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Mutual Information Estimation based Data-Driven Partitions

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Introduction

- Mutual information (MI) fundamental quantity in information theory
  - (Shannon's coding theorems): channel capacity, achievable rate-distortion curve,....
- Statistical learning-decision problems,
  - fidelity indicator for image registration, image segmentation, feature extraction (MPE-SR), detection,...
  - performance limits in Pattern recognition (*Westover et al. 2008*)

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Mutual Information Estimation

- estimation based on empirical data
- a distribution-free framework is fundamental

Introduction

Extensive work on related differential entropy estimation (*Beirlant et al. 1997*)

- non-adaptive product type of histogram-based approaches
- kernel plug-in estimates
  - ✓ strong consistency is well understood

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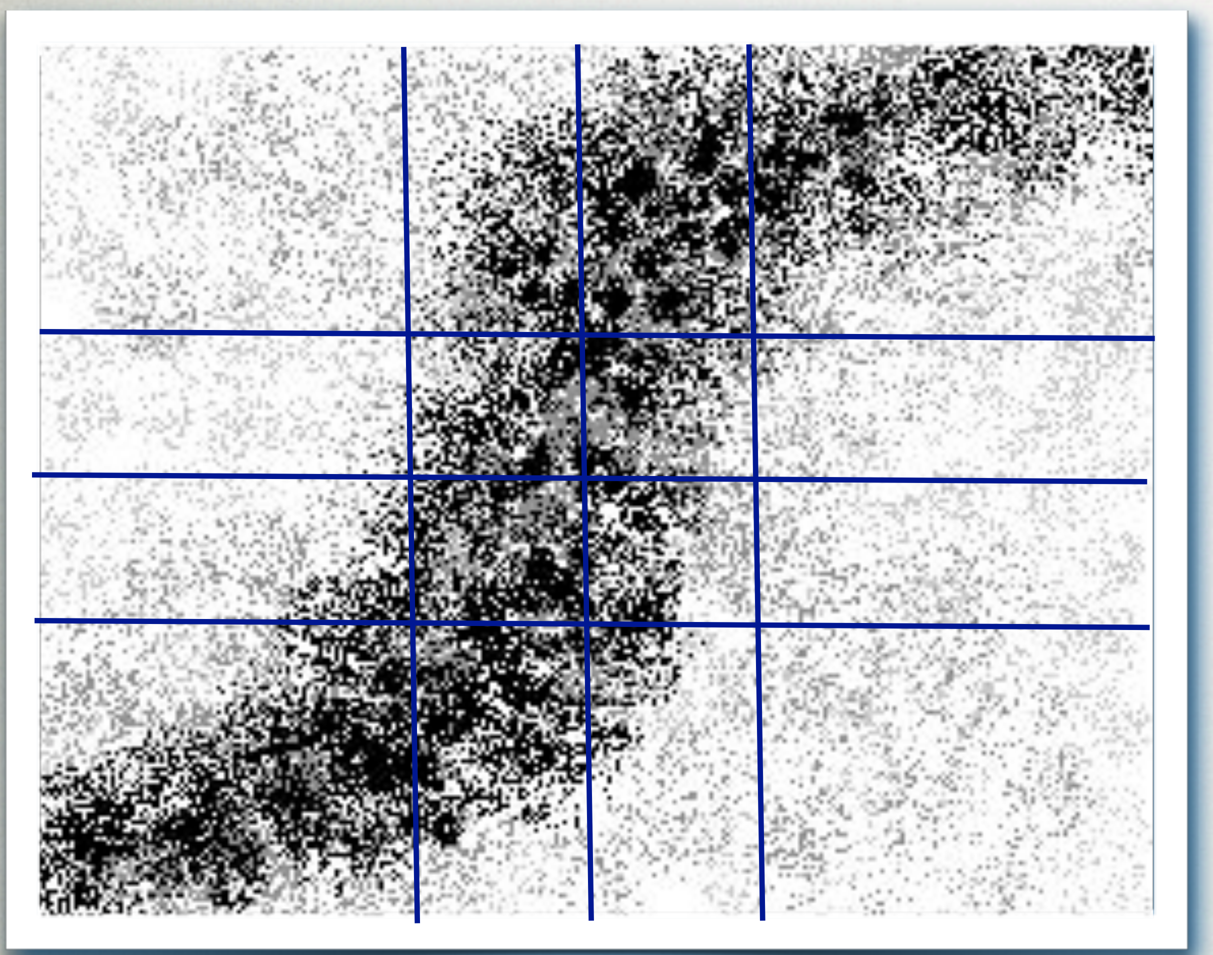
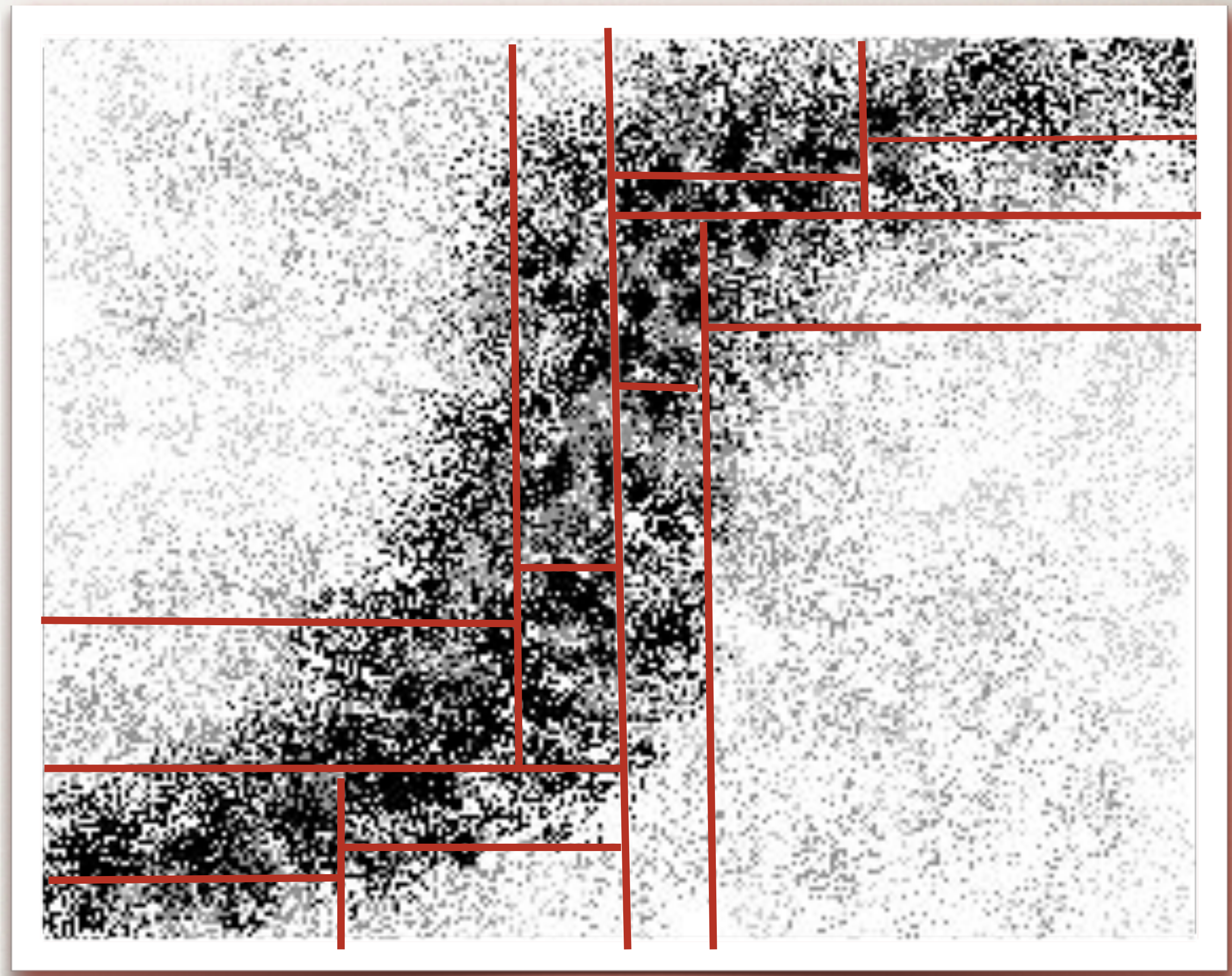
Focus and Motivation of this Work

- ✤ Explore the role of data-dependent partitions -> non-product structure
- ✤ Hypothesis: better adaptation to the data -> better approximation properties -> better estimates
  - ✓ effectiveness demonstrated in other stat. learn. settings (classification, density estimation, *Lugosi et al. 1996*)



PRODUCT PARTITION SCHEME



NON-PRODUCT DATA-DRIVEN PARTITION

Introduction

Work in this direction....

Darbellay et al. 1999 proposed tree-structured data-driven construction

- ✓ based on a local splitting process to adapt to the data
- ✤ consistency an open problem for this setting
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...... on the KL Divergence

- Data-dependent histogram-based approach (Wang et al. IEEE Trans. IT 2005)

Introduction

Proposed directions

- Theory: Find consistency conditions for general partition schemes
- Applications: Propose new concrete data-driven estimates

Content Outline

Main Result

- The Estimator:
  - Approximation Error Analysis
  - Estimation error Analysis
- The Result: Conditions for Strong Consistency

Applications

- Multivariate Statistically Equivalent Block
- Tree-structured Partitions
- Consistency

- Experiments

- Some Extensions

Preliminaries

Let X, Y two random variables with joint distribution $P_{X,Y}$.
The mutual information,

$$I(X;Y) = D(P_{X,Y} || P_X \times P_Y)$$

where $D(P||Q)$ is the Kullback-Leibler divergence,

$$D(P||Q) = \int \log \frac{\partial P}{\partial Q}(x) \cdot \partial P(x).$$

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Main Problem

- joint distribution is unknown
- only i.i.d. realization $(X_1, Y_1), \cdots, (X_n, Y_n)$ available
- a distribution free estimator of $I(X,Y)$ is needed !

