Estimating mutual information for high-dimensional sparse relationships

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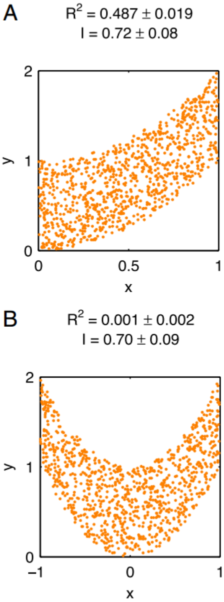
(Joint work with Yuval Benjamini, Hebrew University.)

Overview



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- measures dependence between two random vectors, $\vec{X}$ and $\vec{Y}$

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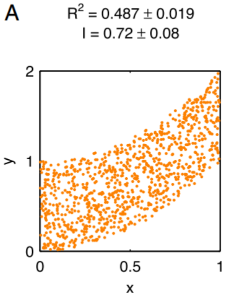

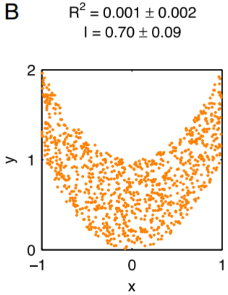

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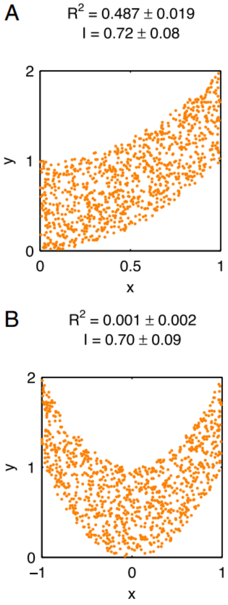

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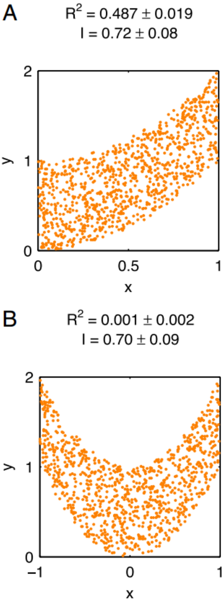

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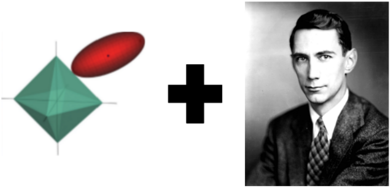
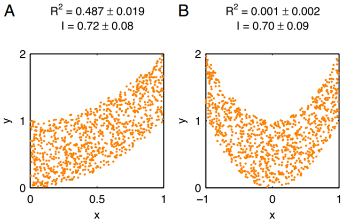
We combine *machine learning* (sparse estimation) with *information theory* to obtain better estimates of $I(\vec{X}; \vec{Y})$



Mutual information $I(X;Y)$



Introduced in Shannon's 1948 paper, "A mathematical theory of communication"

$$I(X;Y) = \int \log\left(\frac{p(x,y)}{p(x)p(y)}\right) p(x,y)dxdy$$

Image credit Kinney et al. 2014.

Applications of $I(X; Y)$

Mutual information has since been applied to many areas outside of information theory

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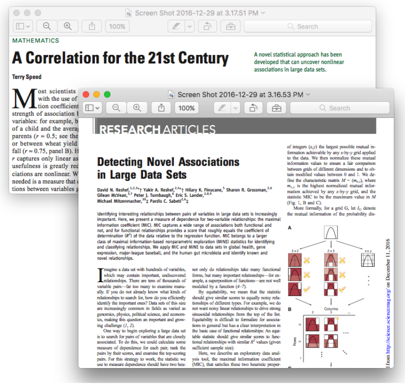
Applications [edit]

In many applications, one wants to maximize mutual information (thus

- In search engine technology, mutual information between phrases
- In telecommunications, the channel capacity is equal to the mutua
- Discriminative training procedures for hidden Markov models have
- RNA secondary structure prediction from a multiple sequence alig
- Phylogenetic profiling prediction from pairwise present and disapp
- Mutual information has been used as a criterion for feature selecti the minimum redundancy feature selection.
- Mutual information is used in determining the similarity of two diffe
- Mutual information of words is often used as a significance functio words; rather, one counts instances where 2 words occur adjacen another, goes up with N.
- Mutual information is used in medical imaging for image registratic reference image, this image is deformed until the mutual informati
- Detection of phase synchronization in time series analysis
- In the infomax method for neural-net and other machine learning,

Engineering, biology, computer science, physics, medicine

Comparing $I(X; Y)$ with Pearson correlation



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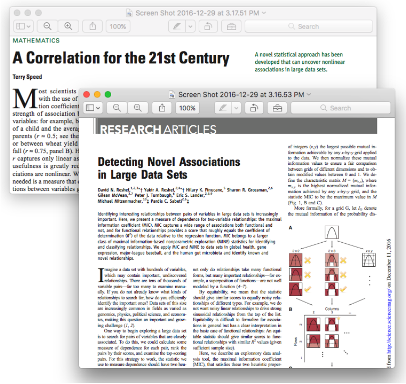

