Estimating mutual information for high-dimensional sparse relationships

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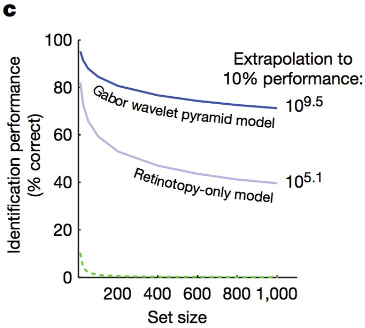
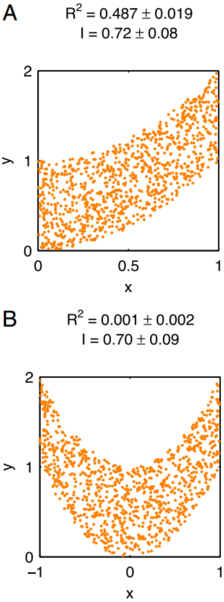
(Joint work with Yuval Benjamini, Hebrew University.)

Introduction



- Much of my work has been inspired by use of machine learning in encoding/decoding models in fMRI (Kay et al. 2008, Nishimoto et al. 2011)
- E.g.: Extrapolating classification accuracy curves (Z., Achanta, and Benjamini 2016)

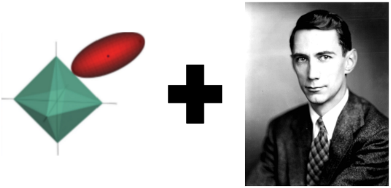
This talk



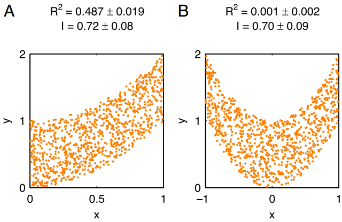
Mutual information $I(\vec{X}; \vec{Y})$

- measures dependence between two random vectors, $\vec{X}$ and $\vec{Y}$
- applies to nonlinear and multidimensional relationships (unlike correlation)
- is *difficult to estimate* in high dimensions

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

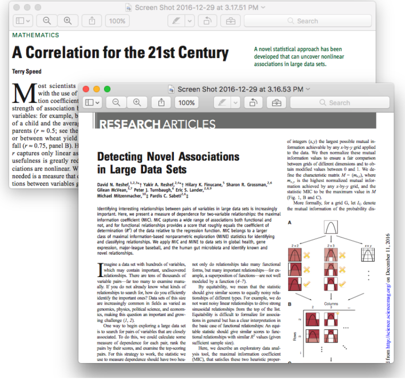
Applications [edit]

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 registratio 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



- In many applications scientists are interested in *dependence*, not *correlation* (Reshef et al. 2011, Speed 2011).
- Only mutual information (and derived quantities) measures dependence directly.

Problems with mutual information

- Hard to interpret (compared to R^2)
  - Define the "informational correlation" (Linfoot 1957)

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

  - Then $\text{Cor}_{Info}(X, Y) \in [0, 1]$.
  - For (X, Y) bivariate normal,

$$|\text{Cor}_{Pearson}(X, Y)| = \text{Cor}_{Info}(X, Y)$$

- Hard to estimate (compared to R^2)

How to estimate $I(X; Y)$

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

- Definition of mutual information:

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

- Kernel density estimate approaches estimate $p(x, y)$ (Beirlant et al. 2001, Ivanov and Rozhkova 1981)
- Nearest neighbor estimators rely on distance-based computations (Mnatsakanov et al. 2008, Goria et al. 2005, Singh et. al. 2003)

How to estimate $I(X; Y)$

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

- **Plug-in estimate**:

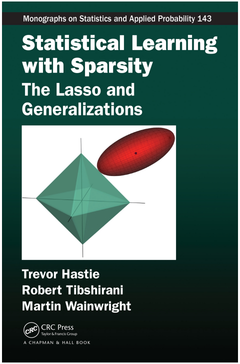
$$\hat{I}(X; Y) = \int \log \left(\frac{\hat{p}(x, y)}{\hat{p}(x)\hat{p}(y)} \right) \hat{p}(x, y) dxdy$$

- Kernel density estimate approaches estimate $p(x, y)$ (Beirlant et al. 2001, Ivanov and Rozhkova 1981)
- Nearest neighbor estimators rely on distance-based computations (Mnatsakanov et al. 2008, Goria et al. 2005, Singh et. al. 2003)

Problems in high dimensions

- Density estimation is known to have *exponential complexity* with respect to dimensionality.
  - E.g. to get the same precision, you need 10 observations for univariate X, Y but 1000 for trivariate $\vec{X}, \vec{Y}$.
- Many applications with high-dimensional X, Y.
  - Gene expression time series
  - Functional magnetic resonance imaging
- 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)

New idea: Use sparsity!



- *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?