$\hat{I}_n(X;Y)$

Preliminaries

Requirements for the Estimate

- ✦ Large sample regime:

  -Universal (distribution free) strongly consistent

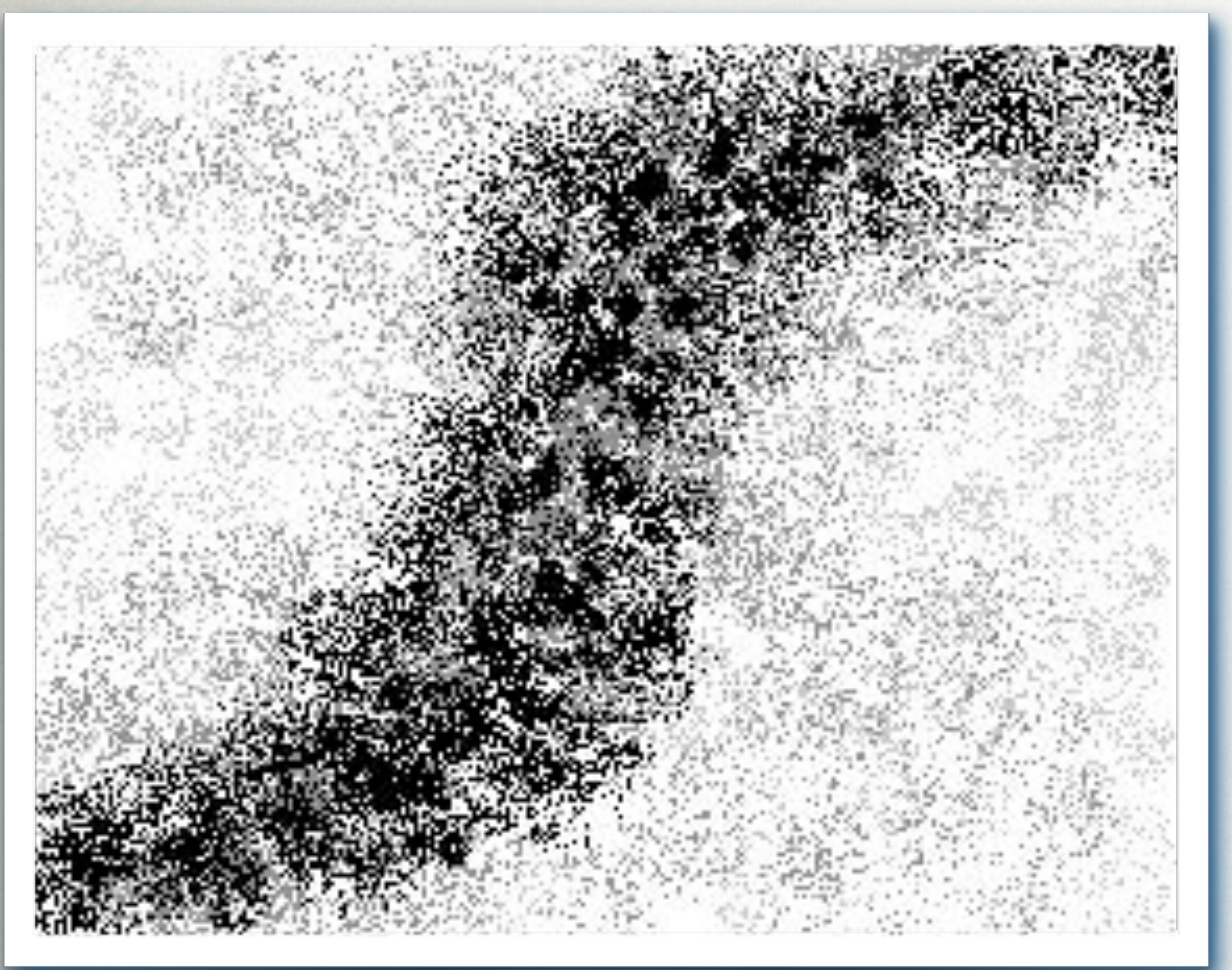
  $$\lim_{n\to\infty} \hat{I}_n(X;Y) = I(X;Y) \text{ almost surely}$$

- ✦ Small sample regime:

  -good approximation to the empirical data

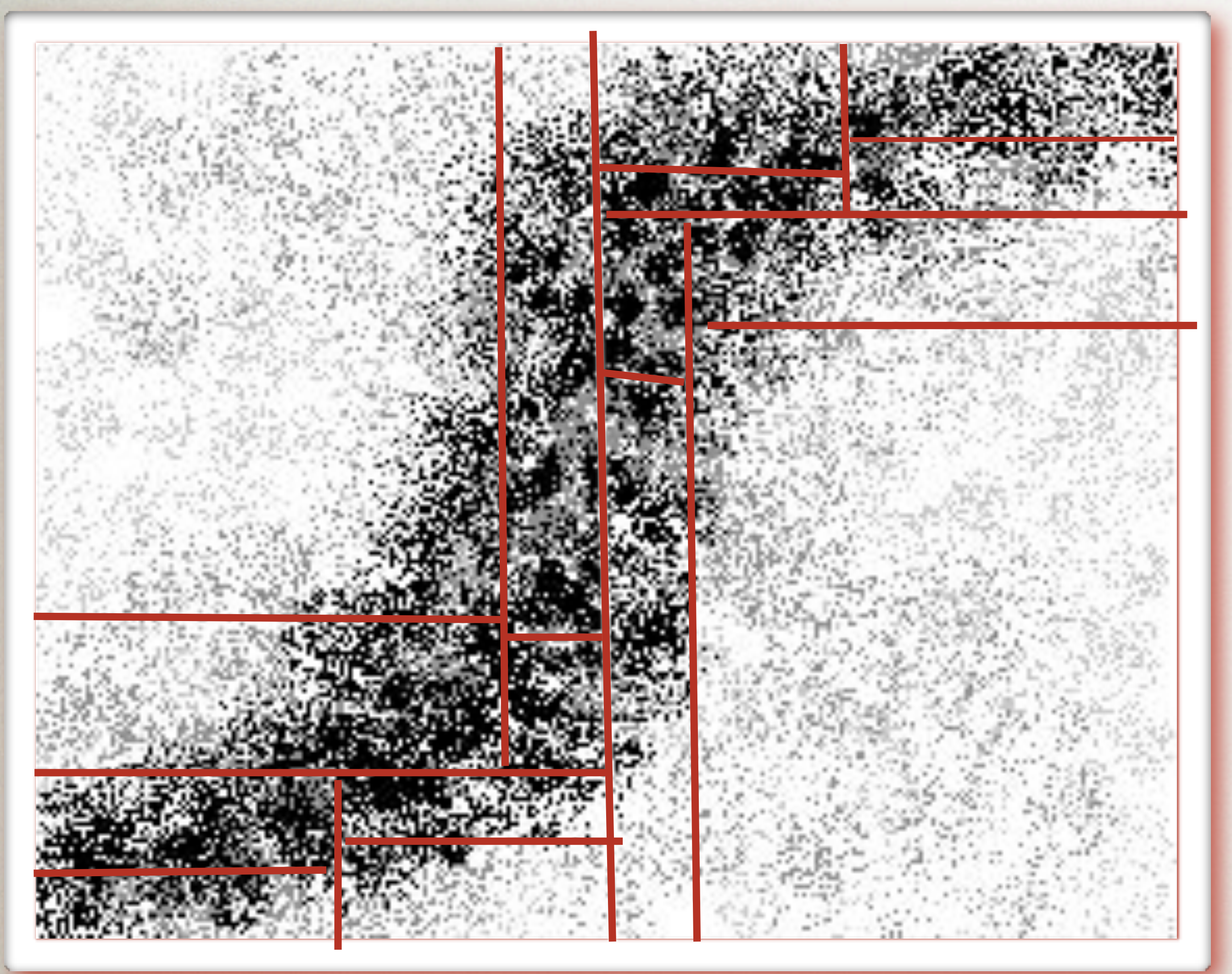
  Bias and stand. dev. of $\left|\hat{I}_n(X;Y) - I(X;Y)\right|$, for finite n

Basic Construction



$$Z_1 = (X_1, Y_1), .., Z_n = (X_n, Y_n)$$

Empirical Data from $P_{X,Y}$



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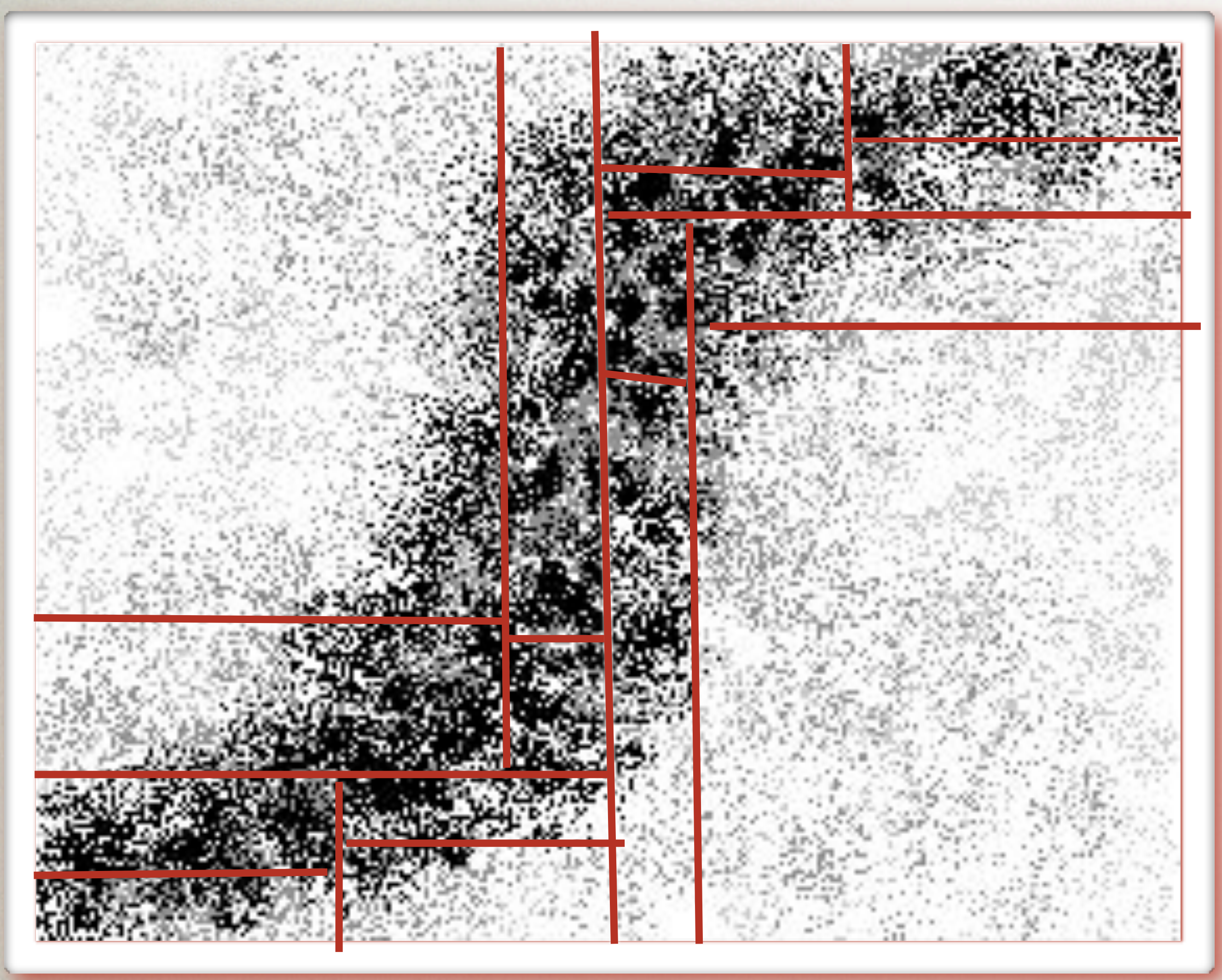
$$\pi_n(Z_1, .., Z_n) = \{A_1, .., A_k\} \in \mathcal{B}\left(\mathbb{R}^d\right)$$

Data-dependent partition rule



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$$\mathrm{P}_n(A) = \frac{1}{n}\sum_{i=1}^{n} \mathbb{I}_A(Z_i),\ \forall A \in \pi_n(Z_1, .., Z_n)$$