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- Only mutual information (and derived quantities) measures dependence directly

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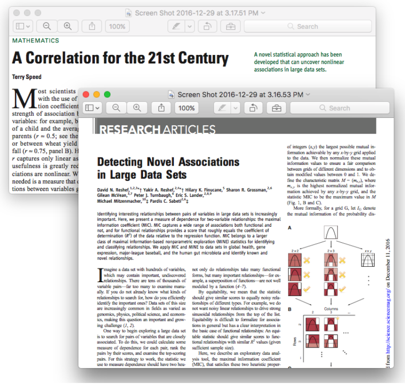

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Problems with mutual information

- Hard to interpret (compared to R^2)
- Hard to estimate (compared to R^2)

Can we make $I(X;Y)$ easier to interpret?

- Define the "informational correlation" (Linfoot 1957)

$$\mathrm{Cor}_{Info}(X,Y) = \sqrt{1 - e^{-2I(X;Y)}}$$

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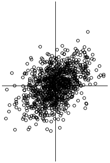
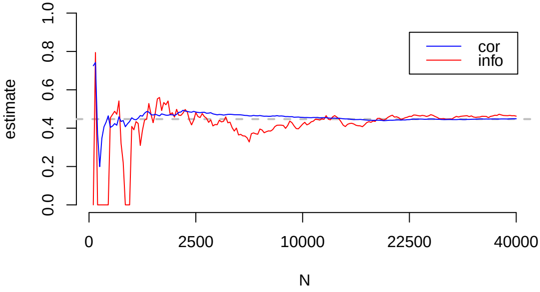
Difficulty of estimating $I(X; Y)$

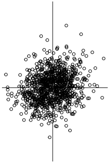
Example with $\text{Cor}_{Pearson}(X, Y) = \text{Cor}_{Info}(X, Y) = 0.44$.

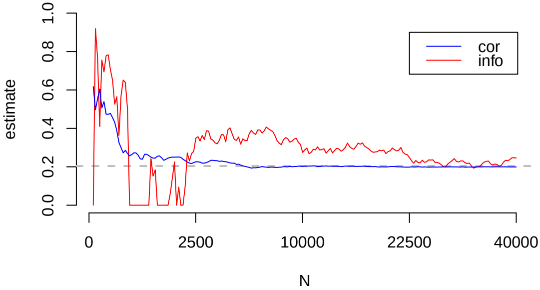




Difficulty of estimating $I(X; Y)$

Example with $\text{Cor}_{Pearson}(X, Y) = \text{Cor}_{Info}(X, Y) = 0.2$.





How to estimate $I(X; Y)$

Suppose we observe pairs $(X_i, Y_i)_{i=1}^n$ iid from density $p(x, y)$

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- Kernel density estimate approaches estimate $p(x, y)$ (Beirlant et al. 2001, Ivanov and Rozhkova 1981)
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Suppose we observe pairs $(X_i, Y_i)_{i=1}^n$ iid from density $p(x,y)$

- **Plug-in estimate**:

$$\hat{I}(X;Y) = \int \log\left(\frac{\hat{p}(x,y)}{\hat{p}(x)\hat{p}(y)}\right)\hat{p}(x,y)dxdy$$

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Problems in high dimensions

- Density estimation is known to have *exponential complexity* with respect to dimensionality.
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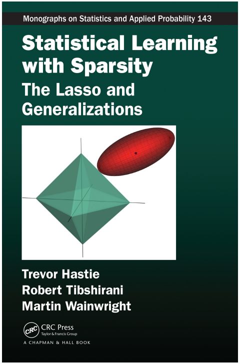
- One approach is to assume joint multivariate normality of X, Y, but this reduces mutual information to a linear statistic.
- Other approaches: binning (Bialek et al. 1991, Paninski 2003), confusion matrix of a classifier (Treves 1997, Quiroga et al. 2009)

First idea: Use sparsity!



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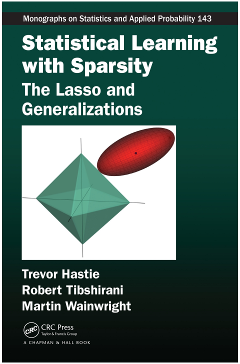

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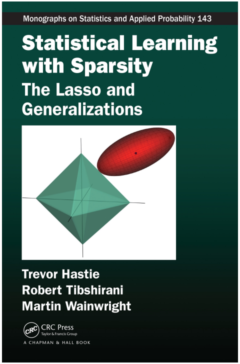
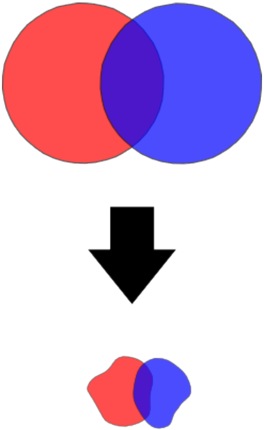


- *Sparsity* refers to existence of low-dimensional structure hidden in high-dimensional data.
- E.g. suppose X is 100-dimensional but Y is only a function of (X_5, X_9).
- Can we exploit sparsity to obtain a good estimate of $I(X;Y)$ even under low sample sizes?

