note that this measure (159) is invariant, e.g., for multiplication with a positive constant: $r_{c\mathbf{V}} = r_{\mathbf{V}}$ ($\forall c > 0$). Weight matrix $\mathbf{V}$ can be uniform ($V_{ij} = 1$), or one can use weighing according to the size of the subspaces: $V_{ij} = 1/(d_i d_j)$. The Amari-index [Eq. (159)] is available in the ITE package, see Amari_index_ISA.m. The $\mathbf{G}$ global matrix can be visualized by its Hinton-diagram (hinton_diagram.m), Fig. 2 provides an illustration. This illustration has been obtained by running demo_ISA.m.

The Amari-index can also be used to measure the efficiency of the estimators of the IPA problem family detailed in Section 4.1.2. The demo files in the ITE toolbox (see Table 19) contain detailed examples for the usage of the Amari-index in the extensions of ISA.

[24]Alternative norms could also be used.

## 4.4 Dataset-, Model Generators

One can generate observations from the ISA model and its extensions (Section 4.1.2) by the functions listed in Table 23. The sources/driving noises can be chosen from many different types in ITE (see `sample_subspaces.m`):

**3D-geom:** In the *3D-geom* test [95] $\mathbf{e}^m$s are random variables uniformly distributed on 3-dimensional geometric forms ($d_m = 3$, $M \leq 6$), see Fig. 3(a). The dataset generator is `sample_subspaces_3D_geom.m`.

**Aw, ABC, GreekABC:** In the $A\omega$ database [134] the distribution of the hidden sources $\mathbf{e}^m$ are uniform on 2-dimensional images ($d_m = 2$) of the English ($M_1 = 26$) and Greek alphabet ($M_2 = 24$). The number of components can be $M = M_1 + M_2 = 50$. Special cases of the database are the *ABC* ($M \leq 26$) [94] and the *GreekABC* ($M \leq 24$) [134] subsets. For illustration, see Fig. 3(d). The dataset generators are called `sample_subspaces_Aw.m`, `sample_subspaces_ABC.m` and `sample_subspaces_GreekABC.m`, respectively.

**mosaic:** The *mosaic* test [131] has 2-dimensional source components ($d_m = 2$) generated from mosaic images. Sources $\mathbf{e}^m$ are generated by sampling 2-dimensional coordinates proportional to the corresponding pixel intensities. In other words, 2-dimensional images are considered as density functions. For illustration, see Fig. 3(h). The dataset generator is `sample_subspaces_mosaic.m`.

**IFS:** Here [133], components $\mathbf{s}^m$ are realizations of IFS[25] based 2-dimensional ($d = 2$) self-similar structures. For all $m$ a $(\{\mathbf{h}_k\}_{k=1,\dots,K}, \mathbf{p} = (p_1, \dots, p_K), \mathbf{v}_1\}$ triple is chosen, where

- $\mathbf{h}_k : \mathbb{R}^2 \to \mathbb{R}^2$ are affine transformations: $\mathbf{h}_k(\mathbf{z}) = \mathbf{C}_k\mathbf{z} + \mathbf{d}_k$ ($\mathbf{C}_k \in \mathbb{R}^{2\times 2}, \mathbf{d}_k \in \mathbb{R}^2$),
- $\mathbf{p}$ is a distribution over the indices $\{1, \dots, K\}$ ($\sum_{k=1}^K p_k = 1, p_k \geq 0$), and
- for the initial value we chose $\mathbf{v}_1 := \left(\frac{1}{2}, \frac{1}{2}\right)$.

In the *IFS* dataset, $T$ samples are generated in the following way: (i) $\mathbf{v}_1$ is given ($t = 1$), (ii) an index $k(t) \in \{1, \dots, K\}$ is drawn according to the distribution $\mathbf{p}$ and (iii) the next sample is generated as $\mathbf{v}_{t+1} := \mathbf{h}_{k(t)}(\mathbf{v}_t)$. The resulting series $\{\mathbf{v}_1, \dots, \mathbf{v}_T\}$ was taken as a hidden source component $\mathbf{s}^m$ and this way 9 components ($M = 9$, $D = 18$) were constructed (see Fig. 3(c)). The generator of the dataset is `sample_subspaces_IFS.m`.

**ikeda:** In the *ikeda* test [127], the hidden $\mathbf{s}_t^m = [s_{t,1}^m, s_{t,2}^m] \in \mathbb{R}^2$ sources realize the ikeda map

$$s_{t+1,1}^m = 1 + \lambda_m[s_{t,1}^m \cos(w_t^m) - s_{t,2}^m \sin(w_t^m)], \tag{160}$$

$$s_{t+1,2}^m = \lambda_m[s_{t,1}^m \sin(w_t^m) + s_{t,2}^m \cos(w_t^m)], \tag{161}$$

where $\lambda_m$ is a parameter of the dynamical system and

$$w_t^m = 0.4 - \frac{6}{1 + (s_{t,1}^m)^2 + (s_{t,2}^m)^2}. \tag{162}$$

There are 2 components ($M = 2$) with initial points $\mathbf{s}_1^1 = [20; 20]$, $\mathbf{s}_1^2 = [-100; 30]$ and parameters $\lambda_1 = 0.9994$, $\lambda_2 = 0.998$, see Fig. 3(f) for illustration. Observation can be generated from this dataset using `sample_subspaces_ikeda.m`.

**lorenz:** In the *lorenz* dataset [131], the sources ($\mathbf{s}^m$) correspond to 3-dimensional ($d_m = 3$) deterministic chaotic time series, the so-called Lorenz attractor [68] with different initial points $(x_0, y_0, z_0)$ and parameters ($a$, $b$, $c$). The Lorenz attractor is described by the following ordinary differential equations:

$$\dot{x}_t = a(y_t - x_t), \tag{163}$$

$$\dot{y}_t = x_t(b - z_t) - y_t, \tag{164}$$

$$\dot{z}_t = x_t y_t - c z_t. \tag{165}$$

The differential equations are computed by the explicit Runge-Kutta (4,5) method in ITE. The number of components can be $M = 3$. The dataset generator is `sample_subspaces_lorenz.m`. For illustration, see Fig. 3(g).

[25] IFS stands for iterated function system.

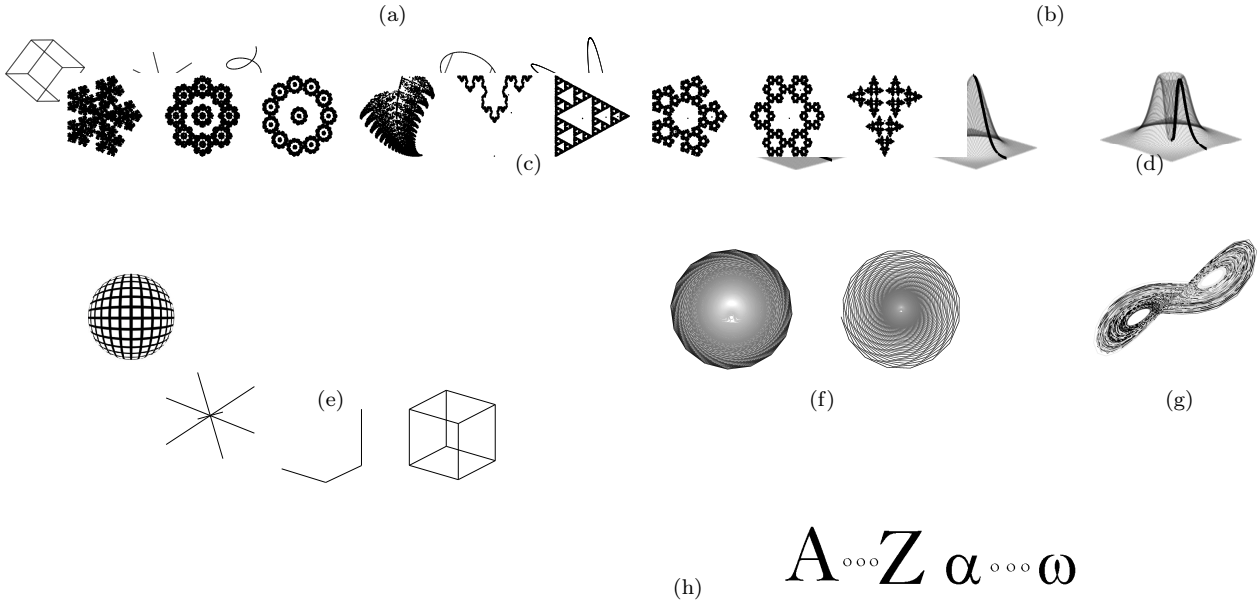



Figure 3: Illustration of the *3D-geom* (a), *multiD-spherical (multi$D_1$-...-$D_M$-spherical)* (b), *IFS* (c), *Aw* (subset on the left: *ABC*, right: *GreekABC*) (d), *multiD-geom (multi$D_1$-...-$D_M$-geom)* (e), *ikeda* (f), *lorenz* (g), and *mosaic* (h) datasets.

**all-k-independent:** In the *all-k-independent* database [94, 128], the $d_m$-dimensional hidden components $\mathbf{v} := \mathbf{e}^m$ are created as follows: coordinates $v_i$ $(i = 1, \ldots, k)$ are independent uniform random variables on the set {0,...,k-1}, whereas $v_{k+1}$ is set to $mod(v_1 + \ldots + v_k, k)$. In this construction, every $k$-element subset of $\{v_1, \ldots, v_{k+1}\}$ is made of independent variables and $d_m = k + 1$. The database generator is `sample_subspaces_all_k_independent.m`.

**multiD-geom (multi$D_1$-...-$D_M$-geom):** In this dataset $\mathbf{e}^m$s are random variables uniformly distributed on $d_m$-dimensional geometric forms. Geometrical forms were chosen as follows: (i) the surface of the unit ball, (ii) the straight lines that connect the opposing corners of the unit cube, (iii) the broken line between $d_m + 1$ points $\mathbf{0} \to \mathbf{e}_1 \to \mathbf{e}_1 + \mathbf{e}_2 \to \ldots \to \mathbf{e}_1 + \ldots + \mathbf{e}_{d_m}$ (where $\mathbf{e}_i$ is the $i$ canonical basis vector in $\mathbb{R}^{d_m}$, i.e., all of its coordinates are zero except the $i^{th}$, which is 1), and (iv) the skeleton of the unit square. Thus, the number of components $M$ can be equal to 4 ($M \leq 4$), and the dimension of the components ($d_m$) can be scaled. In the *multiD-geom* case the dimensions of the subspaces are equal ($d_1 = \ldots = d_M$); in case of the *multi$D_1$-...-$D_M$-geom* dataset, the $d_m$ subspace dimensions can be different. For illustration, see Fig. 3(e). The associated dataset generator is called `sample_subspaces_multiD_geom`.

**multiD-spherical (multi$D_1$-...-$D_M$-spherical):** In this case hidden sources $\mathbf{e}^m$ are spherical random variables [30]. Since spherical variables assume the form $\mathbf{v} = \rho\mathbf{u}$, where $\mathbf{u}$ is uniformly distributed on the $d_m$-dimensional unit sphere, and $\rho$ is a non-negative scalar random variable independent of $\mathbf{u}$, they can be given by means of $\rho$. 3 pieces of stochastic representations $\rho$ were chosen: $\rho$ was uniform on $[0, 1]$, exponential with parameter $\mu = 1$ and lognormal with parameters $\mu = 0, \sigma = 1$. For illustration, see Fig. 3(b). In this case, the number of component can be 3 ($M \leq 3$) The dimension of the source components ($d_m$) is fixed (can be varied) in the *multiD-spherical* (*multi$D_1$-...-$D_M$-spherical*) dataset. Observations can be obtained from these datasets by `sample_subspaces_multiD_spherical.m`.

The datasets and their generators are summarized in Table 24 and Table 25. The `plot_subspaces.m` function can be used to plot the databases (samples/estimations).

| Model | Generator |
|---|---|
| ISA | `generate_ISA.m` |
| complex ISA | `generate_complex_ISA.m` |
| AR-IPA | `generate_AR_IPA.m` |
| ARX-IPA | `generate_ARX_IPA_parameters.m` |
| (u)MA-IPA | `generate_MA_IPA.m` |
| mAR-IPA | `generate_mAR_IPA.m` |
| fAR-IPA | `generate_fAR_IPA.m.m` |

Table 23: IPA model generators. Note: in case of the ARX-IPA model, the observations are generated online in accordance with the online D-optimal ARX identification method.

| Dataset (`data_type`) | Description | Subspace dimensions | # of components | i.i.d. |
|---|---|---|---|---|
| `'3D-geom'` | uniformly distributed (U) on 3D forms | $d_m = 3$ | $M \leq 6$ | Y |
| `'Aw'` | U on English and Greek letters | $d_m = 2$ | $M \leq 50$ | Y |
| `'ABC'` | U on English letters | $d_m = 2$ | $M \leq 26$ | Y |
| `'GreekABC'` | U on Greek letters | $d_m = 2$ | $M \leq 24$ | Y |
| `'mosaic'` | distributed according to mosaic images | $d_m = 2$ | $M \leq 4$ | Y |
| `'IFS'` | self-similar construction | $d_m = 2$ | $M \leq 9$ | N |
| `'ikeda'` | Ikeda map | $d_m = 2$ | $M = 2$ | N |
| `'lorenz'` | Lorenz attractor | $d_m = 3$ | $M \leq 3$ | N |
| `'all-k-independent'` | k-tuples in the subspaces are independent | scalable ($d_m = k + 1$) | $M \geq 1$ | Y |
| `'multid-geom'` | U on $d$-dimensional geometrical forms | scalable ($d = d_m \geq 1$) | $M \leq 4$ | Y |
| `'multid`$_1$`-d`$_2$`-...-d`$_M$`-geom'` | U on $d_m$-dimensional geometrical forms | scalable ($d_m \geq 1$) | $M \leq 4$ | Y |
| `'multid-spherical'` | spherical subspaces | scalable ($d = d_m \geq 1$) | $M \leq 3$ | Y |
| `'multid`$_1$`-d`$_2$`-...-d`$_M$`-spherical'` | spherical subspaces | scalable ($d_m \geq 1$) | $M \leq 3$ | Y |

Table 24: Description of the datasets. Last column: Y – yes, N – no.

| Dataset (`data_type`) | Generator |
|---|---|
| `'3D-geom'` | `sample_subspaces_3D_geom.m` |
| `'Aw'` | `sample_subspaces_Aw.m` |
| `'ABC'` | `sample_subspaces_ABC.m` |
| `'GreekABC'` | `sample_subspaces_GreekABC.m` |
| `'mosaic'` | `sample_subspaces_mosaic.m` |
| `'IFS'` | `sample_subspaces_IFS.m` |
| `'ikeda'` | `sample_subspaces_ikeda.m` |
| `'lorenz'` | `sample_subspaces_lorenz.m` |
| `'all-k-independent'` | `sample_subspaces_all_k_independent.m` |
| `'multid-geom'`, `'multid`$_1$`-d`$_2$`-...-d`$_M$`-geom'` | `sample_subspaces_multiD_geom.m` |
| `'multid-spherical'`, `'multid`$_1$`-d`$_2$`-...-d`$_M$`-spherical'` | `sample_subspaces_multiD_spherical.m` |

Table 25: Generators of the datasets. The high-level sampling function of the datasets is `sample_subspaces.m`.

# 5 Directory Structure of the Package

In this section, we describe the directory structure of the ITE toolbox. Directory

- *code*: code of ITE,
  - *H_I_D_A_C_K*: estimators of entropy, mutual information, divergence, association and cross measures, kernels on distributions (see Section 3).
    - *base*: contains the base estimators; initialization and estimation functions (see Section 3.1).
    - *meta*: the folder of meta estimators; initialization and estimation functions (see Section 3.2).
    - *utilities*: code shared by *base* and *meta*.
  - *IPA*: application of the information theoretical estimators in ITE (see Section 4):
    - *data_generation*: IPA generators corresponding to different datasets and models.
      - *datasets*: sampling from and plotting of the sources (see Table 24, Table 25, Fig. 3).
      - *models*: IPA model generators, see Table 23.
    - *demos*: IPA demonstrations and estimators, see Table 19 and Table 20.
    - *optimization*: IPA optimization methods (see Table 14, Table 15, Table 16, Table 17, and Table 18).
  - *shared*: code shared by *H_I_D_A_C_K* and *IPA*.
    - *downloaded*, *embedded*: downloaded and embedded packages (see Section 2).
- *doc*: contains a link to this manual.