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 $\mathbf{E}[\vec{Y}|\vec{X}]$.
2. Assess the *prediction accuracy* of the model using *identification loss* (Kay et al. 2008)
3. Use the identification loss to obtain a lower bound for the mutual information $I(X; Y)$

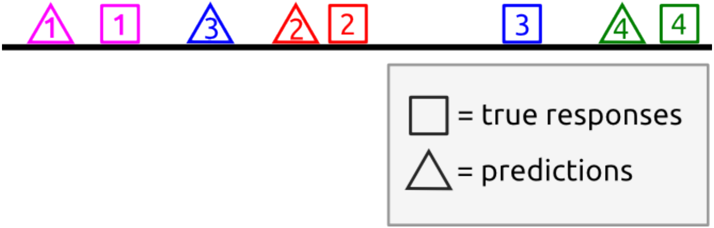
Multiple-response regression

- 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),

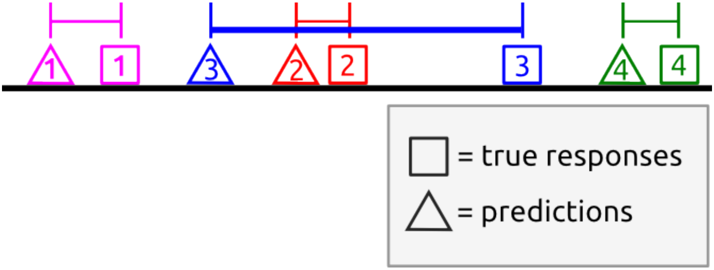
$$\hat{\beta}^{(i)} = \text{argmin}_\beta ||\boldsymbol{X}^T\beta^{(i)} - Y^{(i)}||^2 + \lambda_2||\beta^{(i)}||_2^2 + \lambda_1||\beta^{(i)}||_1$$

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

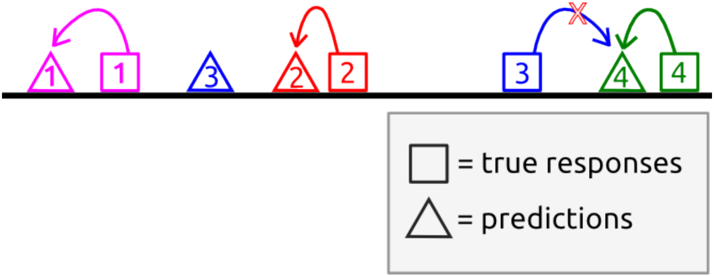
Regression vs Identification loss



Mean-squared error



Identification loss



- First used by Kay et al. (2008) to compare accuracy of center-surround model of V1 versus Gabor filter model of V1.
- We are the first to explore theoretical properties of the loss (e.g. connection to mutual information)

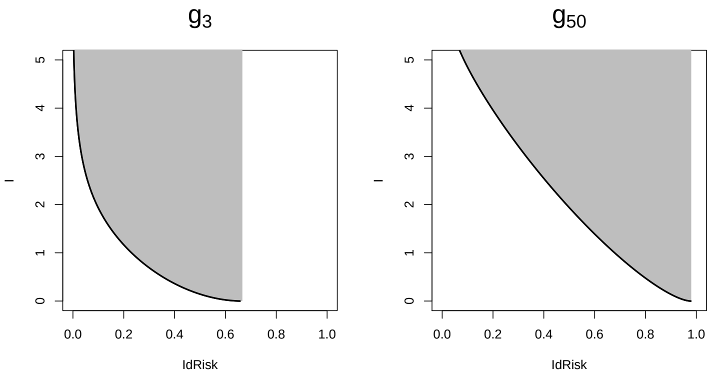
Identification loss and mutual information

- Define the identification risk as the expected identification loss

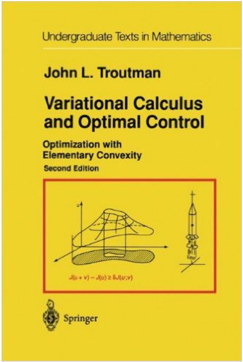
$$\mathrm{IdRisk}_k = \mathbf{E}[\mathrm{IdLoss}_k]$$

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

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



Proof details



- Variational calculus allows optimization of *functionals*.
- Mutual information is a functional of $p(x, y)$.

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

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

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

- $g_k(u)$ obtained by minimizing $\mathrm{I}[p(x,y)]$ subject to $\mathrm{BayesRisk}_k[p(x,y)] \leq u$.

Result

Theorem. (Z., Benjamini 2017) For any $\iota > 0$ and $k = 2, 3, \ldots$, 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, there exists a function g_k such that

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

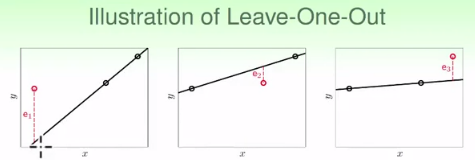
defined by

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

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 $\mathbf{E}[\vec{Y}|\vec{X}]$.
2. Compute *identification loss*, IdLoss_k, using *leave-k-out*.