Dimension reduction vs. sparsity?



Unsupervised dimension reduction

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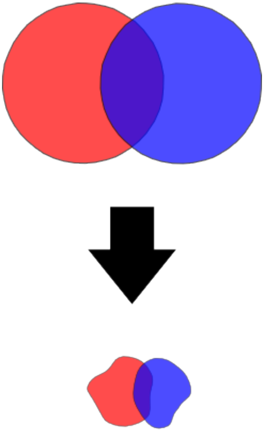

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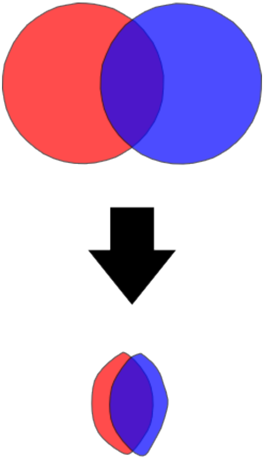

Sparsity = supervised dim. reduction

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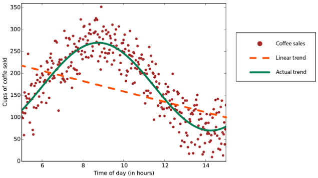
- If $I(X; Y) > 0$, then X carries information about Y and vice-versa.
- Therefore, we can *predict* Y from X (or X from Y)
- We know that often *prediction accuracy* implies a lower bound for *mutual information* (e.g. Fano 1952)

Background: Regression



- Suppose you observe $(\vec{X}^{(i)}, Y^{(i)})_{i=1}^n$ where $Y^{(i)} = f(\vec{X}^{(i)}) + \epsilon$, where f is an unknown function and ϵ is noise. (Also, assume $\mathbf{E}[\epsilon] = 0$.)

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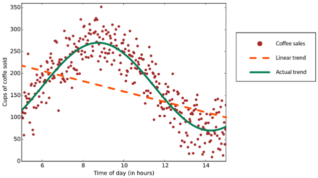

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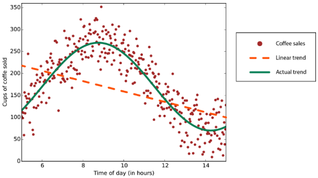

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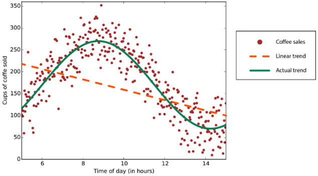

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- The goal in regression is to recover the unknown function f.
- In *linear regression*, we assume f is linear.
- if we do not assume a particular form for f, we can use *nonparametric regression*.

Background: Sparse regression

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	Classical	*Sparse*
Linear	Ordinary Least-Squares (Legendre 1805)	Elastic net (Zou 2008)
Nonpar.	LOWESS (Cleveland 1979)	Random forests (Breiman 2001)

Our proposal

Suppose we observe pairs $(X_i, Y_i)_{i=1}^n$ iid from density $p(x, y)$.

1. Estimate a (sparse) regression model for $\mathbf{E}[y|x]$.
2. Assess the *prediction accuracy* of the model using *identification risk*
3. Use the identification risk to obtain a lower bound for the mutual information $I(X; Y)$

Multiple-response regression

- Pairs $(x_i, y_i)_{i=1}^n$, where X is p-dimensional and Y is q-dimensional.
- Data matrices $\boldsymbol{X}_{n\times p}$, $\boldsymbol{Y}_{n\times q}$.
- For each column of Y, fit sparse model $Y^{(i)} \approx X^T\beta^{(i)} + \epsilon$, e.g. by using elastic net (Zou 2008),

$$\hat{\beta}^{(i)} = \text{argmin}_\beta ||\boldsymbol{X}^T\beta^{(i)} - Y^{(i)}||^2 + \lambda_2||\beta^{(i)}||_2^2 + \lambda_1||\beta^{(i)}||_1$$

- Or, fit a *random forest* model for each column of Y (Breiman 2001)

Regression vs Identification loss

- Independent *test set* $(x_i^*, y_i^*)_{i=1}^k$.
- Use model to predict $\hat{y}_i^* = (x_i^*)^T \hat{B}$ for $i = 1, \ldots, k$.

Two ways to evaluate the predictive accuracy of the regression model:

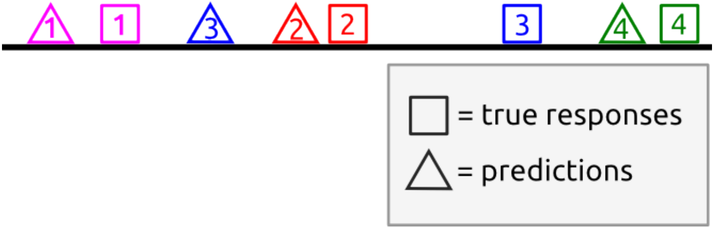
- Regression (mean squared-error) loss:

$$\text{MSE} = \frac{1}{k} \sum_{i=1}^k ||y_i^* - \hat{y}_i^*||^2.$$

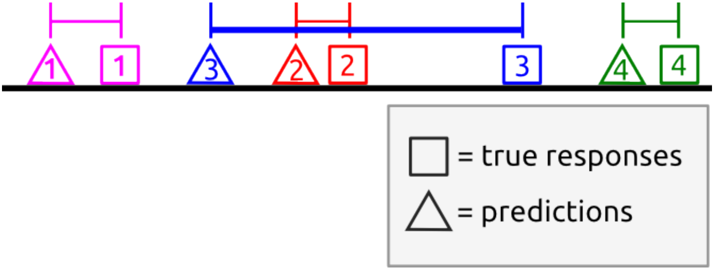
- Identification loss (Kay 2008):

$$\text{IdLoss}_k = \frac{1}{k} \sum_{i=1}^k (1 - I\{\hat{y}_i^* \text{ is nearest neighbor of } y_i^*\}).$$

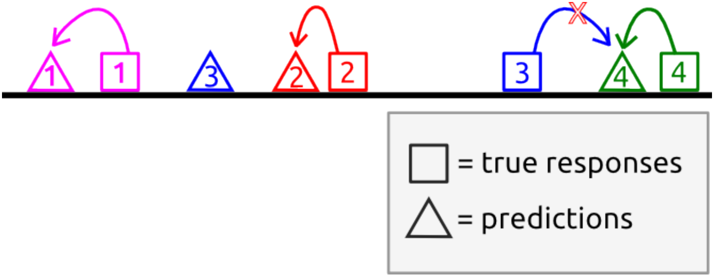
Regression vs Identification loss



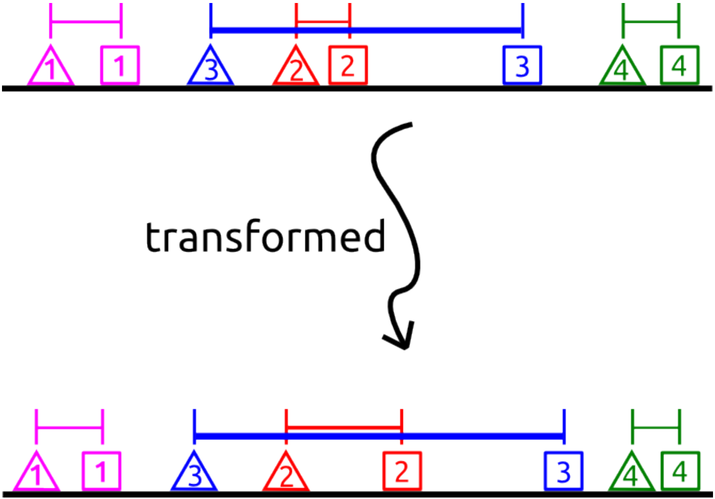
Mean-squared error



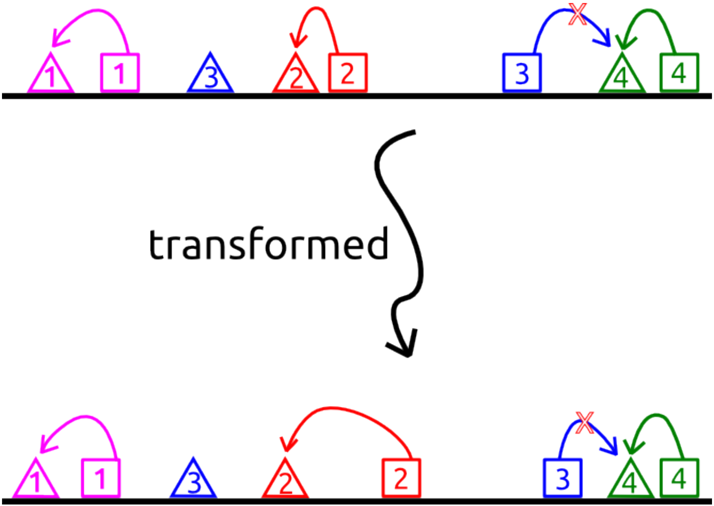
Identification loss



Mean-squared error changes under nonlinear scaling



Identification loss robust under nonlinear scaling



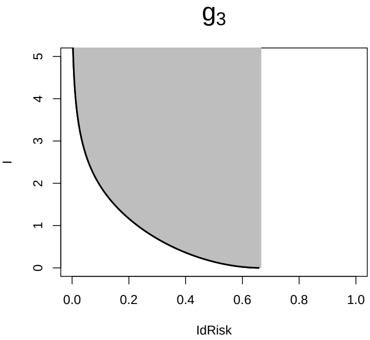
Identification loss and mutual information

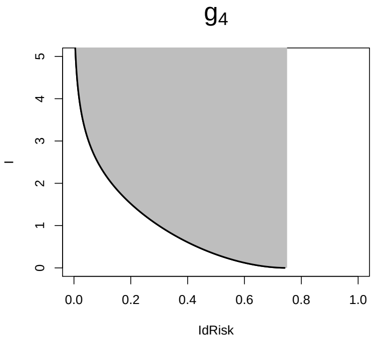
- Define the identification risk as the expected identification loss

$$\text{IdRisk}_k = \mathbf{E}[\text{IdLoss}_k]$$

- **Theorem.** (Z., Benjamini 2017) There exists a function g_k such that

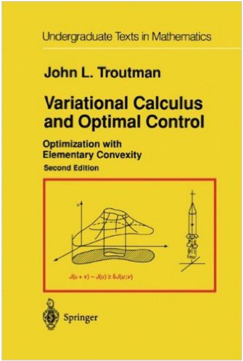
$$I(X;Y) \geq g_k(\text{IdRisk}_k).$$





Proof details

We use *calculus of variations* to obtain this result.