# A Citation of the ITE Toolbox

The citing information of the ITE toolbox is provided below in BibTeX format:

```
@ARTICLE{szabo12separation,
  AUTHOR =       {Zolt{\'a}n Szab{\'o} and Barnab{\'a}s P{\'o}czos and Andr{\'a}s L{\H{o}}rincz},
  TITLE =        {Separation Theorem for Independent Subspace Analysis and its Consequences},
  JOURNAL =      {Pattern Recognition},
  YEAR =         {2012},
  volume =       {45},
  issue =        {4},
  pages =        {1782-1791},
}

@ARTICLE{szabo07undercomplete,
  AUTHOR =       {Zolt{\'a}n Szab{\'o} and Barnab{\'a}s P{\'o}czos and Andr{\'a}s L{\H{o}}rincz},
  TITLE =        {Undercomplete Blind Subspace Deconvolution},
  JOURNAL =      {Journal of Machine Learning Research},
  YEAR =         {2007},
  volume =       {8},
  pages =        {1063-1095},
}
```

# B Abbreviations

The abbreviations used in the paper are listed in Table 26.

# C Functions with Octave-Specific Adaptations

Functions with Octave-specific adaptations are summarized in Table 27.

# D Further Definitions

Below, some further definitions are enlisted for the self-containedness of the documentation:

**Definition 1 (concordance ordering)** *In two dimensions ($d = 2$) a $C_1$ copula is said to be smaller than the $C_2$ copula ($C_1 \prec C_2$) [80], if*

$$C_1(\mathbf{u}) \leq C_2(\mathbf{u}), \quad \left(\forall \mathbf{u} \in [0,1]^2\right). \tag{166}$$

*This pointwise partial ordering on the set of copulas is called* concordance ordering.

*In the general ($d \geq 2$) case, a $C_1$ copula is said to be smaller than the $C_2$ copula ($C_1 \prec C_2$) [52], if*

$$C_1(\mathbf{u}) \leq C_2(\mathbf{u}), \text{ and } \bar{C}_1(\mathbf{u}) \leq \bar{C}_2(\mathbf{u}) \quad \left(\forall \mathbf{u} \in [0,1]^d\right). \tag{167}$$

*Note:*

- *'$\prec$' is called* concordance ordering*; it again defines a partial ordering.*
- *The rationale behind requiring $C_1 \leq C_2$* and *$\bar{C}_1 \leq \bar{C}_2$ is that we want to capture 'simultaneously large'* and *'simultaneously small' tendencies.*
- *The two definitions [(166), (167)] coincide only in the two-dimensional ($d = 2$) case.*

**Definition 2 (measure of concordance [103, 79, 80])** *A $\kappa$ numeric measure of association on pairs of random variables ($y^1$, $y^2$ whose joint copula is $C$) is called a* measure of concordance*, if it satisfies the following properties:*

| Abbreviation | Meaning |
|---|---|
| ANN | approximate nearest neighbor |
| AR | autoregressive |
| ARIMA | integrated ARMA |
| ARMA | autoregressive moving average |
| ARX | AR with exogenous input |
| BFGS | Broyden-Fletcher-Goldfarb-Shannon |
| BSD | blind source deconvolution |
| BSSD | blind subspace deconvolution |
| CDSS | continuously differentiable sample spacing |
| CE | cross-entropy |
| EASI | equivariant adaptive separation via independence |
| fAR | functional AR |
| GV | generalized variance |
| HS | Hilbert-Schmidt |
| HSIC | Hilbert-Schmidt independence criterion |
| ICA/ISA/IPA | independent component/subspace/process analysis |
| i.i.d. | independent identically distributed |
| IFS | iterated function system |
| IPM | integral probability metrics |
| ITE | information theoretical estimators |
| JFD | joint f-decorrelation |
| KCCA | kernel canonical correlation analysis |
| KDE | kernel density estimation |
| KL | Kullback-Leibler |
| KGV | kernel generalized variance |
| kNN | k-nearest neighbor |
| LPA | linear prediction approximation |
| MA | moving average |
| mAR | AR with missing values |
| MMD | maximum mean discrepancy |
| NIW | normal-inverted Wishart |
| NN | nearest neighbor |
| PCA | principal component analysis |
| PNL | post nonlinear |
| QMI | quadratic mutual information |
| RBF | radial basis function |
| RKHS | reproducing kernel Hilbert space |
| RP | random projection |

Table 26: Abbrevations.

| Function | Role |
|---|---|
| `ITE_install.m` | installation of the ITE package |
| `hinton_diagram.m` | Hinton-diagram |
| `estimate_clustering_UD1_S.m` | spectral clustering |
| `control.m` | D-optimal control |
| `sample_subspaces_lorenz.m` | sampling from the *lorenz* dataset |
| `clinep.m` | the core of the 3D trajectory plot |
| `plot_subspaces_3D_trajectory.m` | 3D trajectory plot |
| `IGV_similarity_matrix.m` | similarity matrix for the GV measure |
| `calculateweight.m` | weight computation in the weighted kNN method |
| `kNN_squared_distances.m` | kNN computation |
| `initialize_Octave_ann_wrapper_if_needed.m` | ann Octave wrapper initialization |
| `IGV_estimation.m` | generalized variance estimation |
| `SpectralClustering.m` | spectral clustering |

Table 27: Functions with Octave-specific adaptations, i.e, the functions calling `working_environment_Matlab.m` (directly).

***A1. Domain****: it is defined for every $(y^1, y^2)$ pair of continuous random variables,*

***A2. Range****: $\kappa\left(y^1, y^2\right) \in [-1, 1]$, [$\kappa\left(y^1, y^1\right) = 1$, and $\kappa\left(y^1, -y^1\right) = -1$],*

***A3. Symmetry****: $\kappa\left(y^1, y^2\right) = \kappa\left(y^2, y^1\right)$,*

***A4. Independence****: if $y^1$ and $y^2$ are independent, then $\kappa\left(y^1, y^2\right) = \kappa(\Pi) = 0$,*

***A5. Change of sign****: $\kappa\left(-y^1, y^2\right) = -\kappa\left(y^1, y^2\right)$ [$= \kappa\left(y^1, -y^2\right)$],*

***A6. Coherence****: if $C_1 \prec C_2$, then $\kappa(C_1) \leq \kappa(C_2)$,*[26]

***A7. Continuity****: if $\left(y_t^1, y_t^2\right)$ is a sequence of continuous random variables with copula $C_t$, and if $C_t$ converges to $C$ pointwise*[27]*, then $\lim_{t\to\infty} \kappa(C_t) = \kappa(C)$.*

*Note: properties in the parentheses ('[]') can be derived from the others.*

**Definition 3 (multivariate measure of concordance [25, 140])** *A* multivariate measure of concordance *is a $\kappa$ function that assigns to every continuous random variable $\mathbf{y}$ a real number and satisfies the following properties:*

***B1. Normalization****:*

*B1a : $\kappa\left(y^1, \ldots, y^d\right) = 1$ if each $y^i$ is an increasing function of every other $y^j$ (or in terms of copulas $\kappa(M) = 1$), and*

*B1b : $\kappa\left(y^1, \ldots, y^d\right) = 0$ if $y^i$-s are independent (or in terms of copulas $\kappa(\Pi) = 1$).*

***B2. Monotonicity****: $C_1 \prec C_2 \Rightarrow \kappa(C_1) \leq \kappa(C_2)$.*

***B3. Continuity****: If the cdf of the random variable sequence $\mathbf{y}_t$ ($F_t$) converges to $F$, the cdf of $\mathbf{y}$ ($\lim_{t\to\infty} F_t = F$), then*

$$\lim_{t\to\infty} \kappa(\mathbf{y}_t) = \kappa(\mathbf{y}). \tag{168}$$

*[In terms of copulas: $\lim_{t\to\infty} C_t = C$ (uniformly) $\Rightarrow \lim_{t\to\infty} \kappa(C_t) = \kappa(C)$.]*

***B4. Permutation invariance****: if $\{i_1, ..., i_d\}$ is permutation of $\{1, \ldots, d\}$, then*

$$\kappa\left(y^{i_1}, \ldots, y^{i_d}\right) = \kappa\left(y^1, \ldots, y^d\right). \tag{169}$$

[26] Hence the name concordance ordering.

[27] In fact uniform convergence of the copulas also holds, see [78] and B3 in Def. 3.

***B5. Duality**:*

$$\kappa\left(-y^1,\ldots,-y^d\right)=\kappa\left(y^1,\ldots,y^d\right). \tag{170}$$

***B6. Reflection symmetry property**:*

$$\sum_{\epsilon_1,\ldots,\epsilon_d=\pm 1}\kappa\left(\epsilon_1 y^1,\ldots,\epsilon_d y^d\right)=0, \tag{171}$$

*where the sum is over all the $2^d$ possibilities.*

***B7. Transition property**: there exists a sequence of $r_d$ numbers such that for all* $\mathbf{y}$

$$r_{d-1}\kappa\left(y^2,\ldots,y^d\right)=\kappa\left(y^1,\ldots,y^d\right)+\kappa\left(-y^1,\ldots,y^d\right). \tag{172}$$

**Definition 4 (measure of dependence)** *[80] defined a numeric measure $\kappa$ between two random variables $y^1$ and $y^2$ whose copula is $C$ as a* measure of dependence *if it satisfies the following properties:*

***C1. Domain**: $\kappa$ is defined for every $\left(y^1,y^2\right)$ pair.*

***C2. Symmetry**: $\kappa\left(y^1,y^2\right)=\kappa\left(y^2,y^1\right)$.*

***C3. Range**: $\kappa\left(y^1,y^2\right)\in[0,1]$.*

***C4. Independence**: $\kappa\left(y^1,y^2\right)=0$ if and only if $y^1$ and $y^2$ are independent.*

***C5. Strictly monotone functional dependence**: $\kappa\left(y^1,y^2\right)=1$ if and only each of $y^1$ and $y^2$ is a strictly monotone function of the other.*

***C6. Invariance to strictly monotone functions**: if $f_1$ and $f_2$ are strictly monotone functions, then*

$$\kappa\left(y^1,y^2\right)=\kappa\left(f_1(y^1),f_2(y^2)\right). \tag{173}$$

***C7. Continuity**: if $\left(y_t^1,y_t^2\right)$ is a sequence of random variables with copula $C_n$, and if $\lim_{t\to\infty}C_t=C$ (pointwise), then*

$$lim_{t\to\infty}\kappa(C_t)=\kappa(C). \tag{174}$$

**Definition 5 (multivariate measure of dependence)** *[153] defined the notion of measure of dependence in case of $d$ dimension as follows. A $\kappa$ real-valued function is called a* measure of dependence *if it satisfies the properties:*

***D1. Domain**: $\kappa$ is defined for any continuously distributed* $\mathbf{y}$*,*

***D2. Permutation invariance**: if $\{i_1,...,i_d\}$ is permutation of $\{1,\ldots,d\}$, then*

$$\kappa\left(y^{i_1},\ldots,y^{i_d}\right)=\kappa\left(y^1,\ldots,y^d\right). \tag{175}$$

***D3. Normalization**: $0\leq\kappa\left(y^1,\ldots,y^d\right)\leq 1$.*

***D4. Independence**: $\kappa\left(y^1,\ldots,y^d\right)=0$ if and only if $y^i$-s are independent.*

***D5. Strictly monotone functional dependence**: $\kappa\left(y^1,\ldots,y^d\right)=1$ if and only if each $y^i$ is an increasing function of each of the others.*

***D6. Invariance to strictly monotone functions**: If $f_1,\ldots,f_d$ are all strictly increasing functions, then*

$$\kappa\left(y^1,\ldots,y^d\right)=\kappa\left(f_1\left(y^1\right),\ldots,f_d\left(y^d\right)\right). \tag{176}$$

***D7. Normal case**: Let* $\mathbf{y}$ *be normally distributed and $\rho_{ij}=cov\left(y^i,y^j\right)$. If $r_{ij}$-s are either all non-negative, or all non-positive then $\kappa$ is a strictly increasing function of each of the $|r_{ij}|$-s.*

***D8. Continuity**: If the random variable sequence $\mathbf{y}_t$ converges in distribution to $\mathbf{y}$, then*

$$\lim_{t\to\infty} \kappa(\mathbf{y}_t) = \kappa(\mathbf{y}). \tag{177}$$

**Definition 6 (semimetric space of negative type)** *Let $\mathcal{Z}$ be a non-empty set and let $\rho : \mathcal{Z} \times \mathcal{Z} \to [0, \infty)$ be a function for which the following properties hold for all $z, z' \in \mathcal{Z}$:*

1. *$\rho(z, z') = 0$ if and only if $z = z'$,*
2. *$\rho(z, z') = \rho(z', z)$.*

*Then $(Z, \rho)$ is called a* semimetric space.[28] *A semimetric space is said to be of* negative type *if*

$$\sum_{i=1}^{T}\sum_{j=1}^{T} a_i a_j \rho(z_i, z_j) \leq 0 \tag{178}$$

*for $\forall T \geq 2$, $\forall z_1, \ldots, z_T \in \mathcal{Z}$ and $\forall a_1, \ldots, a_T \in \mathbb{R}$ with $\sum_{i=1}^{T} a_i = 0$.*
*Example:*

- *Euclidean spaces are of negative type.*
- *Let $\mathcal{Z} \subseteq \mathbb{R}^d$ and $\rho(z, z') = \|z - z'\|_2^q$. Then $(\mathcal{Z}, \rho)$ is a semimetric space of negative type for $q \in (0, 2]$.*

**Definition 7 ((covariant) Hilbertian metric)** *A $\rho : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ metric is Hilbertian if there exist a Hilbert space $\mathcal{H}$ and an $f : \mathcal{X} \to \mathcal{H}$ isometry [41]:*

$$\rho^2(x, y) = \langle f(x) - f(y), f(x) - f(y)\rangle_{\mathcal{H}} = \|f(x) - f(y)\|_{\mathcal{H}}^2 \quad (\forall x, y \in \mathcal{X}). \tag{179}$$

*Additionally, if $\mathcal{X}$ is the set of distributions ($\boldsymbol{\mathcal{M}}_+^1(\mathcal{X})$) and $\rho$ is independent of the dominating measure, then $d$ is called* covariant*. Intuitively, this means its value is invariant to arbitrary smooth coordinate transformations of the underlying probability space; for example, it is no matter whether we take RGB, HSV, ... color space.*

**Definition 8 ((Csiszár) f-divergence)** *Let us given a convex function $f$, for which $f(1) = 0$. The f-divergence of the probability densities $f_1$ and $f_2$ on $\mathbb{R}^d$ is defined [22, 74, 2] as*

$$D_f(f_1, f_2) = \int_{\mathbb{R}^d} f\left[\frac{f_1(\mathbf{u})}{f_2(\mathbf{u})}\right] f_2(\mathbf{u})\mathrm{d}\mathbf{u}. \tag{180}$$

*Notes:*

- *The f-divergence is also called Csiszár-Morimoto divergence or Ali-Silvey distance.*
- *$D_f(f_1, f_2) \geq 0$ with equality if and only if $f_1 = f_2$.*

# E Estimation Formulas – Lookup Table

In this section the computations of entropy (Section E.1), mutual information (Section E.2), divergence (Section E.3), association (Section E.4) and cross (Section E.5) measures, and kernels on distributions (Section E.6) are summarized *briefly*. This section is considered to be a quick lookup table. For specific details, please see the referred papers (Section 3).

**Notations**. '$*$' denotes transposition. $\mathbf{1}$ ($\mathbf{0}$) stands for the vector whose all elements are equal to 1 (0); $\mathbf{1}_u$, $\mathbf{0}_u$ explicitly indicate the dimension ($u$). The RBF (radial basis function; also called the Gaussian kernel) is defined as

$$k(\mathbf{u}, \mathbf{v}) = e^{-\frac{\|\mathbf{u}-\mathbf{v}\|^2}{2\sigma^2}}. \tag{181}$$

$tr(\cdot)$ stands for trace. Let $N(\mathbf{m}, \boldsymbol{\Sigma})$ denote the density function of the normal random variable with mean $\mathbf{m}$ and covariance $\boldsymbol{\Sigma}$.

$$V_d = \frac{\pi^{d/2}}{\Gamma\left(\frac{d}{2}+1\right)} = \frac{2\pi^{d/2}}{d\Gamma\left(\frac{d}{2}\right)} \tag{182}$$

[28] In contrast to a metric space, the triangle equality is not required.

is the volume of the d-dimensional unit ball. $\psi$ is the digamma function. Let

$$I_\alpha = \int_{\mathbb{R}^d} [f(\mathbf{u})]^\alpha \, \mathrm{d}\mathbf{u}, \tag{183}$$

where $f$ is a probability density on $\mathbb{R}^d$. The scalar product of $\mathbf{A} \in \mathbb{R}^{L_1 \times L_2}$, $\mathbf{B} \in \mathbb{R}^{L_1 \times L_2}$ is $\langle \mathbf{A}, \mathbf{B} \rangle = \sum_i \sum_j A_{ij} B_{ij}$. The Hadamard product of $\mathbf{A} \in \mathbb{R}^{L_1 \times L_2}$, $\mathbf{B} \in \mathbb{R}^{L_1 \times L_2}$ is $(\mathbf{A} \circ \mathbf{B})_{ij} = A_{ij} B_{ij}$. Let $\mathbb{I}$ be the indicator function. Let $y_{(t)}$ denote the order statistics of $\{y_t\}_{t=1}^T$, $(y_t \in \mathbb{R})$, i.e., $y_{(1)} \leq \ldots \leq y_{(T)}$; for $y_{(i)} = y_{(1)}$ $(i < 1)$ and $y_{(i)} = y_{(T)}$ $(i > T)$.