Computation of empirical frequencies

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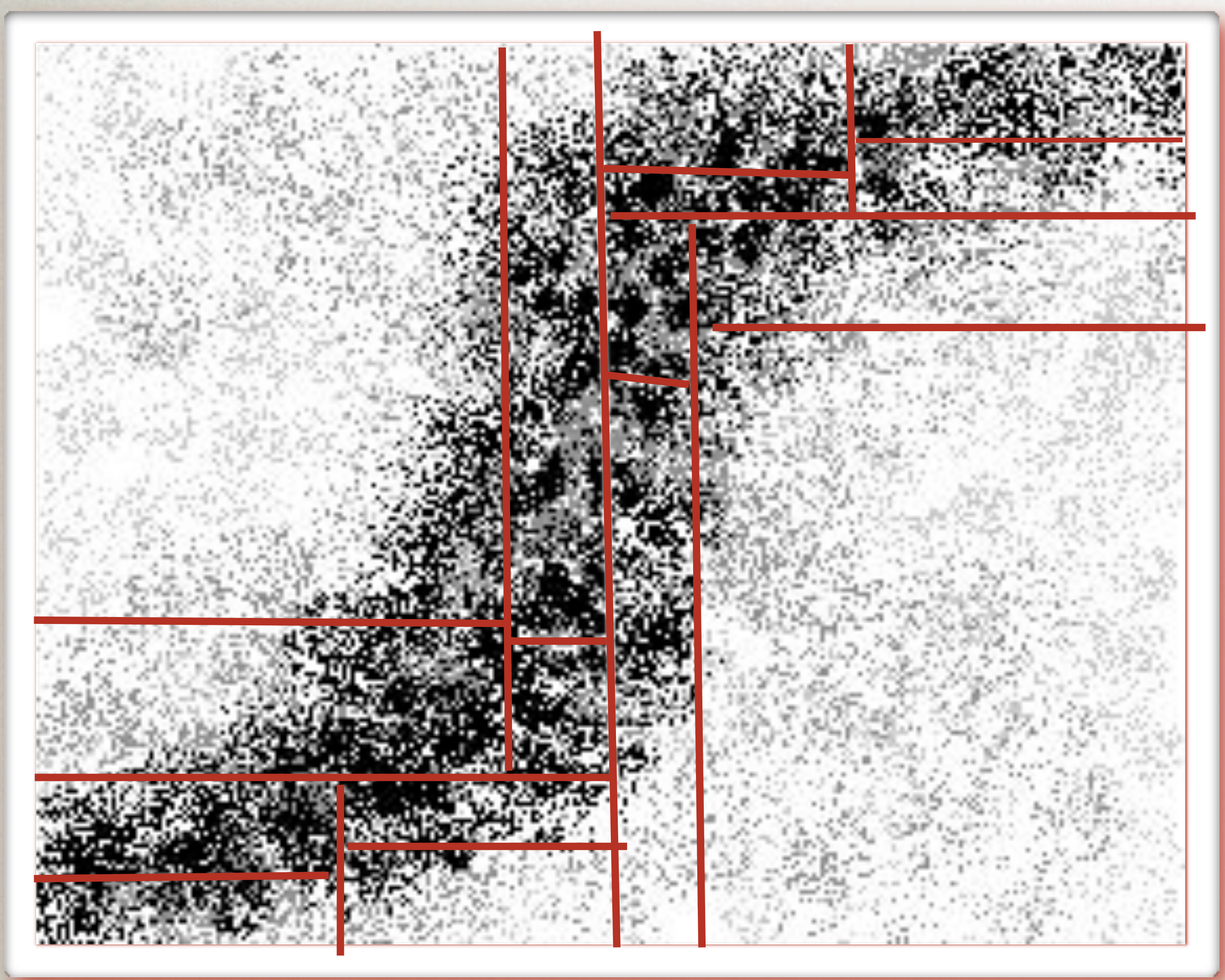
Computation of empirical frequencies

$$\hat{I}_n(X;Y) = \sum_{A\in\pi_n(Z_1^n)} P_n(A) \cdot \log \frac{P_n(A)}{P_n(A_1 \times \mathbb{R}^q) \cdot P_n(\mathbb{R}^p \times A_2)};$$

Empirical mutual information



Product Bin Structure

All $A \in \pi_n(Z_1^n)$ have a product structure $A = A_1 \times A_2$ with $A_1 \in \mathbb{R}^p, A_2 \in \mathbb{R}^q$.
to estimate the product of marginals !
$P_X \times P_Y$

Consistency

Problem

$\Pi = \{\pi_1(\cdot) \cdots \pi_n(\cdot) \cdots\}$

Find the sufficient conditions on the partition scheme to get,

$$\lim_{n\to\infty} \hat{I}_n(X;Y) = I(X;Y) \text{ almost surely}$$

distribution free.

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Main Inequality

$$\left|\hat{I}_n(X;Y) - I(X;Y)\right| \leq$$

estimation error

$$\left|\sum_{A\in\pi_n(Z_1^n)} P_n(A)\cdot\log\frac{P_n(A)}{P_n(A_1\times\mathbb{R}^q)\cdot P_n(\mathbb{R}^p\times A_2)} - \sum_{A\in\pi_n(Z_1^n)} P(A)\cdot\log\frac{P(A)}{P(A_1\times\mathbb{R}^q)\cdot P(\mathbb{R}^p\times A_2)}\right|$$

$$+\left|\sum_{A\in\pi_n(Z_1^n)} P(A)\cdot\log\frac{P(A)}{P(A_1\times\mathbb{R}^q)\cdot P_n(\mathbb{R}^p\times A_2)} - I(X,Y)\right|$$

approximation error

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Estimation Error:

Deviation of empirical measures from probabilities in the MI functional

approximation error

Consistency

Problem

Find the sufficient conditions on the partition scheme to get,

$\Pi = \{\pi_1(\cdot) \cdots \pi_n(\cdot) \cdots\}$

$$\lim_{n\to\infty} \hat{I}_n(X;Y) = I(X;Y) \text{ almost surely}$$

distribution free.

Main Inequality

$\left|\hat{I}_n(X;Y) - I(X;Y)\right| \le$ estimation error

Approximation error:
The effect of quantization reduces magnitude of information theoretic quantities.

$$+\left|\sum_{A\in\pi_n(Z_1^n)} P(A)\cdot\log\frac{P(A)}{P(A_1\times\mathbb{R}^q)\cdot P_n(\mathbb{R}^p\times A_2)} - I(X,Y)\right|$$

approximation error

Consistency

Our approach considers statistical learning tools and inequalities to bound these two sources of error asymptotically.

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Estimation Error Inequality

Let $\mathcal{A}$ collection of measurable partitions for $\mathbb{R}^d$

Definitions: (*Lugosi et al. 1996*)

- The maximum cell count of $\mathcal{A}$ is given by, $$\mathcal{M}(\mathcal{A}) = \sup_{\pi \in \mathcal{A}} |\pi|$$
- Let $\{x_1, .., x_n\} \subset \mathbb{R}^d$ then we can define $$\Delta(\mathcal{A}, x_1, .., x_n) = |\{\{x_1, .., x_n\} \cup \pi : \pi \in \mathcal{A}\}|$$

  and the growth function of $\mathcal{A}$ by $$\Delta_n^*(\mathcal{A}) = \max_{x_1^n \in \mathbb{R}^{d \cdot n}} \Delta(\mathcal{A}, x_1, .., x_n)$$

Theorem: (*Lugosi et al. 1996*)

Let $\mathcal{A}$ be a collection of measurable partitions for $\mathbb{R}^d$, then $\forall \epsilon > 0, \forall n,$

$$\mathbb{P}\left(\sup_{\pi \in \mathcal{A}} \sum_{A \in \pi} |P_n(A) - P(A)| > \epsilon \right) \leq 4 \Delta_{2n}^*(\mathcal{A}) 2^{\mathcal{M}(\mathcal{A})} \exp^{-\frac{n\epsilon^2}{32}},$$

where $\mathbb{P}$ the distribution of the empirical process.

Consistency

Our approach considers statistical learning tools and inequalities to bound these two sources of error asymptotically.

Approximation error Result

Definitions:

- Let $A \in \mathbb{R}^d$ a measurable event, then its diameter is

$$diam(A) = \sup_{x,y \in A} ||x - y||,$$

Theorem: (*Silva et al. 2007*)

Let $\Pi = \{\pi_1(\cdot), \pi_2(\cdot), \cdots\}$ our data-dependent partition scheme if, driven by iid realizations $Z_1 = (X_1, Y_1), .., Z_n = (X_n, Y_n)$ of $\mathrm{P}_{X,Y}$

$$\lim_{n \to \infty} P_{X,Y}\left(\left\{z \in \mathbb{R}^d : diam(\pi_n(z|Z_1^n)) > \epsilon\right\}\right) \to 0,$$

SHRINKING CELL CONDITION

then,

$$\lim_{n \to \infty} \sum_{A \in \pi_n(Z_1^n)} P_{X,Y}(A) \cdot \log \frac{P_{X,Y}(A)}{P_X \times P_Y(A)} = I(X, Y),$$

$\mathbb{P}$- almost surely.

THE MAIN RESULT

THEOREM

Let $\Pi = \{\pi_1(\cdot), \pi_2(\cdot), \cdots\}$ a partition scheme driven by the i.i.d. realizations $Z_1 = (X_1, Y_1), .., Z_n = (X_n, Y_n)$ of $\mathrm{P}_{X,Y}$. If there exist $\tau \in (0,1)$ such that,

i) $\lim_{n\to\infty} \frac{1}{n^\tau} \log \mathcal{S}_n(\mathcal{C}_{[1-p],n}) = 0,$

$\lim_{n\to\infty} \frac{1}{n^\tau} \log \mathcal{S}_n(\mathcal{C}_{[p+1-d],n}) = 0,$

ii) $$\lim_{n\to\infty} \frac{1}{n^\tau} \log \Delta_n^*(\mathcal{A}_n) = 0$$

iii) $$\lim_{n\to\infty} \frac{1}{n^\tau} \mathcal{M}(\mathcal{A}_n) = 0,$$

iv) $\exists\ (k_n)_{n\in\mathbb{N}}$ a sequence of non-negative numbers, with $(k_n) \approx (n^{0.5+\tau/2})$ such that, $\forall A \in \pi_n(Z_1, .., Z_n)$

$$\mathrm{P}_n(A) \geq \frac{k_n}{n},$$

v) $\forall \epsilon > 0$ (shrinking cell condition)

$$\lim_{n\to\infty} P_{X,Y}\left(\left\{z \in \mathbb{R}^d : diam(\pi_n(z|Z_1^n)) > \epsilon\right\}\right) \to 0,$$

then,

$$\lim_{n\to\infty} \hat{I}_n(X;Y) = I(X,Y),$$

$\mathbb{P}$ (empirical process distribution) - almost surely.

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Main Result

- The Estimator
- Approximation Error results
- Estimation error results
- Conditions for Strong Consistency

Applications

- Multivariate Statistically Equivalent Block
- Tree-structured Partitions
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- Experiments

- Future Work

Statistically equivalent blocks (Gessaman)

Idea: use $Z_1, .., Z_n$ to partition the space in equal empirical mass bins

Pseudo-Algorithm

Let $k_n > 0$ the minimum number of sampled points per bin.