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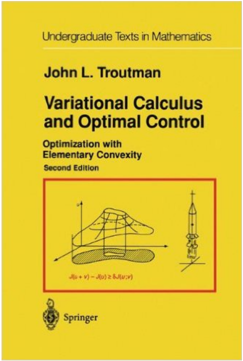

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- Mutual information is a functional of $p(x, y)$.

$$\mathrm{I}[p(x,y)] = \mathbf{E}\left[\log \frac{p(X,Y)}{p(X)p(Y)}\right].$$

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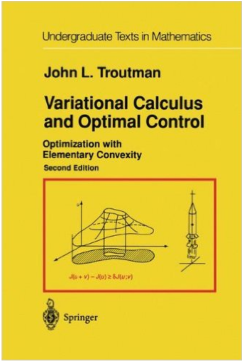

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- Identification risk is *lower-bounded* by another functional–the *Bayes risk*.

$$\mathrm{BayesRisk}_k[p(x,y)] = 1 - \mathbf{E}[\max_{i=1}^{k} p(Y|X_i)].$$

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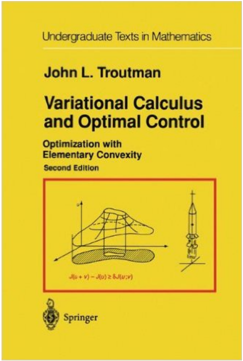

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$$\text{BayesRisk}_k[p(x, y)] = 1 - \mathbf{E}[\max_{i=1}^{k} p(Y|X_i)].$$

- $g_k(u) = \inf_{p(x,y)} I[p(x, y)]$

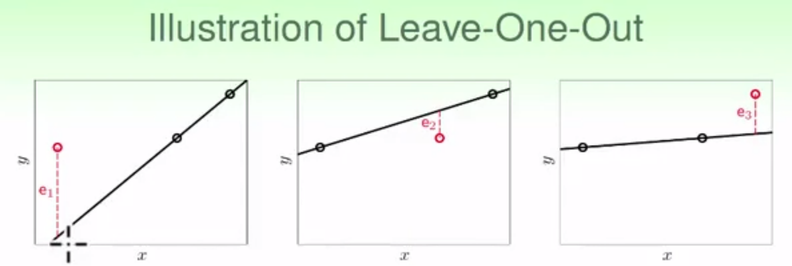
$$\text{subject to } \text{BayesRisk}_k[p(x, y)] \geq u.$$

Our proposal

Suppose we observe pairs $(X_i, Y_i)_{i=1}^n$ iid from density $p(x, y)$.

1. Estimate a (sparse) regression model for $\mathbf{E}[y|x]$.
2. Compute *identification loss*, IdLoss_k, using *leave-k-out*.
3. Estimate mutual information using

$$\hat{I}_{IdLoss}(X; Y) = g_k(\text{IdLoss}_k).$$



- Randomly hold out a subset of size k.
- Use remaining data to predict the held-out data.
- Obtain the average prediction error.