## E.1 Entropy

**Notations**. Let $\mathbf{Y}_{1:T} = (\mathbf{y}_1, \ldots, \mathbf{y}_T)$ $(\mathbf{y}_t \in \mathbb{R}^d)$ stand for our samples. Let $\rho_k(t)$ denote the Euclidean distance of the $k^{th}$ nearest neighbor of $\mathbf{y}_t$ in the sample $\mathbf{Y}_{1:T} \backslash \{\mathbf{y}_t\}$. Let $V \subseteq \mathbb{R}^d$ be a finite set, $S, S_1, S_2 \subseteq \{1, \ldots, k\}$ are index sets. $NN_S(V)$ stands for the $S$-nearest neighbor graph on $V$. $NN_S(V_2, V_1)$ denotes the S-nearest (from $V_1$ to $V_2$) neighbor graph. $\mathbb{E}$ is the expectation operator.

- `Shannon_kNN_k` [59, 115, 34]:

$$\hat{H}(\mathbf{Y}_{1:T}) = \log(T-1) - \psi(k) + \log(V_d) + \frac{d}{T} \sum_{t=1}^{T} \log\left(\rho_k(t)\right). \tag{184}$$

- `Renyi_kNN_k` [155, 64]:

$$C_{\alpha,k} = \left[ \frac{\Gamma(k)}{\Gamma(k+1-\alpha)} \right]^{\frac{1}{1-\alpha}}, \tag{185}$$

$$\hat{I}_\alpha(\mathbf{Y}_{1:T}) = \frac{T-1}{T} V_d^{1-\alpha} C_{\alpha,k}^{1-\alpha} \sum_{t=1}^{T} \frac{[\rho_k(t)]^{d(1-\alpha)}}{(T-1)^\alpha}, \tag{186}$$

$$\hat{H}_{\mathrm{R},\alpha}(\mathbf{Y}_{1:T}) = \frac{1}{1-\alpha} \log\left( \hat{I}_\alpha(\mathbf{Y}_{1:T}) \right). \tag{187}$$

- `Renyi_kNN_1tok` [95]:

$$S = \{1, \ldots, k\}, \tag{188}$$

$$V = \mathbf{Y}_{1:T}, \tag{189}$$

$$L(V) = \sum_{(\mathbf{u},\mathbf{v}) \in edges(NN_S(V))} \|\mathbf{u} - \mathbf{v}\|_2^{d(1-\alpha)}, \tag{190}$$

$$c = \lim_{T \to \infty} \mathbb{E}_{U_{1:T}, u_t : i.i.d., \sim Uniform([0,1]^d)} \left[ \frac{L(U_{1:T})}{T^\alpha} \right], \tag{191}$$

$$\hat{H}_{\mathrm{R},\alpha}(\mathbf{Y}_{1:T}) = \frac{1}{1-\alpha} \log\left[ \frac{L(V)}{cT^\alpha} \right]. \tag{192}$$

- `Renyi_S` [93]:

$$S \subseteq \{1, \ldots, k\}, k \in S, \tag{193}$$

$$V = \mathbf{Y}_{1:T}, \tag{194}$$

$$L(V) = \sum_{(\mathbf{u},\mathbf{v}) \in edges(NN_S(V))} \|\mathbf{u} - \mathbf{v}\|_2^{d(1-\alpha)}, \tag{195}$$

$$c = \lim_{T \to \infty} \mathbb{E}_{U_{1:T}, u_t : i.i.d., \sim Uniform([0,1]^d)} \left[ \frac{L(U_{1:T})}{T^\alpha} \right], \tag{196}$$

$$\hat{H}_{\mathrm{R},\alpha}(\mathbf{Y}_{1:T}) = \frac{1}{1-\alpha} \log\left[ \frac{L(V)}{cT^\alpha} \right]. \tag{197}$$

- `Renyi_weightedkNN` [118]:

$$k_1 = k_1(T) = \left\lceil 0.1\sqrt{T} \right\rceil, \tag{198}$$

$$k_2 = k_2(T) = \left\lceil 2\sqrt{T} \right\rceil, \tag{199}$$

$$N = \left\lfloor \frac{T}{2} \right\rfloor \tag{200}$$

$$M = T - N, \tag{201}$$

$$V_1 = Y_{1:N}, \tag{202}$$

$$V_2 = Y_{N+1:T}, \tag{203}$$

$$S = \{k_1, \ldots, k_2\}, \tag{204}$$

$$\eta_k = \frac{\beta(k, 1-\alpha)}{\Gamma(1-\alpha)} \frac{1}{N} M^{1-\alpha} V_d^{1-\alpha} \sum_{(\mathbf{u},\mathbf{v}) \in edges(NN_S(V_2, V_1))} \|\mathbf{u} - \mathbf{v}\|_2^{d(1-\alpha)}, \tag{205}$$

$$\hat{I}_{\alpha,\mathbf{w}} = \sum_{k \in S} w_k \eta_k, \tag{206}$$

$$\hat{H}_{\mathrm{R},\alpha}(\mathbf{Y}_{1:T}) = \frac{1}{1-\alpha} \log(\hat{I}_{\alpha,\mathbf{w}}), \tag{207}$$

  where the $w_k = w_k(T, d, k_1, k_2)$ weights can be precomputed.

- `Renyi_MST` [155]:

$$V = \mathbf{Y}_{1:T}, \tag{208}$$

$$L(V) = \min_{G \in \text{ spanning trees on } V} \sum_{(\mathbf{u},\mathbf{v}) \in edges(G)} \|\mathbf{u} - \mathbf{v}\|_2^{d(1-\alpha)}, \tag{209}$$

$$c = \lim_{T \to \infty} \mathbb{E}_{U_{1:T}, u_t : i.i.d., \sim Uniform([0,1]^d)} \left[ \frac{L(U_{1:T})}{T^\alpha} \right], \tag{210}$$

$$\hat{H}_{\mathrm{R},\alpha}(\mathbf{Y}_{1:T}) = \frac{1}{1-\alpha} \log \left[ \frac{L(V)}{cT^\alpha} \right]. \tag{211}$$

- `Renyi_GSF` [19]:

$$S = \{1, \ldots, k\}, \tag{212}$$

$$V = \mathbf{Y}_{1:T}, \tag{213}$$

$$L(V) = \min_{G \in \text{ spanning forest on } NN_S(V)} \sum_{(\mathbf{u},\mathbf{v}) \in edges(G)} \|\mathbf{u} - \mathbf{v}\|_2^{d(1-\alpha)}, \tag{214}$$

$$c = \lim_{T \to \infty} \mathbb{E}_{U_{1:T}, u_t : i.i.d., \sim Uniform([0,1]^d)} \left[ \frac{L(U_{1:T})}{T^\alpha} \right], \tag{215}$$

$$\hat{H}_{\mathrm{R},\alpha}(\mathbf{Y}_{1:T}) = \frac{1}{1-\alpha} \log \left[ \frac{L(V)}{cT^\alpha} \right]. \tag{216}$$

- `Tsallis_kNN_k` [64]:

$$C_{\alpha,k} = \left[ \frac{\Gamma(k)}{\Gamma(k+1-\alpha)} \right]^{\frac{1}{1-\alpha}}, \tag{217}$$

$$\hat{I}_\alpha(\mathbf{Y}_{1:T}) = \frac{T-1}{T} V_d^{1-\alpha} C_{\alpha,k}^{1-\alpha} \sum_{t=1}^{T} \frac{[\rho_k(t)]^{d(1-\alpha)}}{(T-1)^\alpha}, \tag{218}$$

$$\hat{H}_{\mathrm{T},\alpha}(\mathbf{Y}_{1:T}) = \frac{1 - \hat{I}_\alpha(\mathbf{Y}_{1:T})}{\alpha - 1}. \tag{219}$$

- `Shannon_Edgeworth` [45]: Since the Shannon entropy is invariant to additive constants ($H(\mathbf{y}) = H(\mathbf{y}+\mathbf{m})$), one can assume without loss of generality that the expectation of $\mathbf{y}$ is zero. The Edgeworth expansion based estimation is

$$\hat{H}(\mathbf{Y}_{1:T}) = H(\phi_d) - \frac{1}{12}\left[\sum_{i=1}^{d}\left(\kappa^{i,i,i}\right)^2 + 3\sum_{i,j=1;i\neq j}^{d}\left(\kappa^{i,i,j}\right)^2 + \frac{1}{6}\sum_{i,j,k=1;i<j<k}^{d}\left(\kappa^{i,j,k}\right)^2\right], \tag{220}$$

where

$$\mathbf{y}_t = \mathbf{y}_t - \frac{1}{T}\sum_{k=1}^{T}\mathbf{y}_k, (t = 1, \ldots, T) \tag{221}$$

$$\mathbf{\Sigma} = \hat{cov}(\mathbf{Y}_{1:T}) = \frac{1}{T-1}\sum_{t=1}^{T}\mathbf{y}_t(\mathbf{y}_t)^*, \tag{222}$$

$$H(\phi_d) = \frac{1}{2}\log\det(\mathbf{\Sigma}) + \frac{d}{2}\log(2\pi) + \frac{d}{2}, \tag{223}$$

$$\sigma_i = \hat{std}(y^i) = \frac{1}{T-1}\sum_{t=1}^{T}\left(y_t^i\right)^2, \quad (i = 1, \ldots, d) \tag{224}$$

$$\kappa^{ijk} = \hat{E}\left[y^i y^j y^k\right] = \frac{1}{T}\sum_{t=1}^{T} y_t^i y_t^j y_t^k, \quad (i, j, k = 1, \ldots, d) \tag{225}$$

$$\kappa^{i,j,k} = \frac{\kappa^{ijk}}{\sigma_i\sigma_j\sigma_k}. \tag{226}$$

- `Shannon_Voronoi` [73]: Let the Voronoi regions associated to samples $\mathbf{y}_1, \ldots, \mathbf{y}_T$ be denoted by $V_1, \ldots, V_T$ ($V_t \subseteq \mathbb{R}^d$). The estimation is as follows:

$$\hat{H}(\mathbf{Y}_{1:T}) = \frac{1}{T-K}\sum_{V_i:vol(V_i)\neq\infty}\log\left[T \times vol(V_i)\right], \tag{227}$$

where 'vol' denotes volume, and $K$ is the number of Voronoi regions with finite volume.

- `Shannon_spacing_V` [147]:

$$m = m(T) = \left\lfloor\sqrt{T}\right\rfloor, \tag{228}$$

$$\hat{H}(\mathbf{Y}_{1:T}) = \frac{1}{T}\sum_{t=1}^{T}\log\left(\frac{T}{2m}\left[y_{(i+m)} - y_{(i-m)}\right]\right). \tag{229}$$

- `Shannon_spacing_Vb` [29]:

$$m = m(T) = \left\lfloor\sqrt{T}\right\rfloor, \tag{230}$$

$$\hat{H}(\mathbf{Y}_{1:T}) = \frac{1}{T-m}\sum_{t=1}^{T-m}\log\left[\frac{T+1}{m}(y_{(t+m)} - y_{(t)})\right] + \sum_{k=m}^{T}\frac{1}{k} + \log\left(\frac{m}{T+1}\right). \tag{231}$$

- `Shannon_spacing_Vpconst` [83]:

$$m = m(T) = \left\lfloor\sqrt{T}\right\rfloor, \tag{232}$$

$$\hat{H}(\mathbf{Y}_{1:T}) = \frac{1}{T}\sum_{t=1}^{T}\log\left[\frac{T}{c_t m}(y_{(t+m)} - y_{(t-m)})\right], \tag{233}$$

where

$$c_t = \begin{cases} 1, & 1 \le t \le m, \\ 2, & m+1 \le t \le T-m, \\ 1 & T-m+1 \le t \le T. \end{cases} \tag{234}$$

It can be shown [83] that (229) = (233)+$\frac{2m\log(2)}{T}$.

- `Shannon_spacing_Vplin` [26]:

$$m = m(T) = \left\lfloor \sqrt{T} \right\rfloor, \tag{235}$$

$$\hat{H}(\mathbf{Y}_{1:T}) = \frac{1}{T}\sum_{t=1}^{T} \log\left[\frac{T}{c_t m}(y_{(t+m)} - y_{(t-m)})\right], \tag{236}$$

where

$$c_t = \begin{cases} 1 + \frac{t-1}{m}, & 1 \le t \le m, \\ 2, & m+1 \le t \le T-m, \\ 1 + \frac{T-t}{m} & T-m+1 \le t \le T. \end{cases} \tag{237}$$

- `Shannon_spacing_LL` [18]:

$$m = m(T) = \left\lfloor \sqrt{T} \right\rfloor, \tag{238}$$

$$\bar{y}_{(i)} = \frac{1}{2m+1}\sum_{j=i-m}^{i+m} y_{(j)}, \tag{239}$$

$$\hat{H}(\mathbf{Y}_{1:T}) = -\frac{1}{T}\sum_{t=1}^{T} \log\left[\frac{\sum_{j=i-m}^{i+m}\left(y_{(j)} - \bar{y}_{(i)}\right)(j-i)}{T\sum_{j=i-m}^{i+m}\left(y_{(j)} - \bar{y}_{(i)}\right)^2}\right]. \tag{240}$$

- `Renyi_spacing_V` [150]:

$$m = m(T) = \left\lfloor \sqrt{T} \right\rfloor, \tag{241}$$

$$\hat{H}_{\mathrm{R},\alpha}(\mathbf{Y}_{1:T}) = \frac{1}{1-\alpha}\log\left[\frac{1}{T}\sum_{t=1}^{T}\left(\frac{T}{2m}\left[y_{(i+m)} - y_{(i-m)}\right]\right)^{1-\alpha}\right]. \tag{242}$$

- `Renyi_spacing_E` [150]:

$$m = m(T) = \left\lfloor \sqrt{T} \right\rfloor, \tag{243}$$

$$t_1 = \sum_{i=2-m}^{0} \frac{y_{(i+m)} - y_{(i+m-1)}}{2}\left(\sum_{j=1}^{i+m-1}\frac{2}{y_{(j+m)} - y_{(j-m)}}\right)^{\alpha}, \tag{244}$$

$$t_2 = \sum_{i=1}^{T+1-m} \frac{y_{(i)} + y_{(i+m)} - y_{(i-1)} - y_{(i+m-1)}}{2}\left(\sum_{j=i}^{i+m-1}\frac{2}{y_{(j+m)} - y_{(j-m)}}\right)^{\alpha}, \tag{245}$$

$$t_3 = \sum_{i=T+2-m}^{T} \frac{y_{(i)} - y_{(i-1)}}{2}\left(\sum_{j=i}^{T}\frac{2}{y_{(j+m)} - y_{(j-m)}}\right)^{\alpha}, \tag{246}$$

$$\hat{H}_{\mathrm{R},\alpha}(\mathbf{Y}_{1:T}) = \frac{1}{1-\alpha}\log\left[\frac{t_1 + t_2 + t_3}{T^{\alpha}}\right]. \tag{247}$$

- `qRenyi_CDSS` [84]:

$$m = m(T) = \left\lfloor \sqrt{T} \right\rfloor, \tag{248}$$

$$\hat{H}_{\mathrm{R},2}(\mathbf{Y}_{1:T}) = -\log\left[\frac{30}{T(T-m)}\sum_{i=1}^{T-m}\sum_{j=i+1}^{i+m-1}\frac{(y_{(j)}-y_{(i+m)})^2(y_{(j)}-y_{(i)})^2}{(y_{(i+m)}-y_{(i)})^5}\right]. \tag{249}$$

- `Shannon_KDP` [120]:

$$\text{adaptive (k-d) partitioning} \Rightarrow \mathcal{A} = \{A_1, \ldots, A_K\}, \tag{250}$$

$$T_k = \#\left\{t : 1 \le t \le T, \mathbf{y}_t \in A_k\right\}, \tag{251}$$

$$\hat{H}(\mathbf{Y}_{1:T}) = \sum_{k=1}^{K}\frac{T_k}{T}\log\left[\frac{T}{T_k}vol(A_k)\right], \tag{252}$$

where 'vol' denotes volume.