★ $T_n = \lfloor (n/k_n)^{1/d} \rfloor$ # axis parallel partition per-coordinate

✤ $\pi_n(Z_1^n)$ induced by T_n statistically equivalent axis - parallel splits per coordinate => $(T_n)^d$ bins

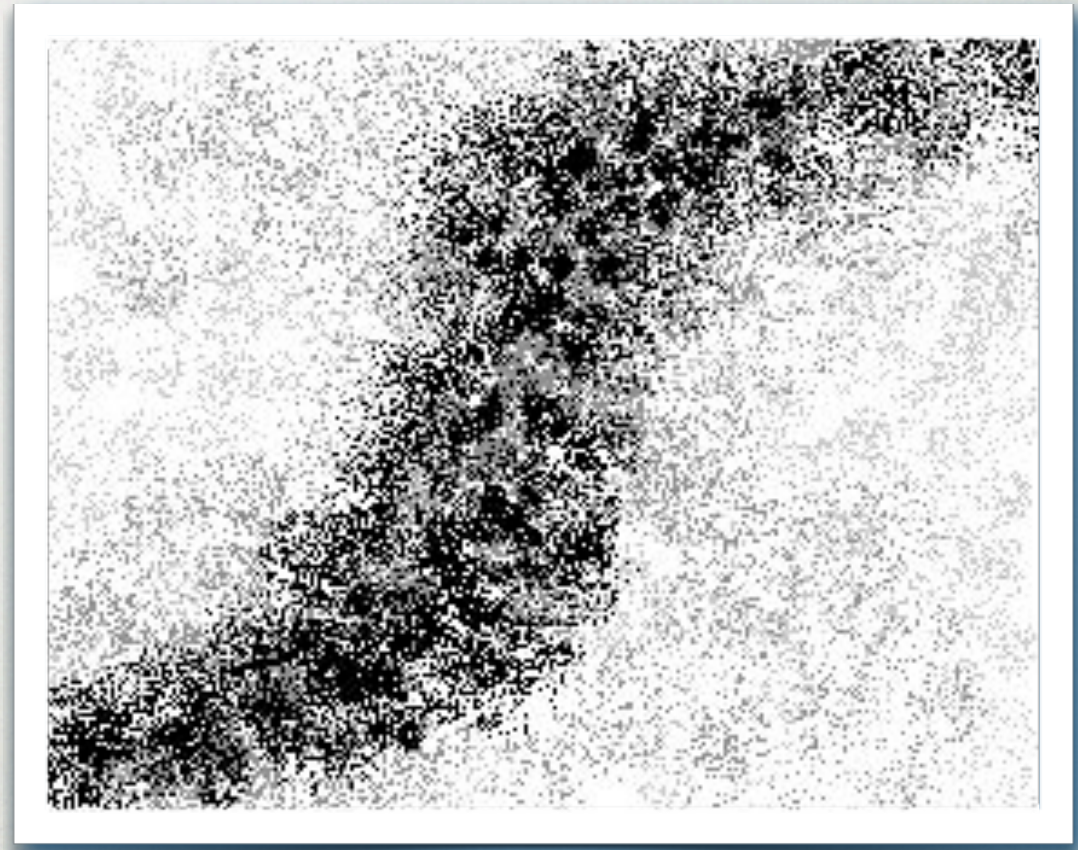

Fig.1: Statistically equivalent blocks

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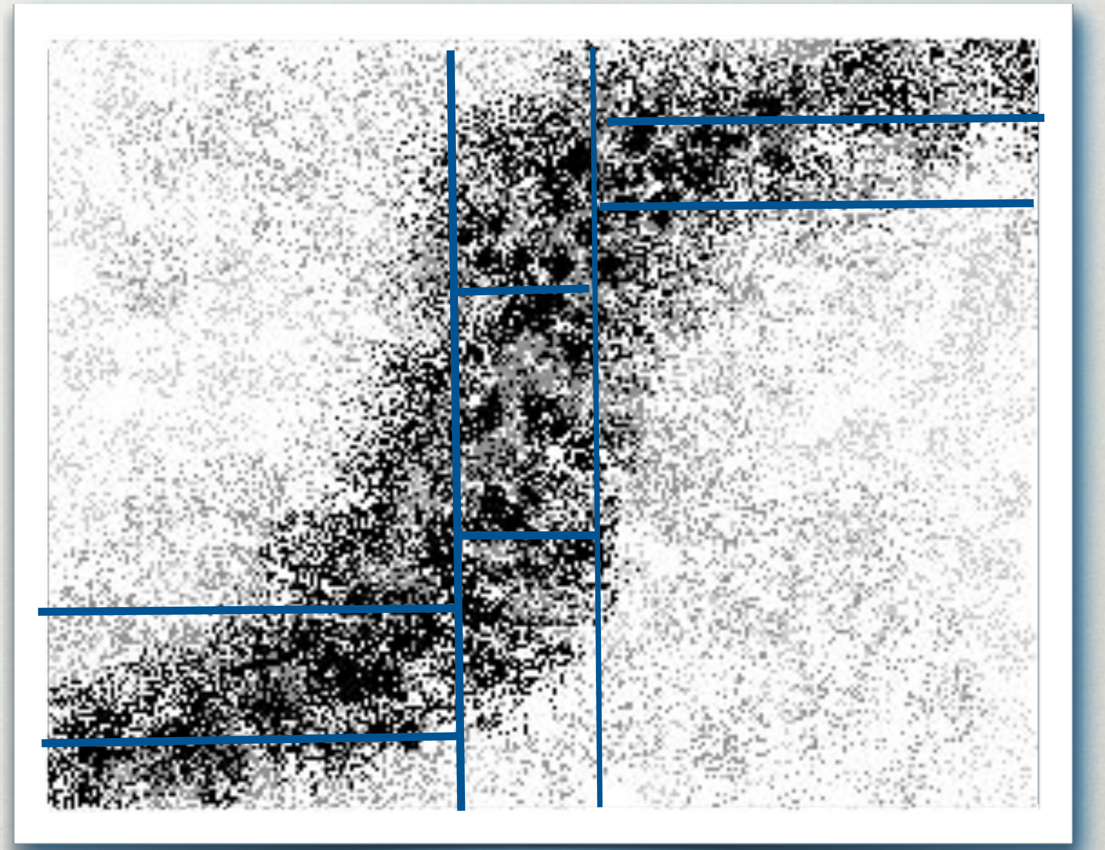

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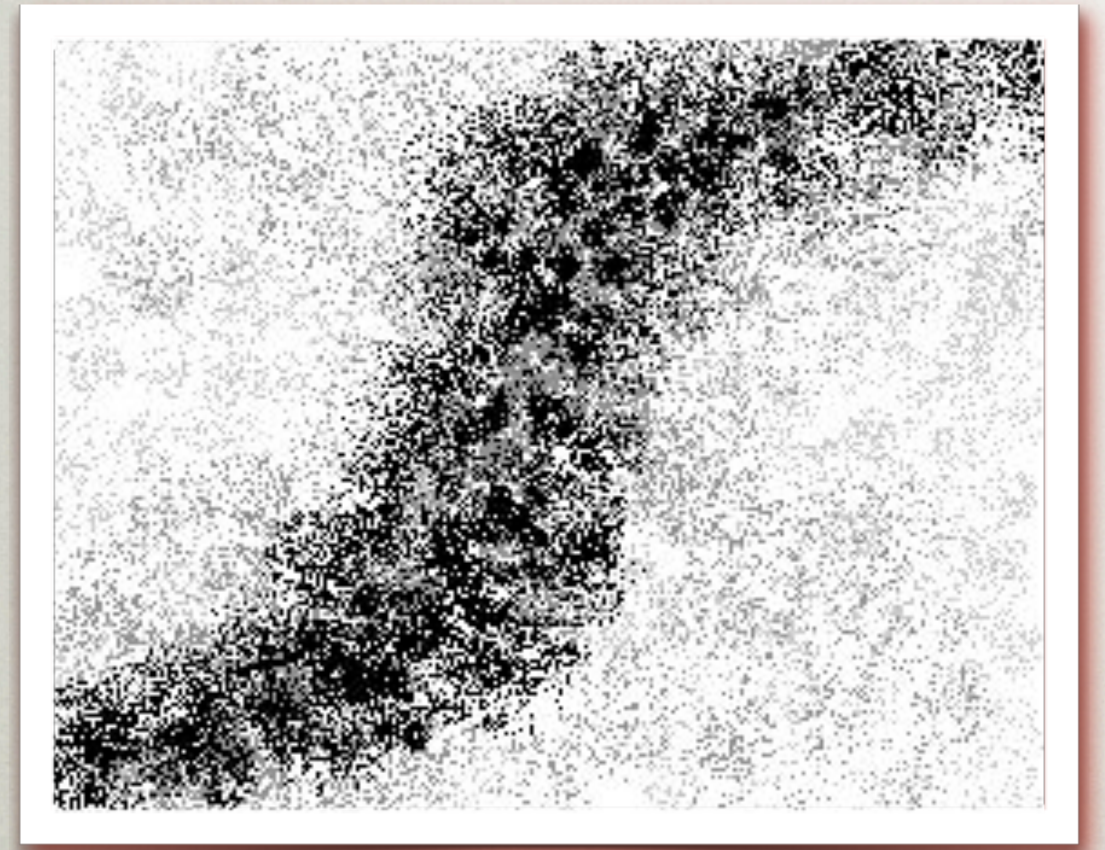


Fig.2: Tree-Structured Partitions

Pseudo-Algorithm

Let $k_n > 0$ the minimum number of sampled points per bin.

★ initialization $U = \{\mathbb{R}^d\}$

✤ For each $A \in U$

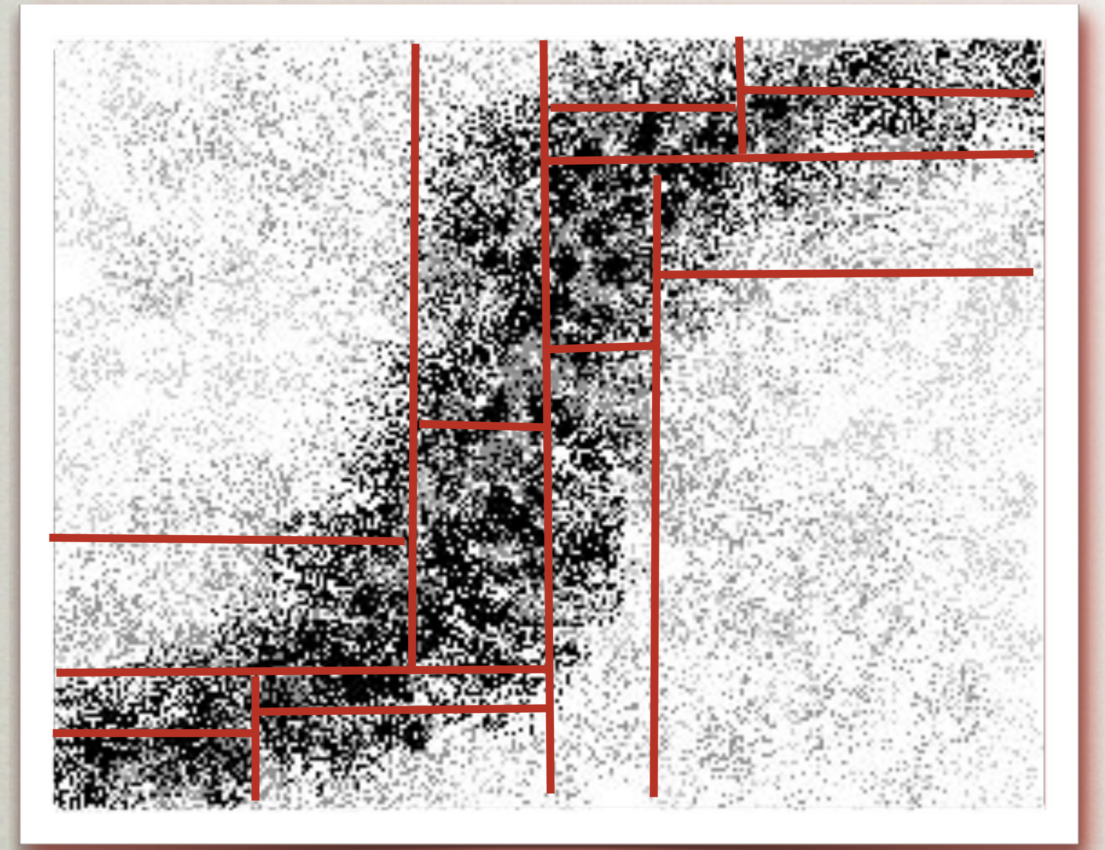
- if $P_n(A) \geq \frac{2 \cdot k_n}{n}$,
  - chose a dimension to partition the space in equal emp. mass, axis-parallel => $A \mapsto B_1, B_2$
  - update $U = U \setminus \{A\} \cup \{B_1, B_2\}$

✤ end For each, $P_n(A) < \frac{2 \cdot k_n}{n}, \forall A \in \mathcal{U}$

✤ finally $\pi_n(Z_1^n) = \mathcal{U}$.