Image credit Hsuan-Tien Lin

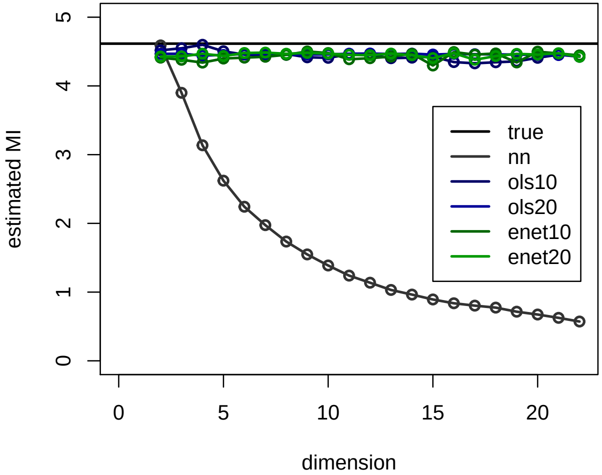
Section 2

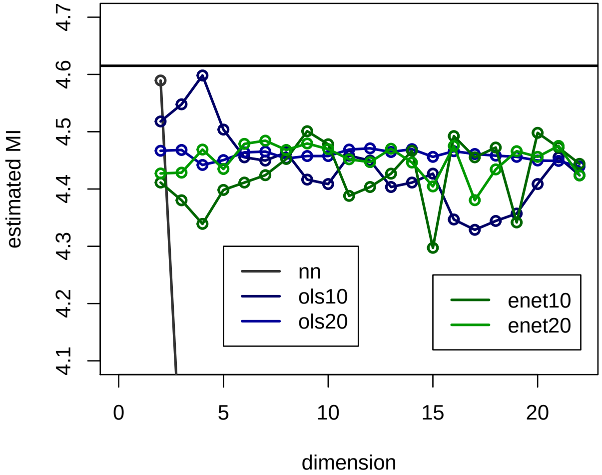
Applications

Simulation

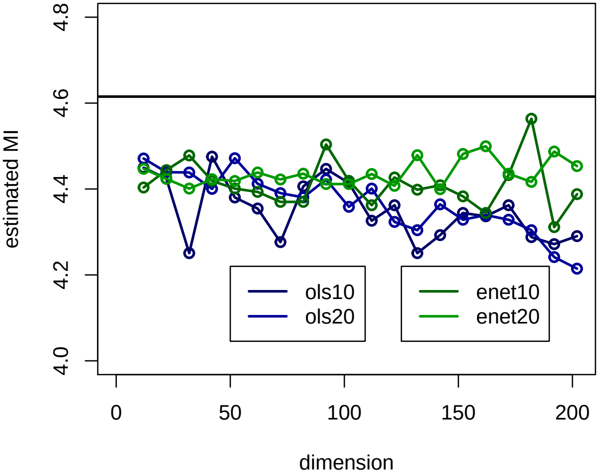
- Generate data: $(Y_1, Y_2) = (X_1, X_2)^T B + \epsilon$ where B is a randomly generated coefficient matrix.
- Add extra noise dimensions $X_3, X_4, \ldots$.
- $n = 1000$.
- Compare Nearest-Neighbor estimator (Mnatsakov et al, 2008, implemented in `FNN`) with our method using OLS and elastic net (sparse).

Simulation Results - I. low dimension

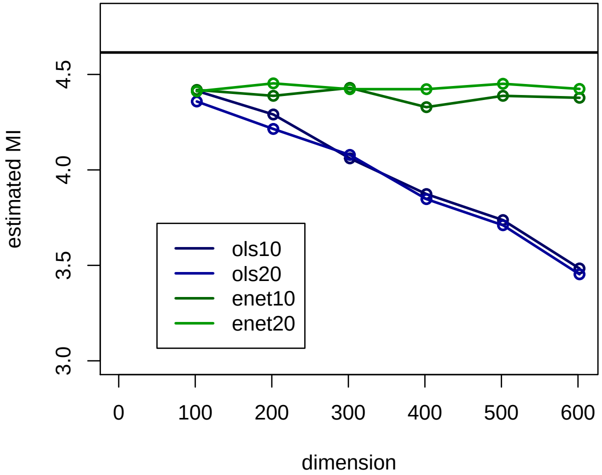



estimated MI
4.1
4.2
4.3
4.4
4.5
4.6
4.7
0
5
10
15
20
dimension
nn
ols10
ols20
enet10
enet20

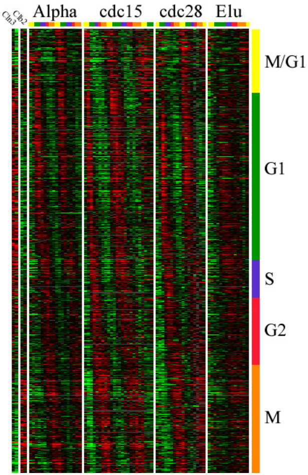
Simulation Results - II. medium dimension



Simulation Results - III. high dimension



Application to gene expression time series



- Data from Spellman et al. 1998
- Expression levels of 6178 yeast genes during cell cycle
- Total 73 time points per gene

Groups of genes

Group	No. genes
unknown	396
cell cycle	27
DNA replication	27
transport	19
cytoskeleton	17
chromatin structure	16

Total 145 different categories (only top 6 shown).

Canonical correlations between time series

Top canonical correlation (Hotelling 1936)

	CC	DR	Tr	Cy	CS
CC		1	1	1	1
DR			1	0.99	0.99
Tr				0.99	0.98
Cy					0.98
CS					

CC = cell cycle, DR = DNA replication, Tr = transport,
Cy = cytoskeleton, CS = chromatin structure

Sparse canonical correlations between time series

Using sparse CCA* (Witten and Tibshirani 2009).

	CC	DR	Tr	Cy	CS
CC		0.96	0.87	0.92	0.94
DR			0.83	0.88	0.95
Tr				0.83	0.78
Cy					0.90
CS					

CC = cell cycle, DR = DNA replication, Tr = transport,
Cy = cytoskeleton, CS = chromatin structure

*: using `CCApermute` in R package `PMA`

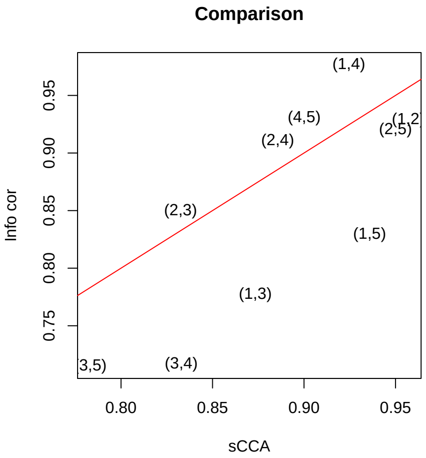
Information correlations between time series

Taking the max of $\hat{I}(X;Y)$ and $\hat{I}(Y;X)$.