- `Shannon_MaxEnt1`, `Shannon_MaxEnt2` [21, 46]: Since the Shannon entropy is invariant to additive constants ($H(y) = H(y+m)$), one can assume without loss of generality that the expectation of $y$ is zero. The maximum entropy distribution based entropy estimators (assuming $y$ with unit standard deviation) take the form

$$H(n) - \left[k_1\mathbb{E}^2\left[G_1(y)\right] + k_2\left(\mathbb{E}\left[G_2(y)\right] - \mathbb{E}\left[G_2(n)\right]\right)^2\right] \tag{253}$$

with suitably chosen $k_i \in \mathbb{R}$ contants and $G_i$ functions ($i = 1, 2$). In Eq. (253),

$$H(n) = \frac{1+\log(2\pi)}{2} \tag{254}$$

denotes the entropy of the standard normal variable ($n$), and in practise expectations are changed to their empirical variants. Particularly,

  - `Shannon_MaxEnt1`:

$$\hat{\sigma} = \hat{\sigma}\left(\mathbf{Y}_{1:T}\right) = \sqrt{\frac{1}{T-1}\sum_{t=1}^{T}\left(y_t\right)^2}, \tag{255}$$

$$y'_t = y_t/\hat{\sigma}, \quad (t = 1, \ldots, T) \tag{256}$$

$$G_1(z) = ze^{\frac{-z^2}{2}}, \tag{257}$$

$$G_2(z) = |z|, \tag{258}$$

$$k_1 = \frac{36}{8\sqrt{3}-9}, \tag{259}$$

$$k_2 = \frac{1}{2-\frac{6}{\pi}}, \tag{260}$$

$$\hat{H}_0 = \hat{H}_0\left(\mathbf{Y}'_{1:T}\right) = H(n) - \left[k_1\left(\frac{1}{T}\sum_{t=1}^{T}G_1\left(y'_t\right)\right)^2 + k_2\left(\frac{1}{T}\sum_{t=1}^{T}G_2\left(y'_t\right) - \sqrt{\frac{2}{\pi}}\right)^2\right], \tag{261}$$

$$\hat{H}\left(\mathbf{Y}_{1:T}\right) = \hat{H}_0 + \log(\hat{\sigma}). \tag{262}$$

– `Shannon_MaxEnt2`:

$$\hat{\sigma} = \hat{\sigma}\left(\mathbf{Y}_{1:T}\right) = \sqrt{\frac{1}{T-1}\sum_{t=1}^{T}\left(y_t\right)^2}, \tag{263}$$

$$y'_t = y_t/\hat{\sigma}, \quad (t = 1, \ldots, T) \tag{264}$$

$$G_1(z) = ze^{\frac{-z^2}{2}}, \tag{265}$$

$$G_2(z) = e^{\frac{-z^2}{2}}, \tag{266}$$

$$k_1 = \frac{36}{8\sqrt{3}-9}, \tag{267}$$

$$k_2 = \frac{24}{16\sqrt{3}-27}, \tag{268}$$

$$\hat{H}_0 = \hat{H}_0\left(\mathbf{Y}'_{1:T}\right) = H(n) - \left[k_1\left(\frac{1}{T}\sum_{t=1}^{T}G_1\left(y'_t\right)\right)^2 + k_2\left(\frac{1}{T}\sum_{t=1}^{T}G_2\left(y'_t\right) - \frac{1}{\sqrt{2}}\right)^2\right], \tag{269}$$

$$\hat{H}\left(\mathbf{Y}_{1:T}\right) = \hat{H}_0 + \log(\hat{\sigma}). \tag{270}$$

## E.2 Mutual Information

**Notations**. For an $\mathbf{Y}_{1:T} = (\mathbf{y}_1, \ldots, \mathbf{y}_T)$ sample set ($\mathbf{y}_t \in \mathbb{R}^d$), let $\hat{F}_m$ denote the empirical estimation of $F_m$, the marginal distribution function of the $m^{th}$ coordinate:

$$\hat{F}_m(y) = \sum_{t=1}^{T}\mathbb{I}_{\{y_t^m \leq y\}}, \tag{271}$$

let the vector of *grades* be defined as

$$\mathbf{U} = \left[F_1\left(y^1\right); \ldots; F_d\left(y^d\right)\right] \in [0,1]^d, \tag{272}$$

and let its empirical analog, the *ranks* be

$$\hat{U}_{mt} = \hat{F}_m(y_t^m) = \frac{1}{T}(\text{rank of } y_t^m \text{ in } y_1^m, \ldots, y_T^m), \quad (m = 1, \ldots, d). \tag{273}$$

Finally, the empirical copula is defined as

$$\hat{C}_T(\mathbf{u}) := \frac{1}{T}\sum_{t=1}^{T}\prod_{i=1}^{d}\mathbb{I}_{\{\hat{U}_{it} \leq u_i\}}, \quad \left(\mathbf{u} = [u_1; \ldots; u_d] \in [0,1]^d\right), \tag{274}$$

specially

$$\hat{C}_T\left(\frac{i_1}{T}, \ldots, \frac{i_T}{T}\right) = \frac{\#\text{ of } \mathbf{y}\text{-s in the sample with } \mathbf{y} \leq \mathbf{y}_{(i_1,\ldots,i_T)}}{T}, \quad (\forall j, i_j = 1, \ldots, T) \tag{275}$$

where $\mathbf{y}_{(i_1,\ldots,i_T)} = [y_{(i_1)}; \ldots; y_{(i_T)}]$ with $y_{(i_j)}$ order statistics in the $j^{th}$ coordinate.

- `HSIC` [37]:

$$H_{ij} = \delta_{ij} - \frac{1}{T}, \tag{276}$$

$$\left(\mathbf{K}_m\right)_{ij} = k_m\left(\mathbf{y}_i^m, \mathbf{y}_j^m\right), \tag{277}$$

$$\hat{I}_{\text{HSIC}}\left(\mathbf{Y}_{1:T}\right) = \frac{1}{T^2}\sum_{u=1}^{M-1}\sum_{v=u+1}^{M} tr(\mathbf{K}_u\mathbf{H}\mathbf{K}_v\mathbf{H}). \tag{278}$$

Currently, $k_m$-s are RBF-s.

- `KCCA`, `KGV` [5, 129]:

$$\kappa_2 = \frac{\kappa T}{2}, \tag{279}$$

$$\mathbf{K}_m = \left[k_m(\mathbf{y}_i^m, \mathbf{y}_j^m)\right]_{i,j=1,\dots,T}, \tag{280}$$

$$\mathbf{H} = \mathbf{I} - \frac{1}{T}\mathbf{1}\mathbf{1}^*, \tag{281}$$

$$\widetilde{\mathbf{K}}_m = \mathbf{H}\mathbf{K}_m\mathbf{H}, \tag{282}$$

$$\begin{pmatrix} (\widetilde{\mathbf{K}}_1 + \kappa_2\mathbf{I}_T)^2 & \widetilde{\mathbf{K}}_1\widetilde{\mathbf{K}}_2 & \cdots & \widetilde{\mathbf{K}}_1\widetilde{\mathbf{K}}_M \\ \widetilde{\mathbf{K}}_2\widetilde{\mathbf{K}}_1 & (\widetilde{\mathbf{K}}_2 + \kappa_2\mathbf{I}_T)^2 & \cdots & \widetilde{\mathbf{K}}_2\widetilde{\mathbf{K}}_M \\ \vdots & \vdots & & \vdots \\ \widetilde{\mathbf{K}}_M\widetilde{\mathbf{K}}_1 & \widetilde{\mathbf{K}}_M\widetilde{\mathbf{K}}_2 & \cdots & (\widetilde{\mathbf{K}}_M + \kappa_2\mathbf{I}_T)^2 \end{pmatrix} \begin{pmatrix} \mathbf{c}_1 \\ \mathbf{c}_2 \\ \vdots \\ \mathbf{c}_M \end{pmatrix} = \tag{283}$$

$$= \lambda \begin{pmatrix} (\widetilde{\mathbf{K}}_1 + \kappa_2\mathbf{I}_T)^2 & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{0} & (\widetilde{\mathbf{K}}_2 + \kappa_2\mathbf{I})^2 & \cdots & \mathbf{0} \\ \vdots & \vdots & & \vdots \\ \mathbf{0} & \mathbf{0} & \cdots & (\widetilde{\mathbf{K}}_M + \kappa_2\mathbf{I})^2 \end{pmatrix} \begin{pmatrix} \mathbf{c}_1 \\ \mathbf{c}_2 \\ \vdots \\ \mathbf{c}_M \end{pmatrix}.$$

Let us write Eq. (283) shortly as $\mathbf{A}\mathbf{c} = \lambda\mathbf{B}\mathbf{c}$. Let the minimal eigenvalue of this generalized eigenvalue problem be $\lambda_{\mathrm{KCCA}}$, and $\lambda_{\mathrm{KGV}} = \frac{\det(\mathbf{A})}{\det(\mathbf{B})}$.

$$\hat{I}_{\mathrm{KCCA}}\left(\mathbf{Y}_{1:T}\right) = -\frac{1}{2}\log(\lambda_{\mathrm{KCCA}}), \tag{284}$$

$$\hat{I}_{\mathrm{KGV}}\left(\mathbf{Y}_{1:T}\right) = -\frac{1}{2}\log(\lambda_{\mathrm{KGV}}). \tag{285}$$

At the moment, $k_m$-s are RBF-s.

- `Hoeffding` [43, 33]: The estimation can be computed as

$$h_2(d) = \left(\frac{2}{(d+1)(d+2)} - \frac{1}{2^d}\frac{d!}{\prod_{i=0}^{d}\left(i+\frac{1}{2}\right)} + \frac{1}{3^d}\right)^{-1}, \tag{286}$$

$$\hat{I}_{\Phi}\left(\mathbf{Y}_{1:T}\right) = \sqrt{h_2(d)\left\{\frac{1}{T^2}\sum_{j=1}^{T}\sum_{k=1}^{T}\prod_{i=1}^{d}\left[1 - \max(\hat{U}_{ij}, \hat{U}_{ik})\right] - \frac{2}{T}\frac{1}{2^d}\sum_{j=1}^{T}\prod_{i=1}^{d}\left(1 - \hat{U}_{ij}^2\right) + \frac{1}{3^d}\right\}}. \tag{287}$$

Under small sample adjustment, one can obtain a similar nice expression:

$$h_2(d,T)^{-1} = \frac{1}{T^2}\sum_{j=1}^{T}\sum_{k=1}^{T}\left[1 - \max\left(\frac{j}{T}, \frac{k}{T}\right)\right]^d - \frac{2}{T}\sum_{j=1}^{T}\left[\frac{T(T-1) - j(j-1)}{2T^2}\right]^d + \frac{1}{3^d}\left[\frac{(T-1)(2T-1)}{2T^2}\right]^d, \tag{288}$$

$$\hat{I}_{\Phi}\left(\mathbf{Y}_{1:T}\right) = \sqrt{h_2(d,T)(t_1 - t_2 + t_3)}, \tag{289}$$

where

$$t_1 = \frac{1}{T^2}\sum_{j=1}^{T}\sum_{k=1}^{T}\prod_{i=1}^{d}\left[1 - \max(\hat{U}_{ij}, \hat{U}_{ik})\right], \quad t_2 = \frac{2}{T}\frac{1}{2^d}\sum_{j=1}^{T}\prod_{i=1}^{d}\left(1 - \hat{U}_{ij}^2 - \frac{1 - \hat{U}_{ij}}{T}\right), \quad t_3 = \frac{1}{3^d}\left[\frac{(T-1)(2T-1)}{2T^2}\right]^d. \tag{290}$$

- `SW1`, `SWinf` [108, 153, 58]:

$$\hat{I}_{\mathrm{SW1}}\left(\mathbf{Y}_{1:T}\right) = \hat{\sigma} = 12\frac{1}{T^2 - 1}\sum_{i_1=1}^{T}\sum_{i_2=1}^{T}\left|\hat{C}_T\left(\frac{i_1}{T}, \frac{i_2}{T}\right) - \frac{i_1}{T}\frac{i_2}{T}\right|. \tag{291}$$

The $\hat{I}_{\mathrm{SWinf}}$ estimation is performed similarly.

- `QMI_CS_KDE_direct`, `QMI_CS_KDE_iChol`, `QMI_ED_KDE_iChol` [111]:

$$I_{\text{QMI-CS}}\left(\mathbf{y}^1,\mathbf{y}^2\right) = \log\left[\frac{L_1 L_2}{(L_3)^2}\right], \tag{292}$$

$$I_{\text{QMI-ED}}\left(\mathbf{y}^1,\mathbf{y}^2\right) = L_1 + L_2 - 2L_3, \tag{293}$$

$$(\mathbf{K}_m)_{ij} = k_m(\mathbf{y}_i^m, \mathbf{y}_j^m), \tag{294}$$

$$\hat{L}_1^{\text{direct}} = \frac{1}{T^2}\left\langle \mathbf{K}_1\mathbf{K}_2\right\rangle, \tag{295}$$

$$\hat{L}_2^{\text{direct}} = \frac{1}{T^4}\left(\mathbf{1}_T^*\mathbf{K}_1\mathbf{1}\right)\left(\mathbf{1}_T^*\mathbf{K}_2\mathbf{1}\right), \tag{296}$$

$$\hat{L}_3^{\text{direct}} = \frac{1}{T^3}\mathbf{1}_T^*\mathbf{K}_1\mathbf{K}_2\mathbf{1}_T, \tag{297}$$

$$\mathbf{K}_m \approx \mathbf{G}_m\mathbf{G}_m^*, \tag{298}$$

$$\hat{L}_1^{\text{iChol}} = \frac{1}{T^2}\mathbf{1}_{d_1}^*\left(\mathbf{G}_1^*\mathbf{G}_2 \circ \mathbf{G}_1^*\mathbf{G}_2\right)\mathbf{1}_{d_2}, \tag{299}$$

$$\hat{L}_2^{\text{iChol}} = \frac{1}{T^4}\left\|\mathbf{1}_T^*\mathbf{G}_1\right\|_2^2\left\|\mathbf{1}_T^*\mathbf{G}_2\right\|_2^2, \tag{300}$$

$$\hat{L}_3^{\text{iChol}} = \frac{1}{T^3}\left(\mathbf{1}_T^*\mathbf{G}_1\right)\left(\mathbf{G}_1^*\mathbf{G}_2\right)\left(\mathbf{G}_2^*\mathbf{1}_T\right). \tag{301}$$

  - `QMI_CS_KDE_direct`:

$$k_m(\mathbf{u},\mathbf{v}) = \frac{1}{\sqrt{2\pi}\sigma}e^{-\frac{\|\mathbf{u}-\mathbf{v}\|^2}{2\sigma^2}} \quad (\forall m), \tag{302}$$

$$\hat{I}_{\text{QMI-CS}}\left(\mathbf{Y}_{1:T}^1,\mathbf{Y}_{1:T}^2\right) = \log\left[\frac{\hat{L}_1^{\text{direct}}\hat{L}_2^{\text{direct}}}{(\hat{L}_3^{\text{direct}})^2}\right]. \tag{303}$$

$$\tag{304}$$

  - `QMI_CS_KDE_iChol`:

$$k_m(\mathbf{u},\mathbf{v}) = e^{-\frac{\|\mathbf{u}-\mathbf{v}\|^2}{2\sigma^2}} \quad (\forall m), \tag{305}$$

$$\hat{I}_{\text{QMI-CS}}\left(\mathbf{Y}_{1:T}^1,\mathbf{Y}_{1:T}^2\right) = \log\left[\frac{\hat{L}_1^{\text{iChol}}\hat{L}_2^{\text{iChol}}}{(\hat{L}_3^{\text{iChol}})^2}\right]. \tag{306}$$

$$\tag{307}$$

  - `QMI_ED_KDE_iChol`:

$$k_m(\mathbf{u},\mathbf{v}) = \frac{1}{\left(\sqrt{2\pi}\sigma\right)^d}e^{-\frac{\|\mathbf{u}-\mathbf{v}\|^2}{2\sigma^2}} \quad (\forall m), \tag{308}$$

$$\hat{I}_{\text{QMI-ED}}\left(\mathbf{Y}_{1:T}^1,\mathbf{Y}_{1:T}^2\right) = \hat{L}_1^{\text{iChol}} + \hat{L}_2^{\text{iChol}} - 2\hat{L}_3^{\text{iChol}}. \tag{309}$$