Tree-structured (dyadic) Partitions

Idea: use $Z_1, .., Z_n$ to partition the space in equal empirical mass bins



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Key question

What is the asymptotic behavior of k_n that guarantee consistency?

Consistency

Statistically equivalent blocks

Tree-structured (dyadic) Partitions k_n

THEOREM

Under the problem setting of Theorem 1, (and respective construction), if $(k_n) \approx (n^{0.5+\tau/2})$ for $\tau \in (1/3, 1)$ then,

$$\lim_{n\to\infty} \hat{I}_n(X;Y) = I(X,Y),$$

$\mathbb{P}$ - almost surely.

Remarks

✳ consistency requires a sub-linear behavior on k_n

✳ the results are stronger than the conditions for L1 consistency

❖ $(a_n) \approx (b_n)$ if an only if $\lim_{n\to\infty} \frac{a_n}{b_n} = C$, for some $C > 0$.

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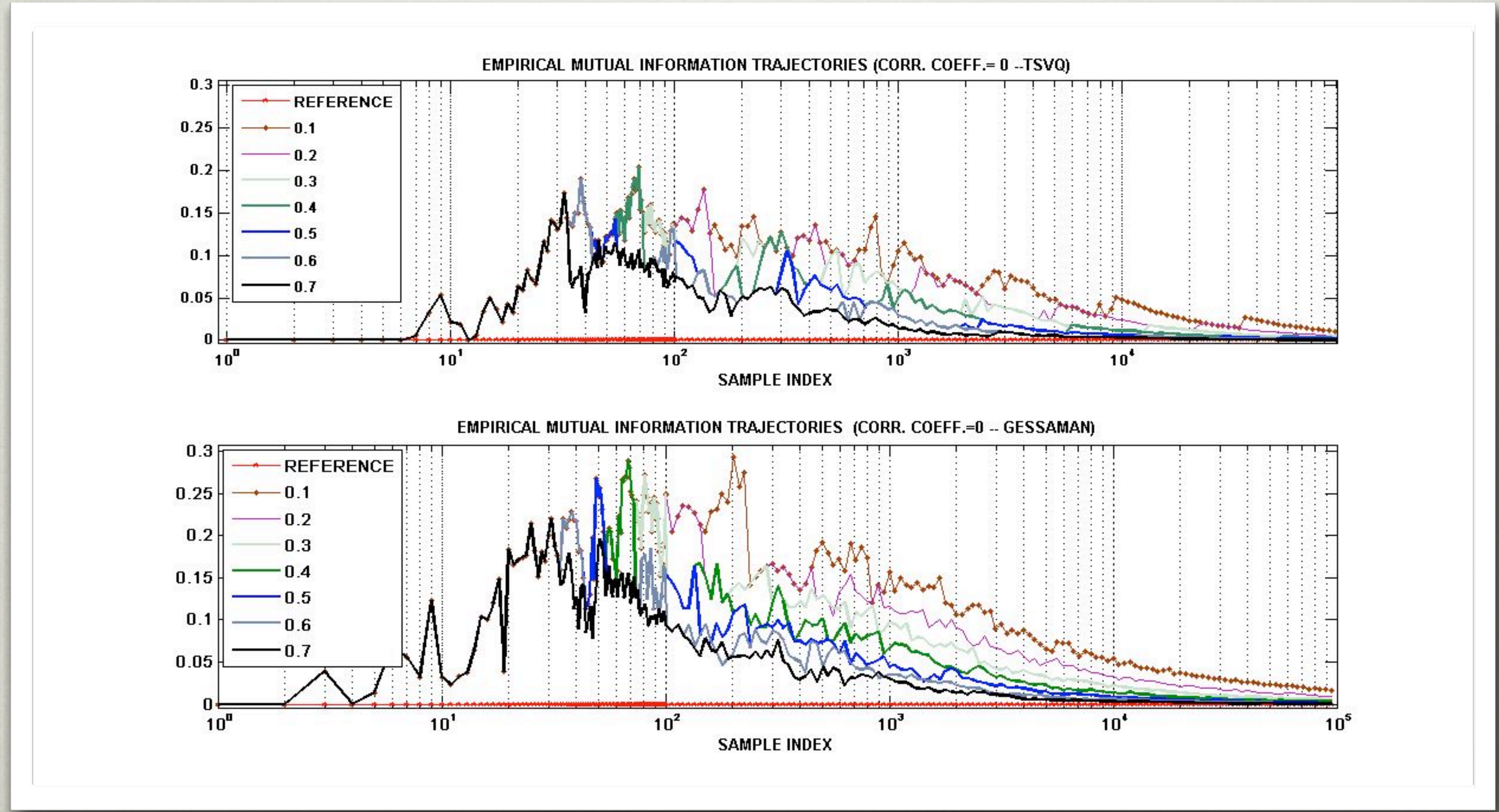
Simulation Analysis

General Setting

- joint Gaussian distribution simulated (two dimensional case)
  - closed form expression for MI
  - ML estimation available (used as a benchmark!)
- evaluation of different level of statistical dependencies
  - correlation coefficient in the range of [0-1]
- across different sampling lengths of the empirical process
- Bias and standard deviations computed using 1000 realizations
- kernel plug-in estimates and non-product histogram based estimates evaluated

Simulation Analysis

Setting i)



Empirical mutual Information trajectories for TSVQ and Gessaman scheme.
Data simulated with correlation coefficient r=0

Simulation Analysis

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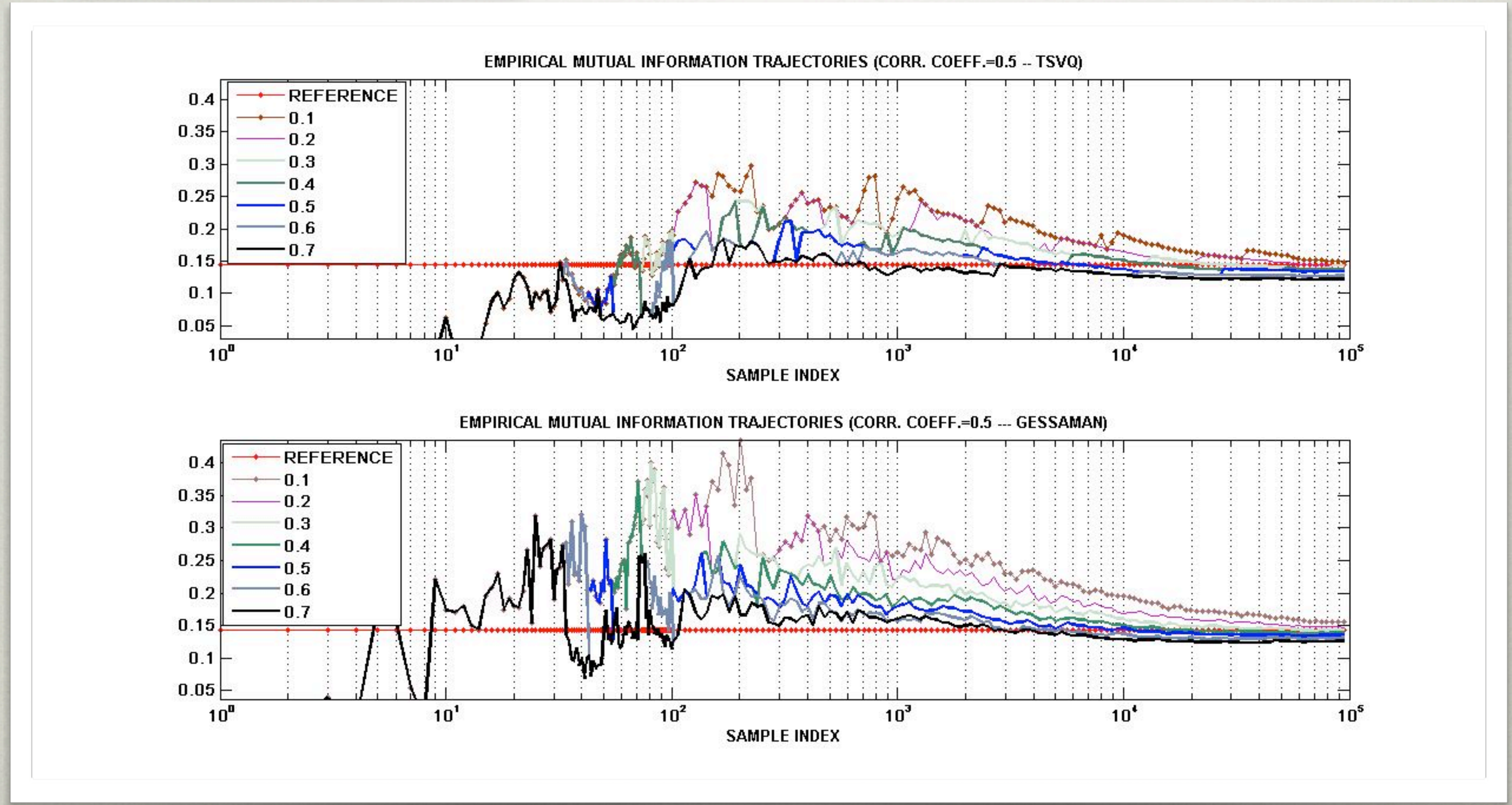


Empirical mutual Information trajectories for TSVQ and Gessaman scheme.
Data simulated with correlation coefficient r=0.5

Simulation Analysis

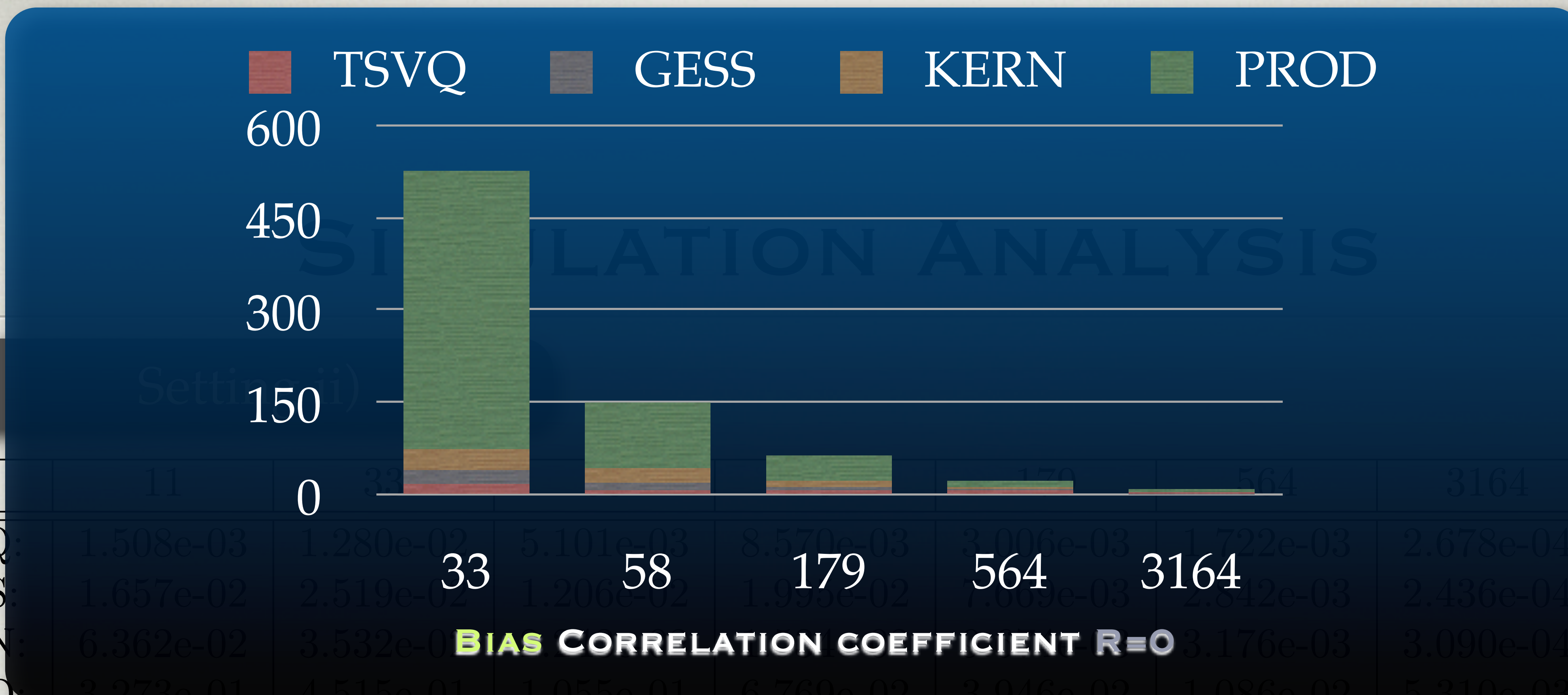
Setting ii)