	CC	DR	Tr	Cy	CS
CC		0.93	0.78	0.98	0.83
DR			0.85	0.91	0.92
Tr				0.72	0.71
Cy					0.93
CS					

CC = cell cycle, DR = DNA replication, Tr = transport,
Cy = cytoskeleton, CS = chromatin structure

Comparing sparse CCA and Cor_{Info}



(1) cell cycle, (2) DNA replication, (3) transport,
(4) cytoskeleton, (5) chromatin structure

Invariance properties

Transform data from each group with random rotation...

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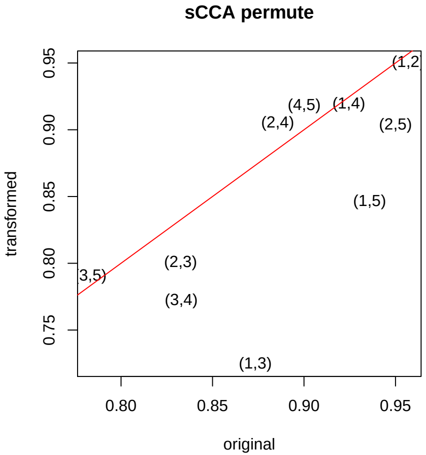
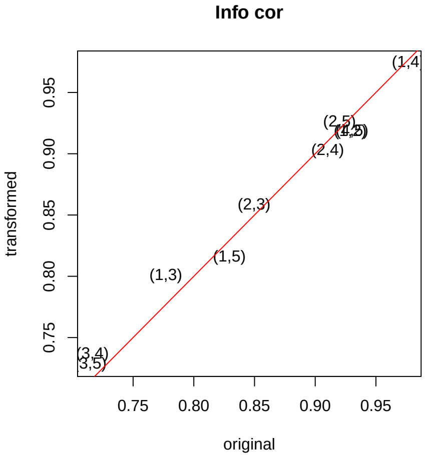


Transform data from each group with random rotation...



Conclusions

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Conclusions

- Mutual information, and derived Cor_{Info} are useful measures of correlation, but hard to estimate.
- Our method targets high-dimensional data with sparsity.
- How to use: choose a regression model suited to the model assumptions. Our method allows you to convert the prediction accuracy of the model, IdLoss_k into an estimate of $I(\vec{X}; \vec{Y})$.
- Example application: measure of joint information between two tables which is robust to transformations.

Related work and future directions

- What if data is high-dimensional, but not sparse? We have another method based on high-dimensional asymptotics (ZB 2016).

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- Estimating quantities related to mutual information, such as *transfer information*, *stimulus-specific information* and *redundancy* (Borst and Theunissen 1999)

Related work and future directions

- What if data is high-dimensional, but not sparse? We have another method based on high-dimensional asymptotics (ZB 2016).
- Estimating quantities related to mutual information, such as *transfer information*, *stimulus-specific information* and *redundancy* (Borst and Theunissen 1999)
- Inferring resting-state brain networks.

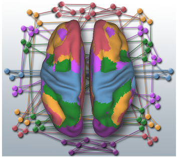

Image credit Simons Foundation

Section 3

The End

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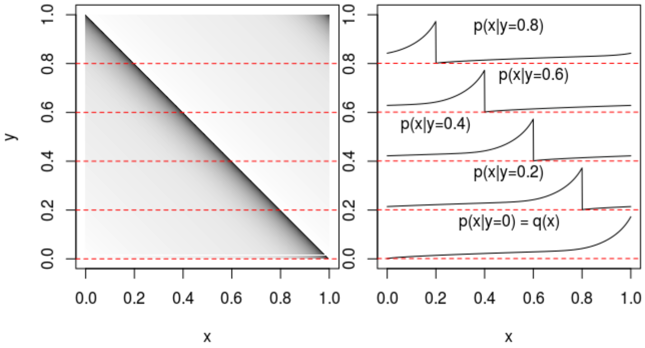
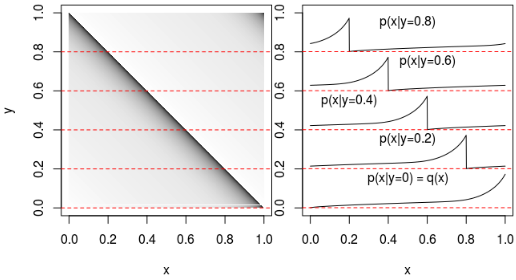
Reduced Problem

Rather than show the whole proof, we consider a simplified problem to illustrate the methods.



Actually, the simplified problem is equivalent to the full problem and we get the same answer (but this is non-trivial).