- `dCov`, `dCor` [138, 135]: The estimation can be carried out on the basis of the pairwise distances of the sample points:

$$a_{kl} = \left\|\mathbf{y}_k^1 - \mathbf{y}_l^1\right\|_2^\alpha, \quad \bar{a}_{k\cdot} = \frac{1}{T}\sum_{l=1}^T a_{kl}, \quad \bar{a}_{\cdot l} = \frac{1}{T}\sum_{k=1}^T a_{kl}, \quad \bar{a}_{\cdot\cdot} = \frac{1}{T^2}\sum_{k,l=1}^T a_{kl}, \quad A_{kl} = a_{kl} - \bar{a}_{k\cdot} - \bar{a}_{\cdot l} + \bar{a}_{\cdot\cdot}, \tag{310}$$

$$b_{kl} = \left\|\mathbf{y}_k^2 - \mathbf{y}_l^2\right\|_2^\alpha, \quad \bar{b}_{k\cdot} = \frac{1}{T}\sum_{l=1}^T b_{kl}, \quad \bar{b}_{\cdot l} = \frac{1}{T}\sum_{k=1}^T b_{kl}, \quad \bar{b}_{\cdot\cdot} = \frac{1}{T^2}\sum_{k,l=1}^T b_{kl}, \quad B_{kl} = b_{kl} - \bar{b}_{k\cdot} - \bar{b}_{\cdot l} + \bar{b}_{\cdot\cdot}, \tag{311}$$

$$\hat{I}_{\mathrm{dCov}}\left(\mathbf{Y}^1_{1:T},\mathbf{Y}^2_{1:T}\right)=\frac{1}{T}\sqrt{\sum_{k,l=1}^{T}A_{kl}B_{kl}}=\frac{1}{T}\sqrt{\langle\mathbf{A},\mathbf{B}\rangle}, \tag{312}$$

$$\hat{I}_{\mathrm{dVar}}\left(\mathbf{Y}^1_{1:T}\right)=\frac{1}{T}\sqrt{\sum_{k,l=1}^{T}(A_{kl})^2}=\frac{1}{T}\sqrt{\langle\mathbf{A},\mathbf{A}\rangle}, \tag{313}$$

$$\hat{I}_{\mathrm{dVar}}\left(\mathbf{Y}^2_{1:T}\right)=\frac{1}{T}\sqrt{\sum_{k,l=1}^{T}(B_{kl})^2}=\frac{1}{T}\sqrt{\langle\mathbf{B},\mathbf{B}\rangle}, \tag{314}$$

$$\hat{I}_{\mathrm{dCor}}\left(\mathbf{Y}^1_{1:T},\mathbf{Y}^2_{1:T}\right)=\begin{cases}\frac{I_{\mathrm{dCov}}\left(\mathbf{Y}^1_{1:T},\mathbf{Y}^2_{1:T}\right)}{\sqrt{I_{\mathrm{dVar}}\left(\mathbf{Y}^1_{1:T},\mathbf{Y}^1_{1:T}\right)I_{\mathrm{dVar}}\left(\mathbf{Y}^2_{1:T},\mathbf{Y}^2_{1:T}\right)}}, & \text{if } \hat{I}_{\mathrm{dVar}}\left(\mathbf{Y}^1_{1:T},\mathbf{Y}^1_{1:T}\right)I_{\mathrm{dVar}}\left(\mathbf{Y}^2_{1:T},\mathbf{Y}^2_{1:T}\right)>0,\\ 0, & \text{otherwise.}\end{cases} \tag{315}$$

## E.3 Divergence

**Notations**. We have $T_1$ and $T_2$ i.i.d. samples from the two distributions ($f_1$, $f_2$) to be compared: $\mathbf{Y}^1_{1:T_1}=\left(\mathbf{y}^1_1,\ldots,\mathbf{y}^1_{T_1}\right)$, $\mathbf{Y}^2_{1:T_2}=\left(\mathbf{y}^2_1,\ldots,\mathbf{y}^2_{T_2}\right)$ ($\mathbf{y}^i_t\in\mathbb{R}^d$). Let $\rho_k(t)$ denote the Euclidean distance of the $k^{th}$ nearest neighbor of $\mathbf{y}^1_t$ in the sample $\mathbf{Y}^1_{1:T_1}\backslash\{\mathbf{y}^1_t\}$, and similarly let $\nu_k(t)$ stand for the Euclidean distance of the $k^{th}$ nearest neighbor of $\mathbf{y}^1_t$ in the sample $\mathbf{Y}^2_{1:T_2}\backslash\{\mathbf{y}^1_t\}$. Let us recall the definitions [Eq. (61), (63)]:

$$D_{\mathrm{temp1}}(\alpha)=\int_{\mathbb{R}^d}\left[f_1(\mathbf{u})\right]^{\alpha}\left[f_2(\mathbf{u})\right]^{1-\alpha}\mathrm{d}\mathbf{u}, \tag{316}$$

$$D_{\mathrm{temp2}}(a,b)=\int_{\mathbb{R}^d}\left[f_1(\mathbf{u})\right]^{a}\left[f_2(\mathbf{u})\right]^{b}f_1(\mathbf{y})\mathrm{d}\mathbf{u}. \tag{317}$$

The definition of $D_{\mathrm{temp3}}$ is as follows:

$$D_{\mathrm{temp3}}(\alpha)=\int_{\mathbb{R}^d}f_1(\mathbf{u})f_2^{\alpha-1}(\mathbf{u})\mathrm{d}\mathbf{u}. \tag{318}$$

- `L2_kNN_k` [97, 96, 98]:

$$\hat{D}_{\mathrm{L}}\left(\mathbf{Y}^1_{1:T_1},\mathbf{Y}^2_{1:T_2}\right)=\sqrt{\frac{1}{T_1V_d}\sum_{t=1}^{T_1}\left[\frac{k-1}{(T_1-1)\rho_k^d(t)}-\frac{2(k-1)}{T_2\nu_k^d(t)}+\frac{(T_1-1)\rho_k^d(t)(k-2)(k-1)}{(T_2)^2\nu_k^{2d}(t)k}\right]}. \tag{319}$$

- `Tsallis_kNN_k` [97, 96]:

$$B_{k,\alpha}=\frac{\Gamma(k)^2}{\Gamma(k-\alpha+1)\Gamma(k+\alpha-1)}, \tag{320}$$

$$\hat{D}_{\mathrm{temp1}}\left(\alpha;\mathbf{Y}^1_{1:T_1},\mathbf{Y}^2_{1:T_2}\right)=B_{k,\alpha}\frac{(T_1-1)^{1-\alpha}}{(T_2)^{1-\alpha}}\frac{1}{T_1}\sum_{t=1}^{T_1}\left[\frac{\rho_k(t)}{\nu_k(t)}\right]^{d(1-\alpha)}, \tag{321}$$

$$\hat{D}_{\mathrm{T},\alpha}\left(\mathbf{Y}^1_{1:T_1},\mathbf{Y}^2_{1:T_2}\right)=\frac{1}{\alpha-1}\left[\hat{D}_{\mathrm{temp1}}\left(\alpha;\mathbf{Y}^1_{1:T_1},\mathbf{Y}^2_{1:T_2}\right)-1\right]. \tag{322}$$

- `Renyi_kNN_k` [97, 96, 98]:

$$B_{k,\alpha}=\frac{\Gamma(k)^2}{\Gamma(k-\alpha+1)\Gamma(k+\alpha-1)}, \tag{323}$$

$$\hat{D}_{\mathrm{temp1}}\left(\alpha;\mathbf{Y}^1_{1:T_1},\mathbf{Y}^2_{1:T_2}\right)=B_{k,\alpha}\frac{(T_1-1)^{1-\alpha}}{(T_2)^{1-\alpha}}\frac{1}{T_1}\sum_{t=1}^{T_1}\left[\frac{\rho_k(t)}{\nu_k(t)}\right]^{d(1-\alpha)}, \tag{324}$$

$$\hat{D}_{\mathrm{R},\alpha}\left(\mathbf{Y}^1_{1:T_1},\mathbf{Y}^2_{1:T_2}\right)=\frac{1}{\alpha-1}\log\left[\hat{D}_{\mathrm{temp1}}\left(\alpha;\mathbf{Y}^1_{1:T_1},\mathbf{Y}^2_{1:T_2}\right)\right]. \tag{325}$$

- `MMD_Ustat` [36]:

$$k(\mathbf{u},\mathbf{v}) = e^{-\frac{\|\mathbf{u}-\mathbf{v}\|^2}{2\sigma^2}}, \tag{326}$$

$$t_1 = \frac{1}{(T_1)^2}\sum_{i,j=1}^{T_1} k\left(\mathbf{y}_i^1, \mathbf{y}_j^1\right), \tag{327}$$

$$t_2 = \frac{1}{(T_2)^2}\sum_{i,j=1}^{T_2} k\left(\mathbf{y}_i^2, \mathbf{y}_j^2\right), \tag{328}$$

$$t_3 = \frac{2}{T_1 T_2}\sum_{i=1}^{T_1}\sum_{j=1}^{T_2} k\left(\mathbf{y}_i^1, \mathbf{y}_j^2\right), \tag{329}$$

$$\hat{D}_{\mathrm{MMD}}\left(\mathbf{Y}_{1:T_1}^1, \mathbf{Y}_{1:T_2}^2\right) = \sqrt{t_1 + t_2 - t_3}. \tag{330}$$

- `MMD_Vstat` [36]:

$$k(\mathbf{u},\mathbf{v}) = e^{-\frac{\|\mathbf{u}-\mathbf{v}\|^2}{2\sigma^2}}, \tag{331}$$

$$t_1 = \frac{1}{T_1(T_1-1)}\sum_{i=1}^{T_1}\sum_{j=1;j\neq i}^{T_1} k\left(\mathbf{y}_i^1, \mathbf{y}_j^1\right), \tag{332}$$

$$t_2 = \frac{1}{T_2(T_2-1)}\sum_{i=1}^{T_2}\sum_{j=1;j\neq i}^{T_2} k\left(\mathbf{y}_i^2, \mathbf{y}_j^2\right), \tag{333}$$

$$t_3 = \frac{2}{T_1 T_2}\sum_{i=1}^{T_1}\sum_{j=1}^{T_2} k\left(\mathbf{y}_i^1, \mathbf{y}_j^2\right), \tag{334}$$

$$\hat{D}_{\mathrm{MMD}}\left(\mathbf{Y}_{1:T_1}^1, \mathbf{Y}_{1:T_2}^2\right) = \sqrt{t_1 + t_2 - t_3}. \tag{335}$$

- `MMD_online` [36]:

$$T' = \left\lfloor \frac{T_1}{2} \right\rfloor \left( = \left\lfloor \frac{T_2}{2} \right\rfloor \right), \tag{336}$$

$$h((\mathbf{x},\mathbf{y}),(\mathbf{u},\mathbf{v})) = k(\mathbf{x},\mathbf{u}) + k(\mathbf{y},\mathbf{v}) - k(\mathbf{x},\mathbf{v}) - k(\mathbf{y},\mathbf{u}), \tag{337}$$

$$\hat{D}_{\mathrm{MMD}}\left(\mathbf{Y}_{1:T}^1, \mathbf{Y}_{1:T}^2\right) = \frac{1}{T'}\sum_{t=1}^{T'} h\left(\left(\mathbf{y}_{2t-1}^1, \mathbf{y}_{2t-1}^2\right), \left(\mathbf{y}_{2t}^1, \mathbf{y}_{2t}^2\right)\right). \tag{338}$$

  Currently, $k$ is RBF.

- `Hellinger_kNN_k` [92]:

$$B_{k,a,b} = V_d^{-(a+b)}\frac{\Gamma(k)^2}{\Gamma(k-a)\Gamma(k-b)}, \tag{339}$$

$$\hat{D}_{\mathrm{temp2}}\left(a,b;\mathbf{Y}_{1:T_1}^1, \mathbf{Y}_{1:T_2}^2\right) = (T_1-1)^{-a}(T_2)^{-b}B_{k,a,b}\frac{1}{T_1}\sum_{t=1}^{T_1}[\rho_k(t)]^{-da}[\nu_k(t)]^{-db}, \tag{340}$$

$$\hat{D}_{\mathrm{H}}\left(\mathbf{Y}_{1:T_1}^1, \mathbf{Y}_{1:T_2}^2\right) = \sqrt{1 - \hat{D}_{\mathrm{temp2}}\left(-\frac{1}{2},\frac{1}{2};\mathbf{Y}_{1:T_1}^1, \mathbf{Y}_{1:T_2}^2\right)}. \tag{341}$$

- `Bhattacharyya_kNN_k` [8, 92]:

$$B_{k,a,b} = V_d^{-(a+b)} \frac{\Gamma(k)^2}{\Gamma(k-a)\Gamma(k-b)}, \tag{342}$$

$$\hat{D}_{\text{temp2}}\left(a, b; \mathbf{Y}^1_{1:T_1}, \mathbf{Y}^2_{1:T_2}\right) = (T_1-1)^{-a}(T_2)^{-b} B_{k,a,b} \frac{1}{T_1} \sum_{t=1}^{T_1} [\rho_k(t)]^{-da} [\nu_k(t)]^{-db}, \tag{343}$$

$$\hat{D}_{\text{B}}\left(\mathbf{Y}^1_{1:T_1}, \mathbf{Y}^2_{1:T_2}\right) = -\log\left[\hat{D}_{\text{temp2}}\left(-\frac{1}{2}, \frac{1}{2}; \mathbf{Y}^1_{1:T_1}, \mathbf{Y}^2_{1:T_2}\right)\right]. \tag{344}$$

- `KL_kNN_k` [64, 87, 151]:

$$\hat{D}\left(\mathbf{Y}^1_{1:T_1}, \mathbf{Y}^2_{1:T_2}\right) = \frac{d}{T_1} \sum_{t=1}^{T_1} \log\left[\frac{\nu_k(t)}{\rho_k(t)}\right] + \log\left(\frac{T_2}{T_1-1}\right). \tag{345}$$

- `KL_kNN_kiTi` [151]:

$$k_1 = k_1(T_1) = \left\lfloor \sqrt{T_1} \right\rfloor, \tag{346}$$

$$k_2 = k_2(T_2) = \left\lfloor \sqrt{T_2} \right\rfloor, \tag{347}$$

$$\hat{D}\left(\mathbf{Y}^1_{1:T_1}, \mathbf{Y}^2_{1:T_2}\right) = \frac{1}{T_1} \sum_{t=1}^{T_1} \log\left[\frac{k_1}{k_2} \frac{T_2}{T_1-1} \frac{\nu^d_{k_2}(t)}{\rho^d_{k_1}(t)}\right] = \frac{d}{T_1} \sum_{t=1}^{T_1} \log\left[\frac{\nu_{k_2}(t)}{\rho_{k_1}(t)}\right] + \log\left(\frac{k_1}{k_2}\frac{T_2}{T_1-1}\right). \tag{348}$$

- `CS_KDE_iChol`, `ED_KDE_iChol` [111];

$$\mathbf{Z}_{1:2T} = \left[\mathbf{Y}^1_{1:T}, \mathbf{Y}^2_{1:T}\right], \tag{349}$$

$$k(\mathbf{u}, \mathbf{v}) = \frac{1}{\left(\sqrt{2\pi}\sigma\right)^d} e^{\frac{-\|\mathbf{u}-\mathbf{v}\|_2^2}{2\sigma^2}}, \tag{350}$$

$$(\mathbf{K})_{ij} = k(\mathbf{z}_i, \mathbf{z}_j), \tag{351}$$

$$\mathbf{K} = \begin{bmatrix} \mathbf{K}_{11} & \mathbf{K}_{12} \\ \mathbf{K}_{21} & \mathbf{K}_{22} \end{bmatrix} \in \mathbb{R}^{(2T)\times(2T)}, \tag{352}$$

$$\mathbf{K} \approx \mathbf{G}\mathbf{G}^*, \tag{353}$$

$$D_{\text{CS}}(f_1, f_2) = \log\left[\frac{L_1 L_2}{(L_3)^2}\right], \tag{354}$$

$$D_{\text{ED}}(f_1, f_2) = L_1 + L_2 - 2L_3, \tag{355}$$

$$\mathbf{e}_1 = [\mathbf{1}_T; \mathbf{0}_T], \tag{356}$$

$$\mathbf{e}_2 = [\mathbf{0}_T; \mathbf{1}_T], \tag{357}$$

$$\hat{L}_1 = \frac{1}{T^2}(\mathbf{e}_1^*\mathbf{G})(\mathbf{G}^*\mathbf{e}_1), \tag{358}$$

$$\hat{L}_2 = \frac{1}{T^2}(\mathbf{e}_2^*\mathbf{G})(\mathbf{G}^*\mathbf{e}_2), \tag{359}$$

$$\hat{L}_3 = \frac{1}{T^2}(\mathbf{e}_1^*\mathbf{G})(\mathbf{G}^*\mathbf{e}_2), \tag{360}$$

$$\hat{D}_{\text{CS}}\left(\mathbf{Y}^1_{1:T}, \mathbf{Y}^2_{1:T}\right) = \log\left[\frac{\hat{L}_1\hat{L}_2}{(\hat{L}_3)^2}\right], \tag{361}$$

$$\hat{D}_{\text{ED}}\left(\mathbf{Y}^1_{1:T}, \mathbf{Y}^2_{1:T}\right) = \hat{L}_1 + \hat{L}_2 - 2\hat{L}_3. \tag{362}$$

- `EnergyDist` [136, 137]:

$$\hat{D}_{\text{EnDist}}(f_1, f_2) = \frac{2}{T_1 T_2} \sum_{t_1=1}^{T_1}\sum_{t_2=1}^{T_2} \rho\left(\mathbf{y}^1_{t_1}, \mathbf{y}^2_{t_2}\right) - \frac{1}{(T_1)^2} \sum_{t_1=1}^{T_1}\sum_{t_2=1}^{T_1} \rho\left(\mathbf{y}^1_{t_1}, \mathbf{y}^1_{t_2}\right) - \frac{1}{(T_2)^2} \sum_{t_1=1}^{T_2}\sum_{t_2=1}^{T_2} \rho\left(\mathbf{y}^2_{t_1}, \mathbf{y}^2_{t_2}\right). \tag{363}$$

- `Bregman_kNN_k` [11, 23, 64]:

$$\hat{D}_{\text{temp3}}\left(\alpha;\mathbf{Y}^1_{1:T_1},\mathbf{Y}^2_{1:T_2}\right)=\frac{1}{T_1}\sum_{t=1}^{T_1}\left[T_2C_{\alpha,k}V_d\nu_k^d(t)\right]^{1-\alpha}=\frac{T_2^{1-\alpha}C_{\alpha,k}^{1-\alpha}V_d^{1-\alpha}}{T_1}\sum_{t=1}^{T_1}\nu_k^{d(1-\alpha)}(t), \tag{364}$$

$$\hat{D}_{\text{NB},\alpha}\left(\mathbf{Y}^1_{1:T_1},\mathbf{Y}^2_{1:T_2}\right)=\hat{I}_\alpha\left(\mathbf{Y}^2_{1:T_2}\right)+\frac{1}{\alpha-1}\hat{I}_\alpha\left(\mathbf{Y}^1_{1:T_1}\right)-\frac{\alpha}{\alpha-1}\hat{D}_{\text{temp3}}\left(\alpha;\mathbf{Y}^1_{1:T_1},\mathbf{Y}^2_{1:T_2}\right). \tag{365}$$

  where the $I_\alpha$ and the $D_{\text{temp3}}$ quantities are defined in Eq. (183) and Eq. (318).