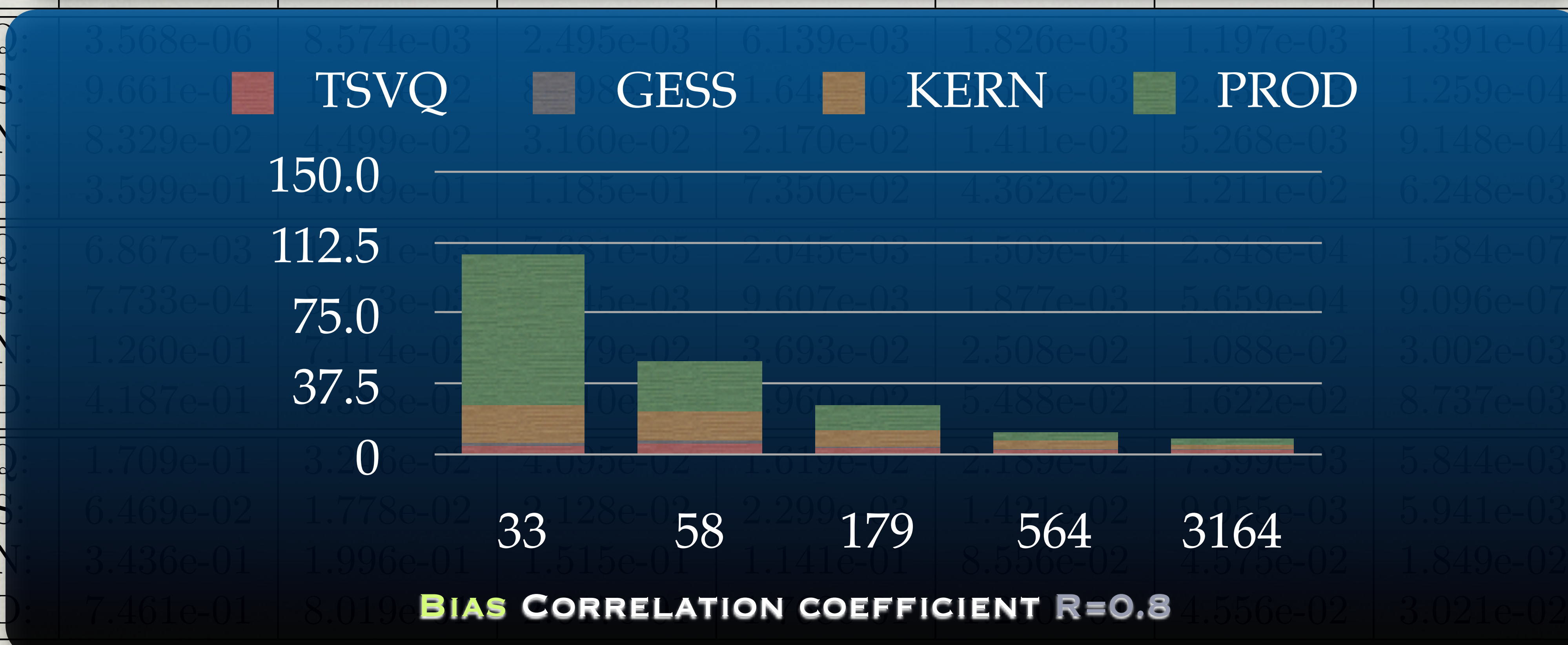
		11	33	58	101	179	564	3164	5626
0	TSVQ:	1.508e-03	1.280e-02	5.101e-03	8.570e-03	3.006e-03	1.722e-03	2.678e-04	8.479e-05
	GESS:	1.657e-02	2.519e-02	1.206e-02	1.995e-02	7.669e-03	2.842e-03	2.436e-04	1.594e-04
	KERN:	6.362e-02	3.532e-02	2.243e-02	1.534e-02	9.674e-03	3.176e-03	3.090e-04	9.035e-05
	PROD:	3.273e-01	4.515e-01	1.055e-01	6.769e-02	3.946e-02	1.086e-02	5.310e-03	5.652e-03
0.3	TSVQ:	3.568e-06	8.574e-03	2.495e-03	6.139e-03	1.826e-03	1.197e-03	1.391e-04	2.359e-05
	GESS:	9.661e-03	1.914e-02	8.498e-03	1.645e-02	5.515e-03	2.037e-03	1.259e-04	8.186e-05
	KERN:	8.329e-02	4.499e-02	3.160e-02	2.170e-02	1.411e-02	5.268e-03	9.148e-04	4.355e-04
	PROD:	3.599e-01	4.769e-01	1.185e-01	7.350e-02	4.362e-02	1.211e-02	6.248e-03	6.680e-03
0.5	TSVQ:	6.867e-03	1.951e-03	7.681e-05	2.045e-03	1.509e-04	2.848e-04	1.584e-07	5.105e-05
	GESS:	7.733e-04	8.473e-03	2.645e-03	9.607e-03	1.877e-03	5.659e-04	9.096e-07	1.270e-06
	KERN:	1.260e-01	7.114e-02	5.079e-02	3.693e-02	2.508e-02	1.088e-02	3.002e-03	1.854e-03
	PROD:	4.187e-01	5.388e-01	1.410e-01	8.960e-02	5.488e-02	1.622e-02	8.737e-03	9.381e-03
0.8	TSVQ:	1.709e-01	3.246e-02	4.095e-02	1.619e-02	2.189e-02	7.399e-03	5.844e-03	6.679e-03
	GESS:	6.469e-02	1.778e-02	2.128e-02	2.299e-03	1.421e-02	9.955e-03	5.941e-03	4.351e-03
	KERN:	3.436e-01	1.996e-01	1.515e-01	1.141e-01	8.556e-02	4.575e-02	1.849e-02	1.354e-02
	PROD:	7.461e-01	8.019e-01	2.617e-01	1.768e-01	1.290e-01	4.556e-02	3.021e-02	3.275e-02

Bias for the non-parametric mutual information estimates (Gessaman partition scheme (GESS), tree-structured partition (TSVQ), classical product partition (PROD) and a kernel plug-in estimate (KERN))

Simulation Analysis

Setting (ii)





R		5626
0	TSVQ:	8.479e-05
	GESS:	1.594e-04
	KERN:	9.035e-05
	PROD:	5.652e-03
0.3	TSVQ:	2.359e-05
	GESS:	8.186e-05
	KERN:	4.355e-04
	PROD:	6.680e-03
0.5	TSVQ:	5.105e-05
	GESS:	1.270e-06
	KERN:	1.854e-03
	PROD:	9.381e-03
0.8	TSVQ:	6.679e-03
	GESS:	4.351e-03
	KERN:	1.354e-02
	PROD:	3.275e-02

Bias for the non-parametric mutual information estimates (Gessaman partition scheme (GESS), tree-structured partition (TSVQ), classical product partition (PROD) and a kernel plug-in estimate (KERN)

Simulation Analysis

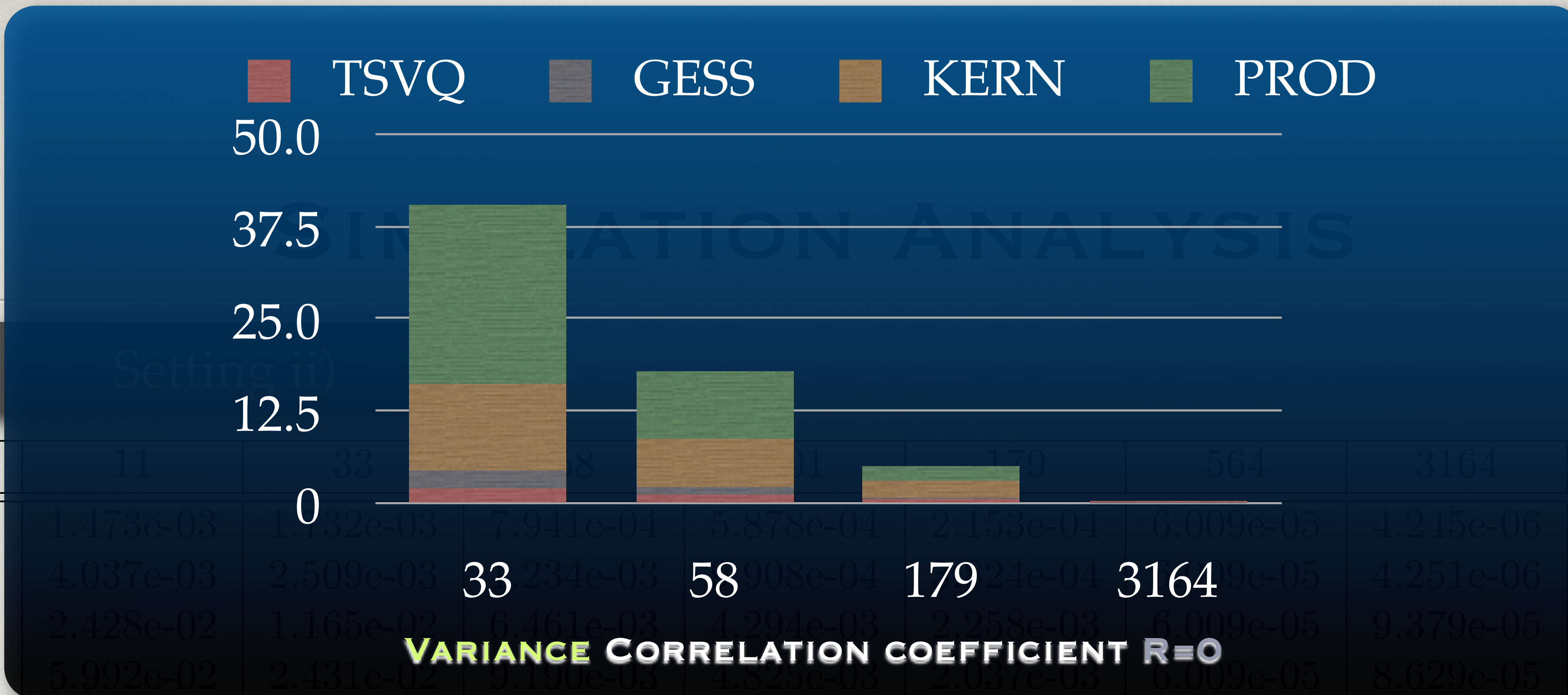
Setting ii)