Reduced Problem



- $p(x, y)$ on unit square with uniform marginals.
- The conditional distributions $p(x|y)$ are just "shifted" copies of a common density, $q(x)$, on $[0, 1]$

$$p(x|y) = q(x - y + I\{x < y\})$$

- Furthermore, $q(x)$ is increasing in x.

Simplified formulae

The information and average Bayes error can be written in terms of $q(x)$.

$$\mathrm{I}[p(x,y)] = \int_0^1 q(x) \log q(x) dx$$

$$\mathrm{BayesAcc}_k[p(x,y)] = \int_{[0,1]^k} \max_{i=1}^{k} q(x_i) dx_1 \cdots dx_k$$

Simplified formulae

Overload the notation and "redefine" information and average Bayes error as functionals of $q(x)$.

$$\mathrm{I}[q(x)] \stackrel{def}{=} \int_0^1 q(x) \log q(x) dx$$

$$\text{BayesAcc}_k[q(x)] \stackrel{def}{=} \frac{1}{k} \int_{[0,1]^k} \max_{i=1}^k q(x_i) dx_1 \cdots dx_k$$

Optimization problem

We now pose the question: how do we find $q(x)$ which maximizes $\text{BayesAcc}_k[q(x)]$ subject to $\text{I}[q(x)] \leq \iota$?

- *Domain of the optimization*: Recall that $q(x)$ satisfies $q(x) \geq 0$, $\int_0^1 q(x)dx = 1$, and is increasing in x. Let $\mathcal{Q}$ denote the space of functions on $[0,1] \to [0,\infty)$ which are increasing in x.
- *Constraints*: We have two remaining constraints, $\text{I}[q(x)] \leq \iota$ and $\int_0^1 q(x)dx = 1$.

Hence the problem is

$$\text{maximize}_{q(x)\in\mathcal{Q}} \text{ BayesAcc}_k[q(x)] \text{ subject to } \int_0^1 q(x)dx = 1 \text{ and } \text{I}[q(x)] \leq \iota.$$

Optimization problem

$$\text{maximize}_{q(x)\in\mathcal{Q}} \text{ BayesAcc}_k[q(x)] \text{ subject to } \int_0^1 q(x)dx = 1 \text{ and } \mathrm{I}[q(x)] \le \iota.$$

- Does a solution exist? *Yes*, because the space of measures with density $q(x)$ satisfying $\mathrm{I}[q(x)] \le \iota$ is tight, and both the constraints and objective are continuous wrt to the topology of weak convergence.
- Given a solution $q^*(x)$ exists, there exist Lagrange multipliers $\lambda \in \mathbb{R}$ and $\nu > 0$ such that q^* minimizes

$$\mathcal{L}[q(x)] = -\text{BayesAcc}_k[q(x)] + \lambda \int_0^1 q(x)dx + \nu \mathrm{I}[q(x)]$$
$$= \int_0^1 (-t^{k-1} + \lambda + \nu \log q(x))q(x)dx.$$

Functional derivatives

- Taylor explansions are a useful trick for computing functional derivatives
- We can compute the functional derivative of $\mathcal{L}[q(x)]$ by writing

$$\begin{aligned}
&\mathcal{L}[q(x) + \epsilon\xi(x)] \\
&\quad = \int_0^1 (-t^{k-1} + \lambda + \nu \log(q(x) + \epsilon\xi(x)))(q(x) + \epsilon\xi(x))dx. \\
&\quad \approx \int (q(x)+\epsilon\xi(x))(-t^{k-1} + \lambda + \nu\{\log q(x) + \frac{\epsilon\xi(x)}{q(x)}\})dx \\
&\quad \approx \mathcal{L}[q(x)] + \int_0^1 (-t^{k-1} + \lambda + \nu(1 + \log q(x))\epsilon\xi(x)dx.
\end{aligned}$$

- Hence

$$\nabla\mathcal{L}[q](x) = -t^{k-1} + \lambda + \nu(1 + \log q(x))$$

Variational magic!

Suppose we set the functional derivative to 0,

$$0 = \nabla \mathcal{L}[q](t) = -t^{k-1} + \lambda + \nu + \nu \log q(t).$$

Then we conclude that the optimal $q^*(t)$ takes the form

$$q^*(t) = \alpha e^{\beta t^{k-1}}$$

for some $\alpha > 0$, $\beta > 0$.
From the constraint $\int q(t)dt = 1$, we get

$$q_\beta(t) = \frac{e^{\beta t^{k-1}}}{\int e^{\beta t^{k-1}} dt}.$$

Result

Theorem. For any $\iota > 0$, there exists $\beta_\iota \geq 0$ such that defining

$$q_\beta(t) = \frac{\exp[\beta t^{k-1}]}{\int_0^1 \exp[\beta t^{k-1}]},$$

we have

$$\int_0^1 q_{\beta_\iota}(t) \log q_{\beta_\iota}(t) dt = \iota.$$

Then,

$$\sup_{I(X;Y)=\iota} \text{BayesAcc}_k = \int_0^1 q_{\beta_\iota}(t) t^{k-1} dt = g_k^{-1}(\iota).$$