- `symBregman_kNN_k` [11, 23, 64], via Eq. (59):

$$\hat{D}_{\text{SB},\alpha}\left(\mathbf{Y}^1_{1:T_1},\mathbf{Y}^2_{1:T_2}\right)=\frac{1}{\alpha-1}\left[\hat{I}_\alpha\left(\mathbf{Y}^1_{1:T_1}\right)+\hat{I}_\alpha\left(\mathbf{Y}^2_{1:T_2}\right)-\hat{D}_{\text{temp3}}\left(\alpha;\mathbf{Y}^1_{1:T_1},\mathbf{Y}^2_{1:T_2}\right)-\hat{D}_{\text{temp3}}\left(\alpha;\mathbf{Y}^2_{1:T_2},\mathbf{Y}^1_{1:T_1}\right)\right], \tag{366}$$

  where the $I_\alpha$ and the $D_{\text{temp3}}$ quantities are defined in Eq. (183) and Eq. (318).

## E.4 Association Measures

**Notations**. We are given $T$ samples from the random variable $\mathbf{y}\in\mathbb{R}^d$ ($\mathbf{Y}_{1:T}=(\mathbf{y}_1,\dots,\mathbf{y}_T)$) and our goal is to estimate the association of its $d_m$-dimensional components ($\mathbf{y}=\left[\mathbf{y}^1;\dots;\mathbf{y}^M\right]$, $\mathbf{y}^m\in\mathbb{R}^{d_m}$).

- `Spearman1`, `Spearman2`, `Spearman3` [117, 153, 78, 105, 52, 80, 79, 106]: One can arrive at explicit formulas by substituting the empirical copula of $\mathbf{y}$ ($\hat{C}_T$, see Eq. (275)) to the definitions of $\hat{A}_{\rho_i}$-s ($i=1,2,3$; see Eqs. (69), (71), (72)). The resulting nonparametric estimators are

$$\hat{A}_{\rho_1}(\mathbf{Y}_{1:T})=\hat{A}_{\rho_1}(\hat{C}_T)=h_\rho(d)\left[2^d\int_{[0,1]^d}\hat{C}_T(\mathbf{u})\mathrm{d}\mathbf{u}-1\right]=h_\rho(d)\left[\frac{2^d}{T}\sum_{j=1}^{T}\prod_{i=1}^{d}(1-\hat{U}_{ij})-1\right], \tag{367}$$

$$\hat{A}_{\rho_2}(\mathbf{Y}_{1:T})=\hat{A}_{\rho_2}(\hat{C}_T)=h_\rho(d)\left[2^d\int_{[0,1]^d}\Pi(\mathbf{u})\mathrm{d}\hat{C}_T(\mathbf{u})-1\right]=h_\rho(d)\left[\frac{2^d}{T}\sum_{j=1}^{T}\prod_{i=1}^{d}\hat{U}_{ij}-1\right], \tag{368}$$

$$\hat{A}_{\rho_3}(\mathbf{Y}_{1:T})=\hat{A}_{\rho_3}(\hat{C}_T)=\frac{\hat{A}_{\rho_1}(\mathbf{Y}_{1:T})+\hat{A}_{\rho_2}(\mathbf{Y}_{1:T})}{2}, \tag{369}$$

  where $h_\rho(d)$ and $\hat{U}_{ij}$ are defined in Eq. (70) and Eq. (273), respectively.

- `Spearman4` [57, 105]:

$$\hat{A}_{\rho_4}(\mathbf{Y}_{1:T})=\hat{A}_{\rho_4}(\hat{C}_T)=\frac{12}{T}\binom{d}{2}^{-1}\sum_{k,l=1;k<l}^{d}\sum_{j=1}^{T}(1-\hat{U}_{kj})(1-\hat{U}_{lj})-3, \tag{370}$$

  where $\hat{U}_{kj}$ and $\hat{U}_{lj}$ are defined in Eq. (273).

- `CorrEntr_KDE_direct` [100]:

$$k(u,v)=e^{-\frac{(u-v)^2}{2\sigma^2}}, \tag{371}$$

$$\mathbf{Y}_{1:T}=\left[\mathbf{y}^1_{1:T};\mathbf{y}^2_{1:T}\right],\quad(\mathbf{y}^i_{1:T}\in\mathbb{R}^{1\times T}) \tag{372}$$

$$\hat{A}_{\text{CorrEntr}}\left(\mathbf{Y}_{1:T}\right)=\frac{1}{T}\sum_{t=1}^{T}k\left(y_t^1,y_t^2\right). \tag{373}$$

- `CCorrEntr_KDE_iChol` [100, 111]:

$$k(u,v) = e^{-\frac{(u-v)^2}{2\sigma^2}}, \tag{374}$$
$$\mathbf{Y}_{1:T} = \left[\mathbf{y}^1_{1:T}; \mathbf{y}^2_{1:T}\right], \quad (\mathbf{y}^i_{1:T} \in \mathbb{R}^{1\times T}) \tag{375}$$
$$\mathbf{Z}_{1:2T} = \left[\mathbf{y}^1_{1:T}, \mathbf{y}^2_{1:T}\right], \tag{376}$$
$$(\mathbf{K})_{ij} = k(\mathbf{z}_i, \mathbf{z}_j), \tag{377}$$
$$\mathbf{K} = \begin{bmatrix} \mathbf{K}_{11} & \mathbf{K}_{12} \\ \mathbf{K}_{21} & \mathbf{K}_{22} \end{bmatrix} \in \mathbb{R}^{(2T)\times(2T)}, \tag{378}$$
$$\mathbf{K} \approx \mathbf{G}\mathbf{G}^*, \tag{379}$$
$$\mathbf{e}_1 = [\mathbf{1}_T; \mathbf{0}_T], \tag{380}$$
$$\mathbf{e}_2 = [\mathbf{0}_T; \mathbf{1}_T], \tag{381}$$
$$L = \sum_{t_1=1}^{T}\sum_{t_2=1}^{T} k\left(y^1_{t_1}, y^2_{t_2}\right), \tag{382}$$
$$\hat{L} = \frac{1}{T^2}(\mathbf{e}_1^*\mathbf{G})(\mathbf{G}^*\mathbf{e}_2), \tag{383}$$
$$\hat{A}_{\mathrm{CCorrEntr}}\left(\mathbf{Y}_{1:T}\right) = \frac{1}{T}\sum_{t=1}^{T} k\left(y^1_t, y^2_t\right) - \frac{\hat{L}}{T^2}. \tag{384}$$

- `CCorrEntr_KDE_Lapl` [100, 16]:

$$k(u,v) = e^{-\frac{|u-v|}{\sigma}}, \tag{385}$$
$$\mathbf{Y}_{1:T} = \left[\mathbf{y}^1_{1:T}; \mathbf{y}^2_{1:T}\right], \quad (\mathbf{y}^i_{1:T} \in \mathbb{R}^{1\times T}) \tag{386}$$
$$L = \sum_{t_1=1}^{T}\sum_{t_2=1}^{T} k\left(y^1_{t_1}, y^2_{t_2}\right) = \sum_{t_1=1}^{T}\sum_{t_2=1}^{T} e^{-\frac{\left|y^1_{t_1} - y^2_{t_2}\right|}{\sigma}} \tag{387}$$
$$= \sum_{t_1=1}^{T}\left[e^{-\frac{y^1_{t_1}}{\sigma}} \sum_{\{t_2: y^2_{t_2} \le y^1_{t_1}\}} e^{\frac{y^2_{t_2}}{\sigma}} + e^{\frac{y^1_{t_1}}{\sigma}} \sum_{\{t_2: y^2_{t_2} > y^1_{t_1}\}} e^{-\frac{y^2_{t_2}}{\sigma}}\right] = [16], \tag{388}$$
$$\hat{A}_{\mathrm{CCorrEntr}}\left(\mathbf{Y}_{1:T}\right) = \frac{1}{T}\sum_{t=1}^{T} k\left(y^1_t, y^2_t\right) - \frac{L}{T^2}. \tag{389}$$

- `CorrEntrCoeff_KDE_direct` [100]:

$$k(u,v) = e^{-\frac{(u-v)^2}{2\sigma^2}}, \tag{390}$$
$$\mathbf{Y}_{1:T} = \left[\mathbf{y}^1_{1:T}; \mathbf{y}^2_{1:T}\right], \quad (\mathbf{y}^i_{1:T} \in \mathbb{R}^{1\times T}) \tag{391}$$
$$C = \frac{1}{T}\sum_{t=1}^{T} k\left(y^1_t, y^2_t\right), \tag{392}$$
$$\hat{A}_{\mathrm{CorrEntrCoeff}}\left(\mathbf{Y}_{1:T}\right) = \frac{C - \frac{\mathbf{1}_T^*\mathbf{K}_{12}\mathbf{1}_T}{T^2}}{\sqrt{\left(1 - \frac{\mathbf{1}_T^* K_{11}\mathbf{1}_T}{T^2}\right)\left(1 - \frac{\mathbf{1}_T^* K_{22}\mathbf{1}_T}{T^2}\right)}}. \tag{393}$$

- `CorrEntrCoeff_KDE_iChol` [100, 111]:

$$\mathbf{Y}_{1:T} = \left[\mathbf{y}^1_{1:T}; \mathbf{y}^2_{1:T}\right], \quad (\mathbf{y}^i_{1:T} \in \mathbb{R}^{1\times T}) \tag{394}$$

$$\mathbf{Z}_{1:2T} = \left[\mathbf{y}^1_{1:T}, \mathbf{y}^2_{1:T}\right], \tag{395}$$

$$k(u,v) = e^{-\frac{(u-v)^2}{2\sigma^2}}, \tag{396}$$

$$(\mathbf{K})_{ij} = k(\mathbf{z}_i, \mathbf{z}_j), \tag{397}$$

$$\mathbf{K} = \begin{bmatrix} \mathbf{K}_{11} & \mathbf{K}_{12} \\ \mathbf{K}_{21} & \mathbf{K}_{22} \end{bmatrix} \in \mathbb{R}^{(2T)\times(2T)}, \tag{398}$$

$$\mathbf{K} \approx \mathbf{G}\mathbf{G}^*, \tag{399}$$

$$C = \frac{1}{T}\sum_{t=1}^{T} k\left(y^1_t, y^2_t\right), \tag{400}$$

$$\mathbf{e}_1 = [\mathbf{1}_T; \mathbf{0}_T]/T, \tag{401}$$

$$\mathbf{e}_2 = [\mathbf{0}_T; \mathbf{1}_T]/T, \tag{402}$$

$$\hat{A}_{\text{CorrEntrCoeff}}\left(\mathbf{Y}_{1:T}\right) = \frac{C - (\mathbf{e}_2^*\mathbf{G})(\mathbf{G}^*\mathbf{e}_1)}{\sqrt{\left[1-(\mathbf{e}_1^*\mathbf{G})(\mathbf{G}^*\mathbf{e}_1)\right]\left[1-(\mathbf{e}_2^*\mathbf{G})(\mathbf{G}^*\mathbf{e}_2)\right]}}. \tag{403}$$

- `Blomqvist` [145, 106]: The empirical estimation of the survival function $\bar{C}$ is

$$\hat{\bar{C}}_T(\mathbf{u}) = \frac{1}{T}\sum_{t=1}^{T}\prod_{i=1}^{d}\mathbb{I}_{\{\hat{U}_{it}>u_i\}}, \quad (\mathbf{u} = [u_1;\ldots;u_d] \in [0,1]^d). \tag{404}$$

The estimation of Blomqvist's $\beta$ is computed as

$$\mathbf{1/2} = \left[\frac{1}{2};\ldots;\frac{1}{2}\right] \in \mathbb{R}^d, \tag{405}$$

$$h_\beta(d) = \frac{2^{d-1}}{2^{d-1}-1}, \tag{406}$$

$$A_\beta\left(y^1,\ldots,y^d\right) = A_\beta(C) = h_\beta(d)\left[\hat{C}_T(\mathbf{1/2}) + \hat{\bar{C}}_T(\mathbf{1/2}) - 2^{1-d}\right]. \tag{407}$$

- `Spearman_lt` [104]:

$$\hat{A}_{\rho_{\text{lt}}}(\mathbf{Y}_{1:T}) = \hat{A}_{\rho_{\text{lt}}}(\hat{C}_T) = \frac{\frac{1}{T}\sum_{j=1}^{T}\prod_{i=1}^{d}(p-\hat{U}_{ij})^+ - \left(\frac{p^2}{2}\right)^d}{\frac{p^{d+1}}{d+1} - \left(\frac{p^2}{2}\right)^d}, \tag{408}$$

where $\hat{U}_{ij}$ is defined in Eq. (273) and $z^+ = \max(z, 0)$.

- `Spearman_L` [104]:

$$k = k(T) = \left\lfloor\sqrt{T}\right\rfloor, \tag{409}$$

$$\hat{A} = \hat{A}_{\rho_{\text{lt}}}(\mathbf{Y}_{1:T}) = \hat{A}_{\rho_{\text{lt}}}(\hat{C}_T) \text{ with } p = \frac{k}{T} \text{ in Eq. (408)}, \tag{410}$$

$$\hat{A}_{\rho_{\text{L}}}(\mathbf{Y}_{1:T}) = \hat{A}_{\rho_{\text{L}}}(\hat{C}_T) = \hat{A}. \tag{411}$$

- `Spearman_ut` [104]: For the estimation we need three quantities, that we provide below (they were not computed in

[104]):

$$\int_{[1-p,1]^d} \hat{C}_T(\mathbf{u})\mathrm{d}\mathbf{u} = \frac{1}{T}\sum_{j=1}^{T}\prod_{i=1}^{d}\left[1-\max(\hat{U}_{ij},1-p)\right] =: c, \tag{412}$$

$$\int_{[1-p,1]^d} \Pi(\mathbf{u})\mathrm{d}\mathbf{u} = \left[\frac{p(2-p)}{2}\right]^d =: c_1(p,d), \tag{413}$$

$$\int_{[1-p,1]^d} M(\mathbf{u})\mathrm{d}\mathbf{u} = \frac{p^d(d+1-pd)}{d+1} =: c_2(p,d), \tag{414}$$

where $\hat{U}_{ij}$ is defined in Eq. (273). Having these expressions at hand, the estimation can be simply written as [see Eq. (85)]:

$$\hat{A}_{\rho_{\mathrm{ut}}}(\mathbf{Y}_{1:T}) = \hat{A}_{\rho_{\mathrm{ut}}}(\hat{C}_T) = \frac{c-c_1(p,d)}{c_2(p,d)-c_1(p,d)}. \tag{415}$$

- `Spearman_U` [104]:

$$k = k(T) = \left\lfloor \sqrt{T} \right\rfloor, \tag{416}$$

$$\hat{A} = \hat{A}_{\rho_{\mathrm{ut}}}(\mathbf{Y}_{1:T}) = \hat{A}_{\rho_{\mathrm{ut}}}(\hat{C}_T) \text{ with } p = \frac{k}{T} \text{ in Eq. (415)}, \tag{417}$$

$$\hat{A}_{\rho_{\mathrm{U}}}(\mathbf{Y}_{1:T}) = \hat{A}_{\rho_{\mathrm{U}}}(\hat{C}_T) = \hat{A}. \tag{418}$$

## E.5 Cross Quantities

**Notations**. We have $T_1$ and $T_2$ i.i.d. samples from the two distributions $(f_1,\ f_2)$ to be compared: $\mathbf{Y}^1_{1:T_1} = \left(\mathbf{y}^1_1,\dots,\mathbf{y}^1_{T_1}\right)$, $\mathbf{Y}^2_{1:T_2} = \left(\mathbf{y}^2_1,\dots,\mathbf{y}^2_{T_2}\right)$ $(\mathbf{y}^i_t \in \mathbb{R}^d)$. Let $\nu_k(t)$ denote the Euclidean distance of the $k^{th}$ nearest neighbor of $\mathbf{y}^1_t$ in the sample $\mathbf{Y}^2_{1:T_2}\backslash\{\mathbf{y}^1_t\}$.