		11	33	58	101	179	564	3164	5626
	TSVQ:	1.473e-03	1.732e-03	7.941e-04	5.878e-04	2.153e-04	6.009e-05	4.245e-06	1.534e-06
0	GESS:	4.037e-03	2.509e-03	1.234e-03	9.908e-04	3.824e-04	6.009e-05	4.251e-06	1.992e-06
	KERN:	2.428e-02	1.165e-02	6.461e-03	4.294e-03	2.258e-03	6.009e-05	9.379e-05	4.941e-05
	PROD:	5.992e-02	2.431e-02	9.190e-03	4.825e-03	2.037e-03	6.009e-05	8.629e-05	6.193e-05
	TSVQ:	1.406e-03	2.563e-03	1.418e-03	1.022e-03	5.302e-04	1.926e-04	3.049e-05	1.437e-05
0.3	GESS:	5.565e-03	3.369e-03	1.729e-03	1.384e-03	6.555e-04	1.926e-04	3.006e-05	1.632e-05
	KERN:	2.565e-02	1.198e-02	6.465e-03	4.127e-03	2.461e-03	1.926e-04	1.145e-04	6.314e-05
	PROD:	6.055e-02	2.276e-02	9.664e-03	5.346e-03	2.454e-03	1.926e-04	1.212e-04	7.653e-05
	TSVQ:	1.563e-03	3.355e-03	2.268e-03	1.697e-03	9.138e-04	3.759e-04	6.863e-05	3.585e-05
0.5	GESS:	6.514e-03	4.386e-03	2.632e-03	2.079e-03	9.792e-04	3.759e-04	7.069e-05	3.894e-05
	KERN:	2.820e-02	1.322e-02	7.290e-03	4.674e-03	2.497e-03	3.759e-04	1.494e-04	7.831e-05
	PROD:	6.687e-02	2.631e-02	1.327e-02	6.010e-03	2.894e-03	3.759e-04	1.769e-04	1.146e-04
	TSVQ:	1.007e-03	3.621e-03	2.464e-03	2.227e-03	1.333e-03	6.586e-04	1.386e-04	7.679e-05
0.8	GESS:	6.426e-03	4.900e-03	3.601e-03	3.257e-03	1.521e-03	6.586e-04	1.418e-04	8.362e-05
	KERN:	3.132e-02	1.534e-02	1.042e-02	6.225e-03	3.412e-03	6.586e-04	2.345e-04	1.244e-04
	PROD:	7.025e-02	2.808e-02	1.602e-02	8.991e-03	4.766e-03	6.586e-04	4.581e-04	3.277e-04

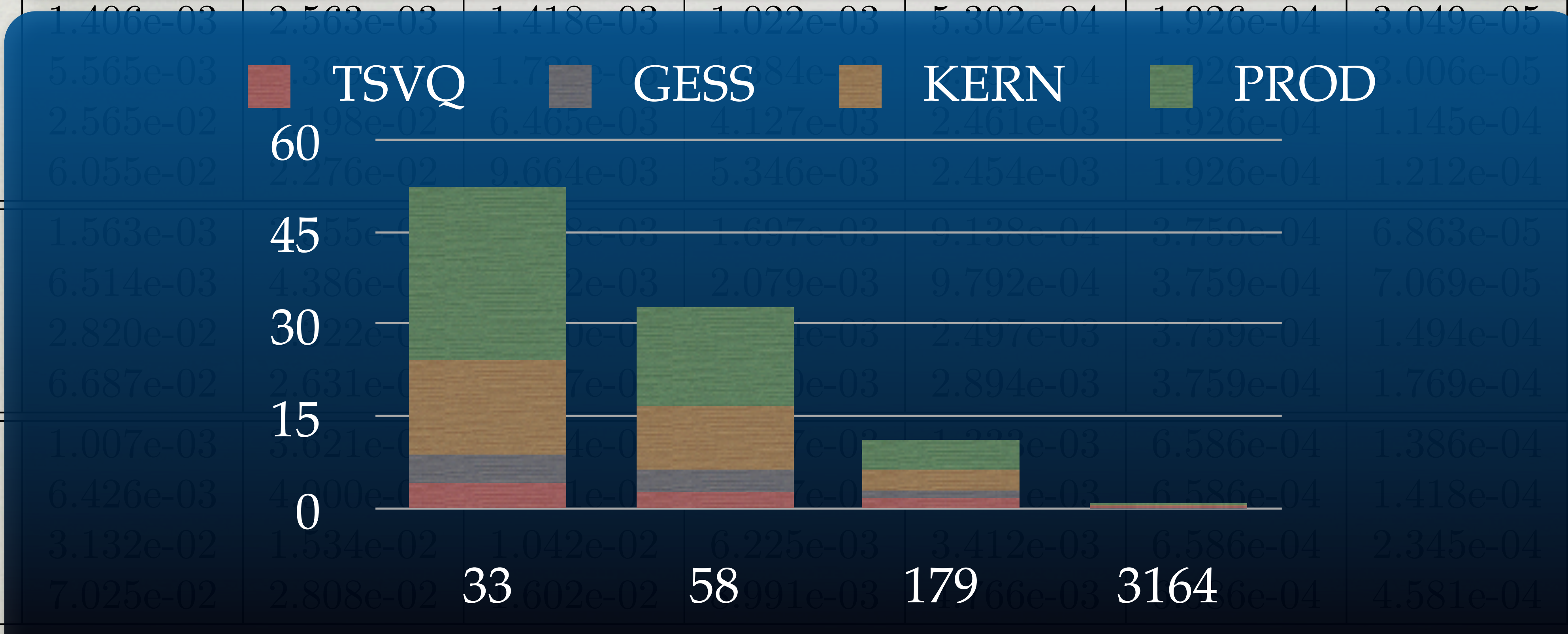
Variance for the non-parametric mutual information estimates (Gessaman partition scheme (GESS), tree-structured partition (TSVQ), classical product partition (PROD) and a kernel plug-in estimate (KERN))

Simulation Analysis

Setting ii)



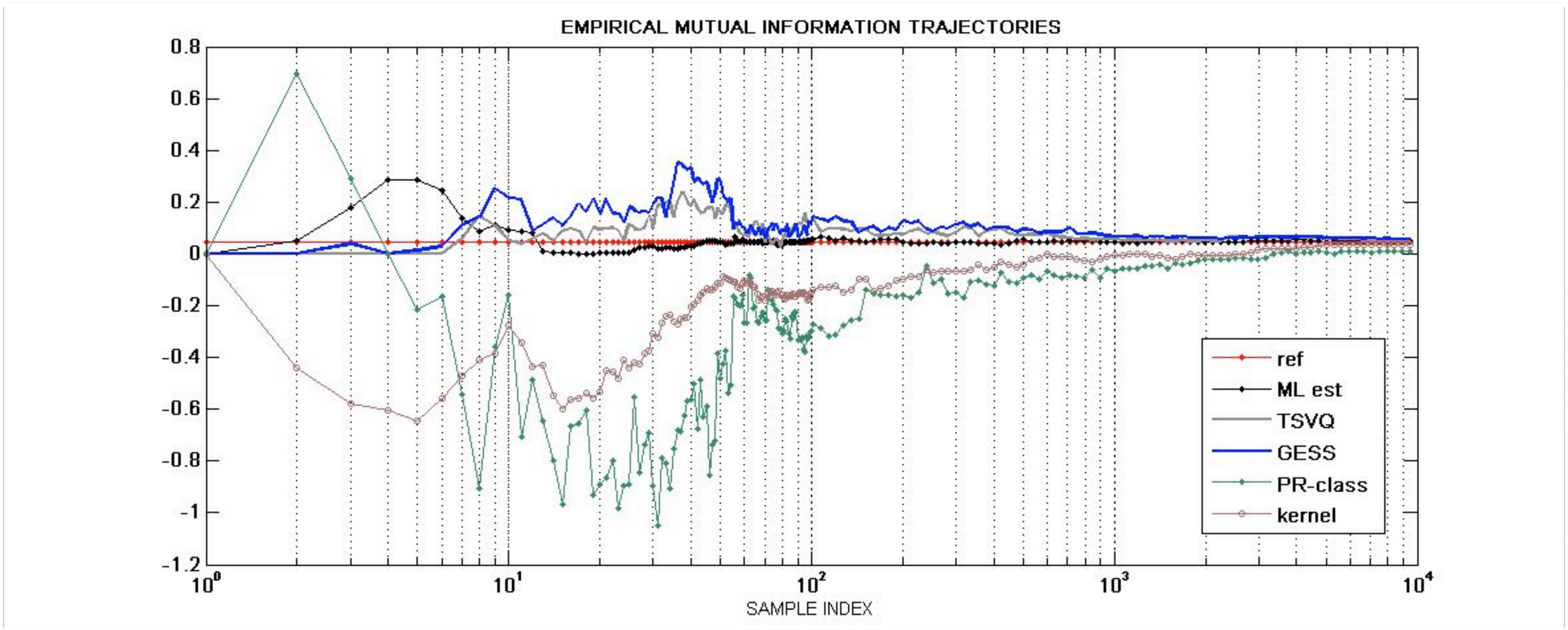
R	Method	5626
0	TSVQ:	1.534e-06
	GESS:	1.992e-06
	KERN:	4.941e-05
	PROD:	6.193e-05
0.3	TSVQ:	1.437e-05
	GESS:	1.632e-05
	KERN:	6.314e-05
	PROD:	7.653e-05
0.5	TSVQ:	3.585e-05
	GESS:	3.894e-05
	KERN:	7.831e-05
	PROD:	1.146e-04
0.8	TSVQ:	7.679e-05
	GESS:	8.362e-05
	KERN:	1.244e-04
	PROD:	3.277e-04



Varia... estimates (Gessaman partition scheme (GESS), tree-structured partition (TSVQ), classical product partition (PROD) and a kernel plug-in estimate (KERN)

Simulation Analysis

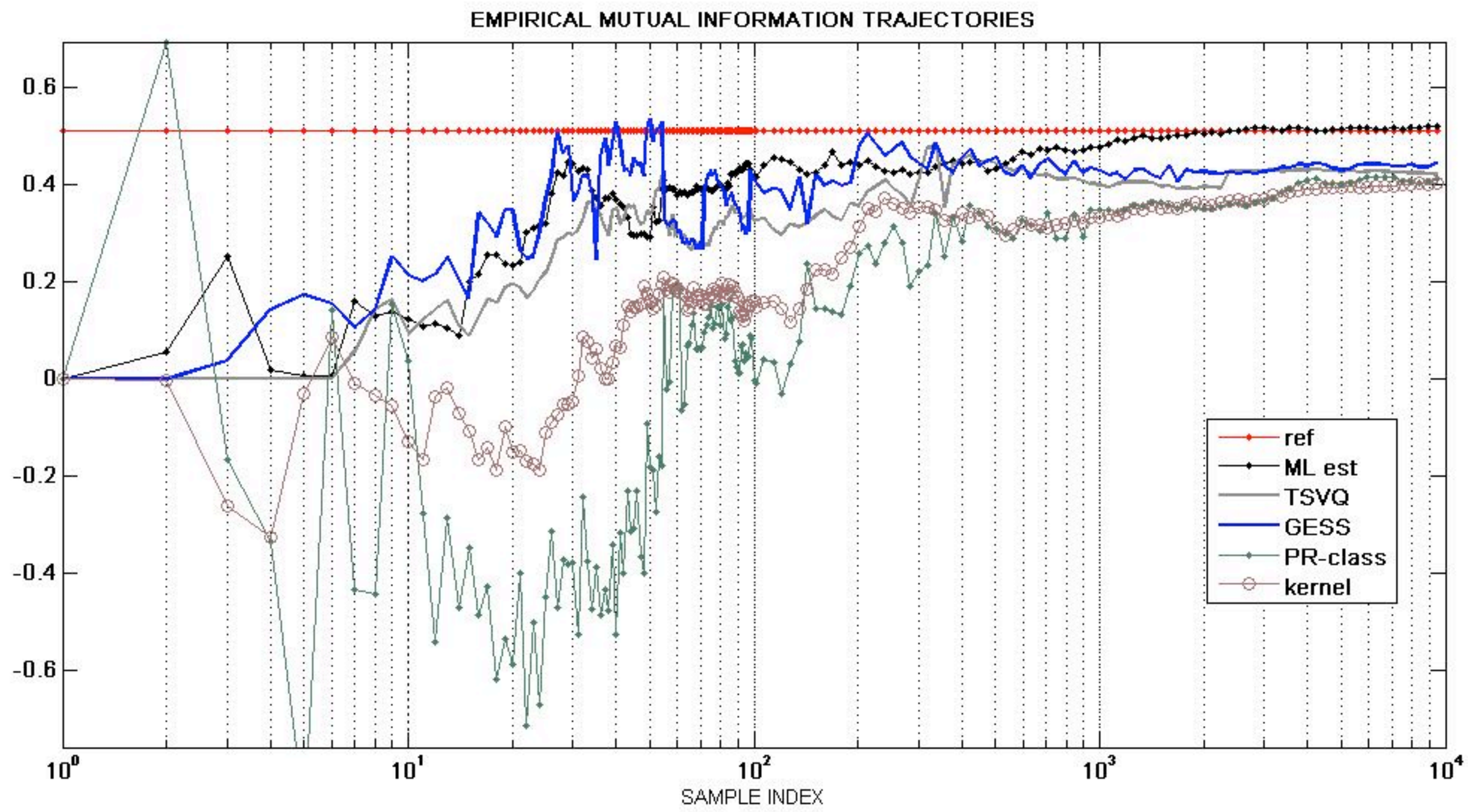
Setting ii)