- `CE_kNN_k` [64]:

$$\hat{C}_{\mathrm{CE}}\left(\mathbf{Y}^1_{1:T_1},\mathbf{Y}^2_{1:T_2}\right) = \log(V_d)+\log(T_2)-\psi(k)+\frac{d}{T_1}\sum_{t=1}^{T_1}\log\left[\nu_k(t)\right]. \tag{419}$$

## E.6 Kernels on Distributions

**Notations**. We have $T_1$ and $T_2$ i.i.d. samples from the two distributions $(f_1,\ f_2)$ whose similarity (kernel value) is to be estimated: $\mathbf{Y}^1_{1:T_1} = \left(\mathbf{y}^1_1,\dots,\mathbf{y}^1_{T_1}\right)$, $\mathbf{Y}^2_{1:T_2} = \left(\mathbf{y}^2_1,\dots,\mathbf{y}^2_{T_2}\right)$ $(\mathbf{y}^i_t \in \mathbb{R}^d)$. Let $\rho_k(t)$ denote the Euclidean distance of the $k^{th}$ nearest neighbor of $\mathbf{y}^1_t$ in the sample $\mathbf{Y}^1_{1:T_1}\backslash\{\mathbf{y}^1_t\}$, and similarly let $\nu_k(t)$ stand for the Euclidean distance of the $k^{th}$ nearest neighbor of $\mathbf{y}^1_t$ in the sample $\mathbf{Y}^2_{1:T_2}\backslash\{\mathbf{y}^1_t\}$.

- '`expected`' [76]:

$$\hat{K}_{\exp}\left(\mathbf{Y}^1_{1:T_1},\mathbf{Y}^2_{1:T_2}\right) = \frac{1}{T_1T_2}\sum_{i=1}^{T_1}\sum_{j=1}^{T_2}k\left(\mathbf{y}^1_i,\mathbf{y}^2_j\right). \tag{420}$$

- '`Bhattacharyya_kNN_k`' [8, 50, 92]:

$$B_{k,a,b} = V_d^{-(a+b)}\frac{\Gamma(k)^2}{\Gamma(k-a)\Gamma(k-b)}, \tag{421}$$

$$\hat{D}_{\mathrm{temp2}}\left(a,b;\mathbf{Y}^1_{1:T_1},\mathbf{Y}^2_{1:T_2}\right) = (T_1-1)^{-a}(T_2)^{-b}B_{k,a,b}\frac{1}{T_1}\sum_{t=1}^{T_1}[\rho_k(t)]^{-da}[\nu_k(t)]^{-db}, \tag{422}$$

$$\hat{K}_{\mathrm{B}}\left(\mathbf{Y}^1_{1:T_1},\mathbf{Y}^2_{1:T_2}\right) = \hat{D}_{\mathrm{temp2}}\left(-\frac{1}{2},\frac{1}{2};\mathbf{Y}^1_{1:T_1},\mathbf{Y}^2_{1:T_2}\right). \tag{423}$$

- 'PP_kNN_k' [50, 92]:

$$B_{k,a,b} = V_d^{-(a+b)} \frac{\Gamma(k)^2}{\Gamma(k-a)\Gamma(k-b)}, \tag{424}$$

$$\hat{D}_{\text{temp2}}\left(a, b; \mathbf{Y}_{1:T_1}^1, \mathbf{Y}_{1:T_2}^2\right) = (T_1 - 1)^{-a}(T_2)^{-b} B_{k,a,b} \frac{1}{T_1} \sum_{t=1}^{T_1} [\rho_k(t)]^{-da} [\nu_k(t)]^{-db}, \tag{425}$$

$$\hat{K}_{\text{PP}}\left(\mathbf{Y}_{1:T_1}^1, \mathbf{Y}_{1:T_2}^2\right) = \hat{D}_{\text{temp2}}\left(\rho - 1, \rho; \mathbf{Y}_{1:T_1}^1, \mathbf{Y}_{1:T_2}^2\right). \tag{426}$$

# References


[1] Dimitris Achlioptas. Database-friendly random projections: Johnson-Lindenstrauss with binary coins. *Journal of Computer and System Sciences*, 66:671–687, 2003.

[2] S. M. Ali and S. D. Silvey. A general class of coefficients of divergence of one distribution from another. *Journal of the Royal Statistical Society, Series B*, 28:131–142, 1966.

[3] Shun-ichi Amari, Andrzej Cichocki, and Howard H. Yang. A new learning algorithm for blind signal separation. *Advances in Neural Information Processing Systems (NIPS)*, pages 757–763, 1996.

[4] Rosa I. Arriga and Santosh Vempala. An algorithmic theory of learning: Robust concepts and random projections. *Machine Learning*, 63:161–182, 2006.

[5] Francis R. Bach and Michael I. Jordan. Kernel independent component analysis. *Journal of Machine Learning Research*, 3:1–48, 2002.

[6] Michéle. Basseville. Divergence measures for statistical data processing - an annotated bibliography. *Signal Processing*, 2012. To appear. `hal.inria.fr/docs/00/54/23/37/PDF/PI-1961.pdf`.

[7] J. Beirlant, E.J. Dudewicz, L. Győrfi, and E.C. van der Meulen. Nonparametric entropy estimation: An overview. *International Journal of Mathematical and Statistical Sciences*, 6:17–39, 1997.

[8] Anil K. Bhattacharyya. On a measure of divergence between two statistical populations defined by their probability distributions. *Bulletin of the Calcutta Mathematical Society*, 35:99–109, 1943.

[9] Ella Bingham and Aapo Hyvärinen. A fast fixed-point algorithm for independent component analysis of complex-valued signals. *International Journal of Neural Systems*, 10(1):1–8, 2000.

[10] Nils Blomqvist. On a measure of dependence between two random variables. *The Annals of Mathematical Statistics*, 21:593–600, 1950.

[11] Lev M. Bregman. The relaxation method of finding the common points of convex sets and its application to the solution of problems in convex programming. *USSR Computational Mathematics and Mathematical Physics*, 7:200–217, 1967.

[12] J. Burbea and C.R. Rao. On the convexity of some divergence measures based on entropy functions. *IEEE Transactions on Information Theory*, 28:489–495, 1982.

[13] Jean-François Cardoso. Multidimensional independent component analysis. In *International Conference on Acoustics, Speech, and Signal Processing (ICASSP)*, pages 1941–1944, 1998.

[14] Jean-François Cardoso and Beate Hvam Laheld. Equivariant adaptive source separation. *IEEE Transactions on Signal Processing*, 44:3017–3030, 1996.

[15] Jean-François Cardoso and Antoine Souloumiac. Blind beamforming for non-gaussian signals. *IEE Proceedings F, Radar and Signal Processing*, 140(6):362–370, 1993.

[16] Aiyou Chen. Fast kernel density independent component analysis. In *Independent Component Analysis and Blind Signal Separation (ICA)*, pages 24–31, 2006.

[17] Pierre Comon. Independent component analysis, a new concept? *Signal Processing*, 36:287–314, 1994.

[18] Juan C. Correa. A new estimator of entropy. *Communications in Statistics - Theory and Methods*, 24:2439–2449, 1995.

[19] Jose A. Costa and Alfred O. Hero. Geodesic entropic graphs for dimension and entropy estimation in manifold learning. *IEEE Transactions on Signal Processing*, 52:2210–2221, 2004.

[20] Timothee Cour, Stella Yu, and Jianbo Shi. Normalized cut segmentation code. Copyright 2004 University of Pennsylvania, Computer and Information Science Department.

[21] Thomas M. Cover and Joy A. Thomas. *Elements of Information Theory*. John Wiley and Sons, New York, USA, 1991.

[22] Imre Csiszár. Eine informationstheoretische ungleichung und ihre anwendung auf den beweis der ergodizitat von markoffschen ketten. *Publications of the Mathematical Institute of Hungarian Academy of Sciences*, 8:85–108, 1963.

[23] Imre Csiszár. Generalized projections for non-negative functions. *Acta Mathematica Hungarica*, 68:161–185, 1995.

[24] Lieven De Lathauwer, Bart De Moor, and Joos Vandewalle. Fetal electrocardiogram extraction by source subspace separation. In *IEEE SP/Athos Workshop on Higher-Order Statistics*, pages 134–138, 1995.

[25] Ali Dolati and Manuel Úbeda-Flores. On measures of multivariate concordance. *Journal of Probability and Statistical Science*, 4:147–164, 2006.

[26] Nader Ebrahimi, Kurt Pflughoeft, and Ehsan S. Soofi. Two measures of sample entropy. *Statistics and Probability Letters*, 20:225–234, 1994.

[27] Dominik M. Endres and Johannes E. Schindelin. A new metric for probability distributions. *IEEE Transactions on Information Theory*, 49:1858–1860, 2003.

[28] Jan Eriksson. Complex random vectors and ICA models: Identifiability, uniqueness and separability. *IEEE Transactions on Information Theory*, 52(3), 2006.

[29] Bert Van Es. Estimating functionals related to a density by a class of statistics based on spacings. *Scandinavian Journal of Statistics*, 19:61–72, 1992.

[30] Kai-Tai Fang, Samuel Kotz, and Kai Wang Ng. *Symmetric multivariate and related distributions*. Chapman and Hall, 1990.

[31] Peter Frankl and Hiroshi Maehara. The Johnson-Lindenstrauss Lemma and the sphericity of some graphs. *Journal of Combinatorial Theory Series A*, 44(3):355 – 362, 1987.

[32] Wayne A. Fuller. *Introduction to Statistical Time Series*. Wiley-Interscience, 1995.

[33] Sandra Gaißer, Martin Ruppert, and Friedrich Schmid. A multivariate version of Hoeffding's phi-square. *Journal of Multivariate Analysis*, 101:2571–2586, 2010.

[34] M. N. Goria, Nikolai N. Leonenko, V. V. Mergel, and P. L. Novi Inverardi. A new class of random vector entropy estimators and its applications in testing statistical hypotheses. *Journal of Nonparametric Statistics*, 17:277–297, 2005.

[35] Arthur Gretton, Karsten M. Borgwardt, Malte Rasch, Bernhard Schölkopf, and Alexander J. Smola. A kernel method for the two sample problem. In *Advances in Neural Information Processing Systems (NIPS)*, pages 513–520, 2007.

[36] Arthur Gretton, Karsten M. Borgwardt, Malte J. Rasch, Bernhard Schölkopf, and Alexander Smola. A kernel two-sample test. *Journal of Machine Learning Research*, 13:723–773, 2012.

[37] Arthur Gretton, Olivier Bousquet, Alexander Smola, and Bernhard Schölkopf. Measuring statistical dependence with Hilbert-Schmidt norms. In *International Conference on Algorithmic Learnng Theory (ALT)*, pages 63–78, 2005.

[38] A.B. Hamza and H. Krim. Jensen-Rényi divergence measure: theoretical and computational perspectives. In *IEEE International Symposium on Information Theory (ISIT)*, page 257, 2003.

[39] Godfrey H. Hardy and Srinivasa I. Ramanujan. Asymptotic formulae in combinatory analysis. *Proceedings of the London Mathematicl Society*, 17(1):75–115, 1918.

[40] Jan Havrda and František Charvát. Quantification method of classification processes. concept of structural $\alpha$-entropy. *Kybernetika*, 3:30–35, 1967.

[41] Matthias Hein and Olivier Bousquet. Hilbertian metrics and positive definite kernels on probability measures. In *International Conference on Artificial Intelligence and Statistics (AISTATS)*, pages 136–143, 2005.

[42] Nadine Hilgert and Bruno Portier. Strong uniform consistency and asymptotic normality of a kernel based error density estimator in functional autoregressive models. *Statistical Inference for Stochastic Processes*, 15(2):105–125, 2012.

[43] W. Hoeffding. Massstabinvariante korrelationstheorie. *Schriften des Mathematischen Seminars und des Instituts für Angewandte Mathematik der Universität Berlin*, 5:181–233, 1940.

[44] Harold Hotelling. Analysis of a complex of statistical variables into principal components. *Journal of Educational Psychology*, 24:417–441, 1933.

[45] Marc Van Hulle. Edgeworth approximation of multivariate differential entropy. *Neural Computation*, 17:1903–1910, 2005.

[46] Aapo Hyvärinen. New approximations of differential entropy for independent component analysis and projection pursuit. In *Advances in Neural Information Processing Systems (NIPS)*, pages 273–279, 1997.

[47] Aapo Hyvärinen. Independent component analysis for time-dependent stochastic processes. In *International Conference on Artificial Neural Networks (ICANN)*, pages 541–546, 1998.

[48] Aapo Hyvärinen and Erkki Oja. A fast fixed-point algorithm for independent component analysis. *Neural Computation*, 9(7):1483–1492, 1997.

[49] Piotr Indyk and Rajeev Motwani. Approximate nearest neighbors: Towards removing the curse of dimensionality. In *ACM Symposium on Theory of Computing, 1998*, pages 604–613.

[50] Tony Jebara, Risi Kondor, and Andrew Howard. Probability product kernels. *Journal of Machine Learning Research*, 5:819–844, 2004.

[51] Miguel Jerez, Jose Casals, and Sonia Sotoca. *Signal Extraction for Linear State-Space Models: Including a free MATLAB Toolbox for Time Series Modeling and Decomposition.* LAP LAMBERT Academic Publishing, 2011.

[52] Harry Joe. Multivariate concordance. *Journal of Multivariate Analysis*, 35:12–30, 1990.

[53] William B. Johnson and Joram Lindenstrauss. Extensions of Lipschitz maps into a Hilbert space. *Contemporary Mathematics*, 26:189–206, 1984.

[54] Christian Jutten and Jeanny Hérault. Blind separation of sources: An adaptive algorithm based on neuromimetic architecture. *Signal Processing*, 24:1–10, 1991.

[55] Christian Jutten and Juha Karhunen. Advances in blind source separation (BSS) and independent component analysis (ICA) for nonlinear systems. *International Journal of Neural Systems*, 14(5):267–292, 2004.

[56] K. Rao Kadiyala and Sune Karlsson. Numerical methods for estimation and inference in bayesian VAR-models. *Journal of Applied Econometrics*, 12:99–132, 1997.

[57] Maurice G. Kendall. *Rank correlation methods.* London, Griffin, 1970.

[58] Sergey Kirshner and Barnabás Póczos. ICA and ISA using Schweizer-Wolff measure of dependence. In *International Conference on Machine Learning (ICML)*, pages 464–471, 2008.

[59] L. F. Kozachenko and Nikolai N. Leonenko. A statistical estimate for the entropy of a random vector. *Problems of Information Transmission*, 23:9–16, 1987.

[60] Solomon Kullback and Richard Leibler. On information and sufficiency. *Annals of Mathematical Statistics*, 22(1):79–86, 1951.

[61] Jan Kybic. High-dimensional mutual information estimation for image registration. In *International Conference on Image Processing (ICIP)*, pages 1779–1782, 2004.

[62] Russell H. Lambert. *Multichannel Blind Deconvolution: FIR matrix algebra and separation of multipath mixtures*. PhD thesis, University of Southern California, 1996.

[63] Erik Learned-Miller and III. John W. Fisher. ICA using spacings estimates of entropy. *Journal of Machine Learning Research*, 4:1271–1295, 2003.

[64] Nikolai Leonenko, Luc Pronzato, and Vippal Savani. A class of Rényi information estimators for multidimensional densities. *Annals of Statistics*, 36(5):2153–2182, 2008.

[65] Ping Li, Trevor J. Hastie, and Kenneth W. Hastie. Very sparse random projections. In *International Conference on Knowledge Discovery and Data Mining (KDD)*, pages 287–296, 2006.

[66] Jianhua Lin. Divergence measures based on the Shannon entropy. *IEEE Transactions on Information Theory*, 37:145–151, 1991.

[67] Weifeng Liu, P.P. Pokharel, and José C. Príncipe. Correntropy: Properties and applications in non-Gaussian signal processing. *IEEE Transactions on Signal Processing*, 55:5286 – 5298, 2007.

[68] Edward Norton Lorenz. Deterministic nonperiodic flow. *Journal of Atmospheric Sciences*, 20:130–141, 1963.

[69] Russell Lyons. istance covariance in metric spaces. *Annals of Probability*, 2012. (To appear. `http://php.indiana.edu/~rdlyons/pdf/dcov.pdf`).

[70] André F. T. Martins, Pedro M. Q. Aguiar, and Mário A. T. Figueiredo. Tsallis kernels on measures. In *Information Theory Workshop (ITW)*, pages 298–302, 2008.

[71] André F. T. Martins, Noah A. Smith, Eric P. Xing, Pedro M. Q. Aguiar, and Mário A. T. Figueiredo. Nonextensive information theoretical kernels on measures. *Journal of Machine Learning Research*, 10:935–975, 2009.

[72] Jiří Matoušek. On variants of the Johnson-Lindenstrauss lemma. *Random Structures and Algorithms*, 33(2):142–156, 2008.

[73] Erik Miller. A new class of entropy estimators for multi-dimensional densities. In *International Conference on Acoustics, Speech, and Signal Processing (ICASSP)*, pages 297–300, 2003.

[74] Tetsuzo Morimoto. Markov processes and the H-theorem. *Journal of the Physical Society of Japan*, 18:328–331, 1963.

[75] Frederick Mosteller. On some useful "inefficient" statistics. *Annals of Mathematical Statistics*, 17:377–408, 1946.

[76] Krikamol Muandet, Kenji Fukumizu, Francesco Dinuzzo, and Bernhard Schölkopf. Learning from distributions via support measure machines. In *Advances in Neural Information Processing Systems (NIPS)*, pages 10–18, 2011.

[77] Alfred Müller. Integral probability metrics and their generating classes of functions. *Advances in Applied Probability*, 29:429–443, 1997.

[78] Roger B. Nelsen. Nonparametric measures of multivariate association. *Lecture Notes-Monograph Series, Distributions with Fixed Marginals and Related Topics*, 28:223–232, 1996.

[79] Roger B. Nelsen. *Distributions with Given Marginals and Statistical Modelling*, chapter Concordance and copulas: A survey, pages 169–178. Kluwer Academic Publishers, Dordrecht, 2002.

[80] Roger B. Nelsen. *An Introduction to Copulas (Springer Series in Statistics)*. Springer, 2006.

[81] Arnold Neumaier and Tapio Schneider. Estimation of parameters and eigenmodes of multivariate autoregressive models. *ACM Transactions on Mathematical Software*, 27(1):27–57, 2001.

[82] Andrew Y. Ng, Michael I. Jordan, and Yair Weiss. On spectral clustering: analysis and an algorithm. In *Advances in Neural Information Processing Systems (NIPS)*, pages 849–856, 2002.

[83] Hadi Alizadeh Noughabi and Naser Reza Arghami. A new estimator of entropy. *Journal of Iranian Statistical Society*, 9:53–64, 2010.

[84] Umut Ozertem, Ismail Uysal, and Deniz Erdogmus. Continuously differentiable sample-spacing entropy estimation. *IEEE Transactions on Neural Networks*, 19:1978–1984, 2008.

[85] Jason A. Palmer and Scott Makeig. Contrast functions for independent subspace analysis. In *International conference on Latent Variable Analysis and Signal Separation (LVA/ICA)*, pages 115–122, 2012.

[86] Michael S. Pedersen, Jan Larsen, Ulrik Kjems, and Lucas C. Parra. A survey of convolutive blind source separation methods. In *Springer Handbook of Speech Processing*. Springer, 2007.

[87] Fernando Pérez-Cruz. Estimation of information theoretic measures for continuous random variables. In *Advances in Neural Information Processing Systems (NIPS)*, pages 1257–1264, 2008.

[88] Barnabás Póczos, Zoubin Ghahramani, and Jeff Schneider. Copula-based kernel dependency measures. In *International Conference on Machine Learning (ICML)*, 2012.

[89] Barnabás Póczos and András Lőrincz. Identification of recurrent neural networks by Bayesian interrogation techniques. *Journal of Machine Learning Research*, 10:515–554, 2009.

[90] Barnabás Póczos, Zoltán Szabó, Melinda Kiszlinger, and András Lőrincz. Independent process analysis without a priori dimensional information. In *International Conference on Independent Component Analysis and Signal Separation (ICA)*, pages 252–259, 2007.

[91] Barnabás Póczos, Bálint Takács, and András Lőrincz. Independent subspace analysis on innovations. In *European Conference on Machine Learning (ECML)*, pages 698–706, 2005.

[92] Barnabás Póczos, Liang Xiong, Dougal Sutherland, and Jeff Schneider. Support distribution machines. Technical report, Carnegie Mellon University, 2012. `http://arxiv.org/abs/1202.0302`.

[93] Dávid Pál, Barnabás Póczos, and Csaba Szepesvári. Estimation of Rényi entropy and mutual information based on generalized nearest-neighbor graphs. In *Advances in Neural Information Processing Systems (NIPS)*, pages 1849–1857, 2011.

[94] Barnabás Póczos and András Lőrincz. Independent subspace analysis using geodesic spanning trees. In *International Conference on Machine Learning (ICML)*, pages 673–680, 2005.

[95] Barnabás Póczos and András Lőrincz. Independent subspace analysis using k-nearest neighborhood estimates. In *International Conference on Artificial Neural Networks (ICANN)*, pages 163–168, 2005.

[96] Barnabás Póczos and Jeff Schneider. On the estimation of $\alpha$-divergences. In *International conference on Artificial Intelligence and Statistics (AISTATS)*, pages 609–617, 2011.

[97] Barnabás Póczos, Zoltán Szabó, and Jeff Schneider. Nonparametric divergence estimators for independent subspace analysis. In *European Signal Processing Conference (EUSIPCO)*, pages 1849–1853, 2011.

[98] Barnabás Póczos, Liang Xiong, and Jeff Schneider. Nonparametric divergence: Estimation with applications to machine learning on distributions. In *Uncertainty in Artificial Intelligence (UAI)*, pages 599–608, 2011.

[99] Ravikiran Rajagopal and Lee C. Potter. Multivariate MIMO FIR inverses. *IEEE Transactions on Image Processing*, 12:458–465, 2003.

[100] Murali Rao, Sohan Seth, Jianwu Xu, Yunmei Chen, Hemant Tagare, and José C. Príncipe. A test of independence based on a generalized correlation function. *Signal Processing*, 91:15–27, 2011.

[101] Reuven Y. Rubinstein and Dirk P. Kroese. *The Cross-Entropy Method*. Springer, 2004.

[102] Alfréd Rényi. On measures of information and entropy. In *Proceedings of the 4th Berkeley Symposium on Mathematics, Statistics and Probability*, pages 547–561, 1961.

[103] Marco Scarsini. On measures of concordance. *Stochastica*, 8:201–218, 1984.

[104] Friedrich Schmid and Rafael Schmidt. Multivariate conditional versions of Spearman's rho and related measures of tail dependence. *Journal of Multivariate Analysis*, 98:1123–1140, 2007.

[105] Friedrich Schmid and Rafael Schmidt. Multivariate extensions of Spearman's rho and related statistics. *Statistics & Probability Letters*, 77:407–416, 2007.

[106] Friedrich Schmid, Rafael Schmidt, Thomas Blumentritt, Sandra Gaißer, and Martin Ruppert. *Copula Theory and Its Applications*, chapter Copula based Measures of Multivariate Association. Lecture Notes in Statistics. Springer, 2010.

[107] Tapio Schneider and Arnold Neumaier. Algorithm 808: ARfit - a Matlab package for the estimation of parameters and eigenmodes of multivariate autoregressive models. *ACM Transactions on Mathematical Software*, 27(1):58–65, 2001.

[108] B. Schweizer and Edward F. Wolff. On nonparametric measures of dependence for random variables. *The Annals of Statistics*, 9:879–885, 1981.

[109] Dino Sejdinovic, Arthur Gretton, Bharath Sriperumbudur, and Kenji Fukumizu. Hypothesis testing using pairwise distances and associated kernels. In *International Conference on Machine Learning (ICML)*, pages 1111–1118, 2012.

[110] Sohan Seth and José C. Príncipe. Compressed signal reconstruction using the correntropy induced metric. In *IEEE International Conference on Acoustics, Speech and Signal Processing (ICASSP)*, pages 3845 – 3848, 2008.

[111] Sohan Seth and José C. Príncipe. On speeding up computation in information theoretic learning. In *International Joint Conference on Neural Networks (IJCNN)*, pages 2883–2887, 2009.

[112] Claude E. Shannon. A mathematical theory of communication. *Bell System Technical Journal*, 27(3):379–423, 1948.

[113] Jianbo Shi and Jitendra Malik. Normalized cuts and image segmentation. *IEEE Transactions on Pattern Analysis and Machine Intelligence*, 22(8):888–905, 2000.

[114] Masaaki Sibuya. Bivariate extreme statistics. *Annals of the Institute of Statistical Mathematics*, 11:195–210, 1959.

[115] Harshinder Singh, Neeraj Misra, Vladimir Hnizdo, Adam Fedorowicz, and Eugene Demchuk. Nearest neighbor estimates of entropy. *American Journal of Mathematical and Management Sciences*, 23:301–321, 2003.

[116] A. Sklar. Fonctions de répartition á n dimensions et leurs marges. *Publications de l'Institut de Statistique de l'Université de Paris*, 8:229–231, 1959.

[117] C. Spearman. The proof and measurement of association between two things. *The American Journal of Psychology*, 15:72–101, 1904.

[118] Kumar Sricharan and Alfred. O. Hero. Weighted k-NN graphs for Rényi entropy estimation in high dimensions. In *IEEE Workshop on Statistical Signal Processing (SSP)*, pages 773–776, 2011.

[119] Bharath K. Sriperumbudur, Kenji Fukumizu, Arthur Gretton, Bernhard Schölkopf, and Gert R. G. Lanckriet. On the empirical estimation of integral probability metrics. *Electronic Journal of Statistics*, 6:1550–1599, 2012.

[120] Dan Stowell and Mark D. Plumbley. Fast multidimensional entropy estimation by k-d partitioning. *IEEE Signal Processing Letters*, 16:537–540, 2009.

[121] Zoltán Szabó. Complete blind subspace deconvolution. In *International Conference on Independent Component Analysis and Signal Separation (ICA)*, pages 138–145, 2009.

[122] Zoltán Szabó. Autoregressive independent process analysis with missing observations. In *European Symposium on Artificial Neural Networks, Computational Intelligence and Machine Learning (ESANN)*, pages 159–164, 2010.

[123] Zoltán Szabó and András Lőrincz. Towards independent subspace analysis in controlled dynamical systems. In *ICA Research Network International Workshop (ICARN)*, pages 9–12, 2008.

[124] Zoltán Szabó and András Lőrincz. Complex independent process analysis. *Acta Cybernetica*, 19:177–190, 2009.

[125] Zoltán Szabó and András Lőrincz. Fast parallel estimation of high dimensional information theoretical quantities with low dimensional random projection ensembles. In *International Conference on Independent Component Analysis and Signal Separation (ICA)*, pages 146–153, 2009.

[126] Zoltán Szabó and András Lőrincz. Distributed high dimensional information theoretical image registration via random projections. *Digital Signal Processing*, 22(6):894–902, 2012.

[127] Zoltán Szabó and Barnabás Póczos. Nonparametric independent process analysis. In *European Signal Processing Conference (EUSIPCO)*, pages 1718–1722, 2011.

[128] Zoltán Szabó, Barnabás Póczos, and András Lőrincz. Cross-entropy optimization for independent process analysis. In *International Conference on Independent Component Analysis and Blind Source Separation (ICA)*, pages 909–916, 2006.

[129] Zoltán Szabó, Barnabás Póczos, and András Lőrincz. Undercomplete blind subspace deconvolution. *Journal of Machine Learning Research*, 8:1063–1095, 2007.

[130] Zoltán Szabó, Barnabás Póczos, and András Lőrincz. Undercomplete blind subspace deconvolution via linear prediction. In *European Conference on Machine Learning (ECML)*, pages 740–747, 2007.

[131] Zoltán Szabó, Barnabás Póczos, and András Lőrincz. Auto-regressive independent process analysis without combinatorial efforts. *Pattern Analysis and Applications*, 13:1–13, 2010.

[132] Zoltán Szabó, Barnabás Póczos, and András Lőrincz. Separation theorem for independent subspace analysis and its consequences. *Pattern Recognition*, 45:1782–1791, 2012.

[133] Zoltán Szabó, Barnabás Póczos, Gábor Szirtes, and András Lőrincz. Post nonlinear independent subspace analysis. In *International Conference on Artificial Neural Networks (ICANN)*, pages 677–686, 2007.

[134] Zoltán Szabó and András Lőrincz. Real and complex independent subspace analysis by generalized variance. In *ICA Research Network International Workshop (ICARN)*, pages 85–88, 2006.

[135] Gábor J. Székely and Maria L. Rizzo and. Brownian distance covariance. *The Annals of Applied Statistics*, 3:1236–1265, 2009.

[136] Gábor J. Székely and Maria L. Rizzo. Testing for equal distributions in high dimension. *InterStat*, 5, 2004.

[137] Gábor J. Székely and Maria L. Rizzo. A new test for multivariate normality. *Journal of Multivariate Analysis*, 93:58–80, 2005.

[138] Gábor J. Székely, Maria L. Rizzo, and Nail K. Bakirov. Measuring and testing dependence by correlation of distances. *The Annals of Statistics*, 35:2769–2794, 2007.

[139] Anisse Taleb and Christian Jutten. Source separation in post-nonlinear mixtures. *IEEE Transactions on Signal Processing*, 10(47):2807–2820, 1999.

[140] M. D. Taylor. Multivariate measures of concordance. *Annals of the Institute of Statistical Mathematics*, 59:789–806, 2007.

[141] Fabian J. Theis. Blind signal separation into groups of dependent signals using joint block diagonalization. In *IEEE International Symposium on Circuits and Systems (ISCAS)*, pages 5878–5881, 2005.

[142] Fabian J. Theis. Towards a general independent subspace analysis. In *Advances in Neural Information Processing Systems (NIPS)*, pages 1361–1368, 2007.

[143] Flemming Topsøe. Some inequalities for information divergence and related measures of discrimination. *IEEE Transactions on Information Theory*, 46:1602–1609, 2000.

[144] Constantino Tsallis. Possible generalization of Boltzmann-Gibbs statistics. *Journal of Statistical Physics*, 52:479–487, 1988.

[145] Manuel Úbeda-Flores. Multivariate versions of Blomqvist's beta and Spearman's footrule. *Annals of the Institute of Statistical Mathematics*, 57:781–788, 2005.

[146] James V. Uspensky. Asymptotic formulae for numerical functions which occur in the theory of partitions. *Bulletin of the Russian Academy of Sciences*, 14(6):199–218, 1920.

[147] Oldrich Vasicek. A test for normality based on sample entropy. *Journal of the Royal Statistical Society, Series B*, 38:54–59, 1976.

[148] T. Villmann and S. Haase. Mathematical aspects of divergence based vector quantization using Fréchet-derivatives. Technical report, University of Applied Sciences Mittweida, 2010.

[149] Ulrike von Luxburg. A tutorial on spectral clustering. *Statistics and Computing*, 17(4), 2007.

[150] Mark P. Wachowiak, Renata Smolikova, Georgia D. Tourassi, and Adel S. Elmaghraby. Estimation of generalized entropies with sample spacing. *Pattern Analysis and Applications*, 8:95–101, 2005.

[151] Quing Wang, Sanjeev R. Kulkarni, and Sergio Verdú. Divergence estimation for multidimensional densities via k-nearest-neighbor distances. *IEEE Transactions on Information Theory*, 55:2392–2405, 2009.

[152] Quing Wang, Sanjeev R. Kulkarni, and Sergio Verdú. Universal estimation of information measures for analog sources. *Foundations And Trends In Communications And Information Theory*, 5:265–353, 2009.

[153] Edward F. Wolff. N-dimensional measures of dependence. *Stochastica*, 4:175–188, 1980.

[154] Donghui Yan, Ling Huang, and Michael I. Jordan. Fast approximate spectral clustering. In *International Conference on Knowledge Discovery and Data Mining (KDD)*, pages 907–916, 2009.

[155] Joseph E. Yukich. Probability theory of classical Euclidean optimization problems. *Lecture Notes in Mathematics*, 1675, 1998.

[156] Andreas Ziehe, Motoaki Kawanabe, Stefan Harmeling, and Klaus-Robert Müller. Blind separation of postnonlinear mixtures using linearizing transformations and temporal decorrelation. *Journal of Machine Learning Research*, 4:1319–1338, 2003.

[157] V. M. Zolotarev. Probability metrics. *Theory of Probability and its Applications*, 28:278–302, 1983.