Empirical mutual Information trajectories for different estimation techniques. Data simulated with correlation coefficient r=0.3

Simulation analysis

Setting ii)



Empirical mutual Information trajectories for different estimation techniques. Data simulated with correlation coefficient r=0.8

Extensions

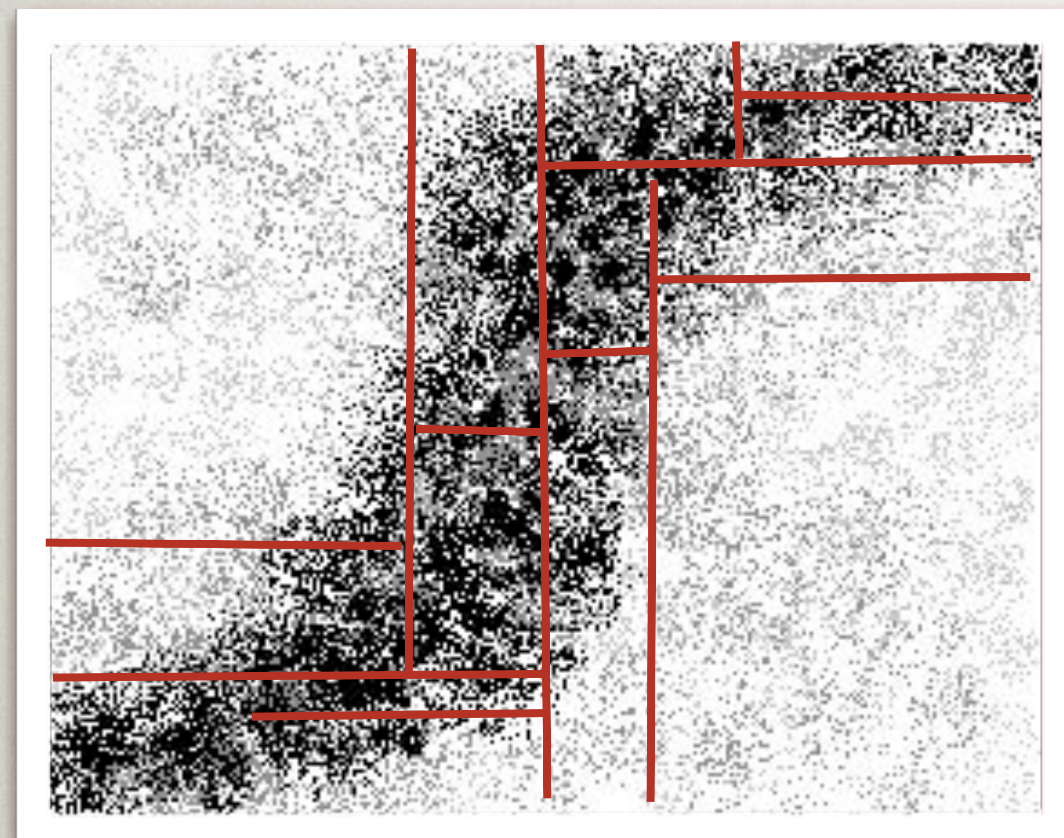
- Working in improvements for the case of TSP
- Applications in test of independence
- Similar results for the case of the KLD

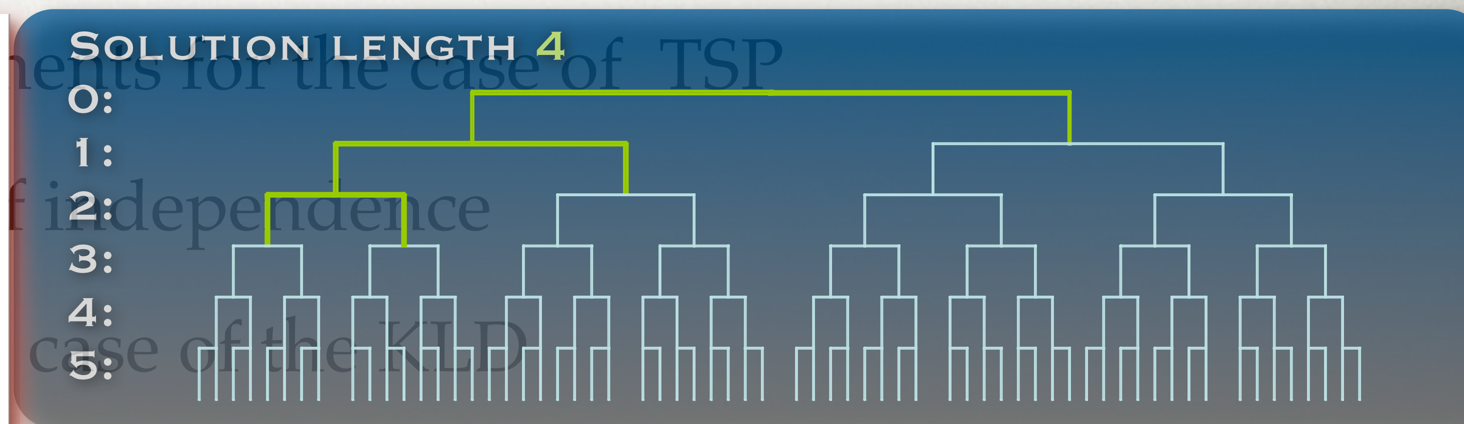
Extensions

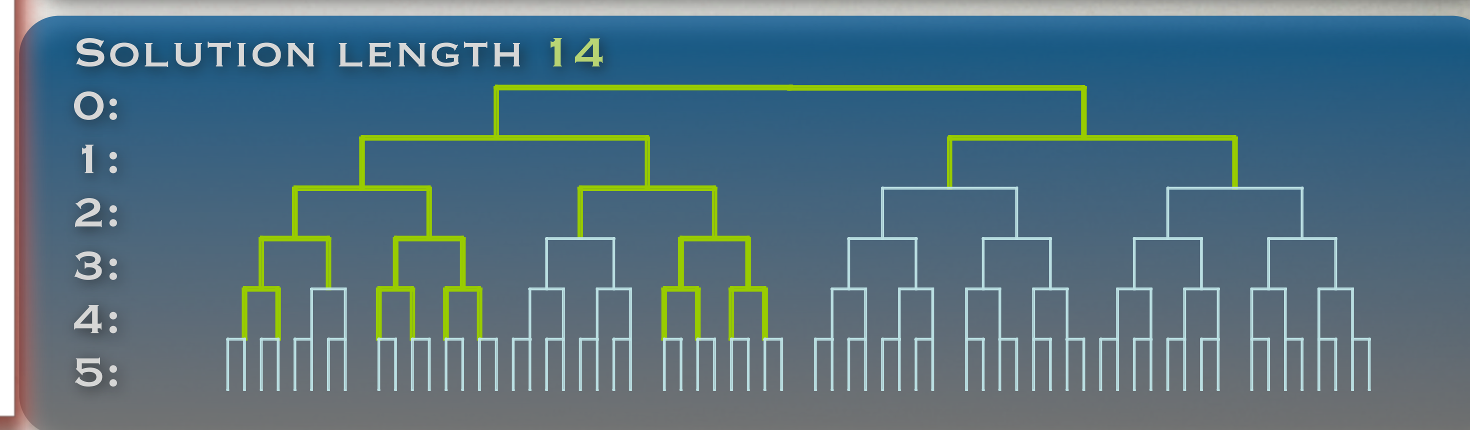
$$\hat{\mathbf{T}}^* = \arg \min_{T \ll \mathbf{T}_{full}} \left[L_{\mathcal{X}_T} - L_{\mathcal{X}} \right] + \Delta(\hat{P}_{X_T,Y}, P_{X_T,Y}).$$

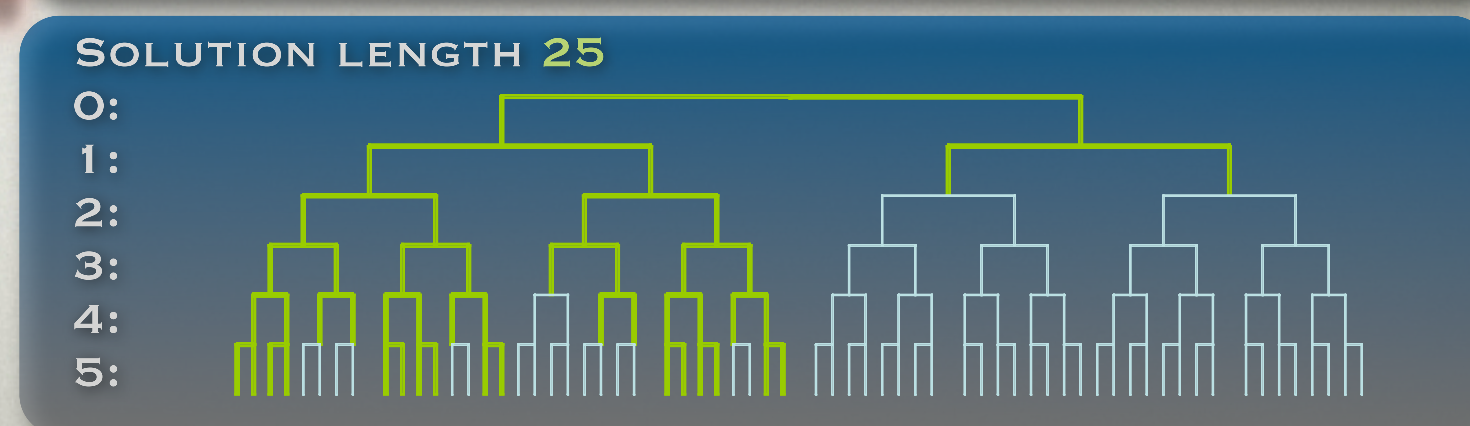
Approximation error

Estimation error









Extensions

- Working in improvements for the case of TSP
- Applications in test of independence
- Similar results for the case of the KLD

Thank you!