3. Estimate mutual information using

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

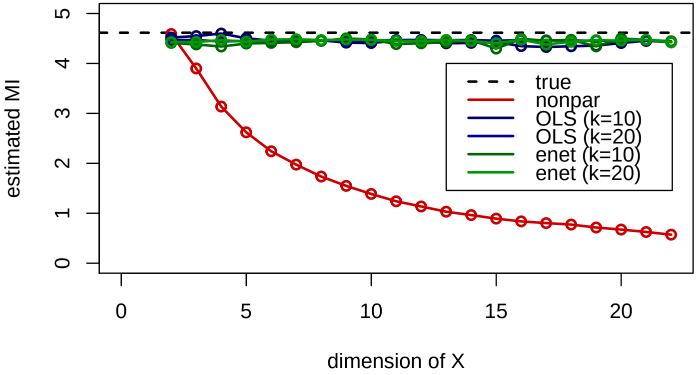
Section 2

Applications

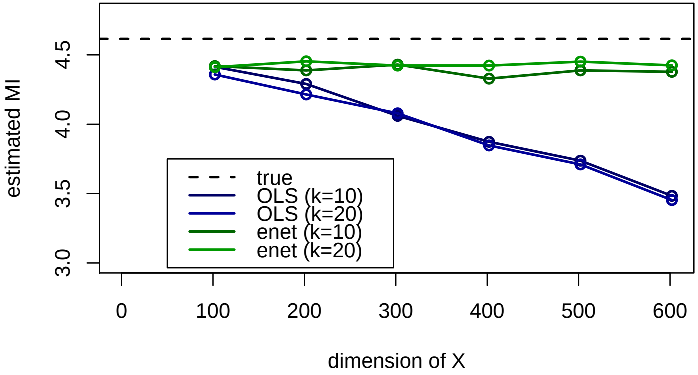
Simulation

- 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



Simulation Results - III. high dimension



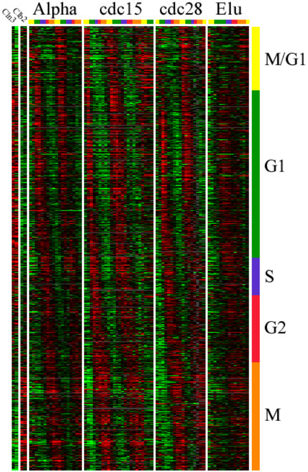
Application to gene expression time series

- Suppose we have *groups* of genes, $\vec{X}^{(1)}, \ldots, \vec{X}^{(m)}$.
- Each group may consist of a different number of genes, p_i.
- Goal: estimate the informational correlation

$$\text{Cor}_{Info}(\vec{X}^{(i)}, \vec{X}^{(j)})$$

  between each pair, $i \neq j$.
- Conclusion: find groups which are high predictive of each other–this may have biological significance.
- Also: we will show that our method is *robust* to rotations.

Application to gene expression time series



- Data from Spellman et al. 1998
- Expression levels of 6178 yeast genes during cell cycle
- Total 73 measurements 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).

Correlations between time series

Cor_{Info} (using OLS)

	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

Using sparse CCA*

	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

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

*Witten and Tibshirani 2009, `PMA::CCApermute`

Invariance properties

Transform data from each group with random rotation...

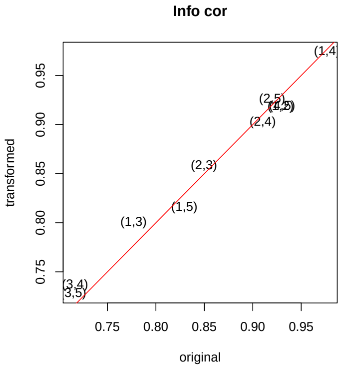
$$\tilde{\boldsymbol{X}} = \boldsymbol{X} E$$

$$\tilde{\boldsymbol{Y}} = \boldsymbol{X} F$$

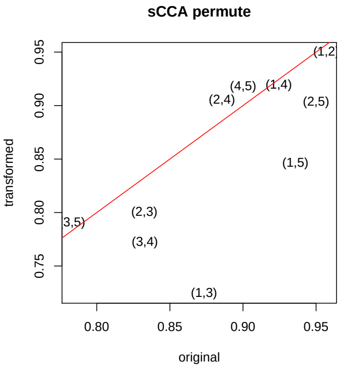
with $E^T E = I$, $F^T F = I$.

Invariance properties

Cor$_{Info}$ (using OLS)



Using sparse CCA*



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).
- Estimating quantities related to mutual information, such as *transfer information*, *stimulus-specific information* and *redundancy* (Borst and Theunissen 1999)
- Inferring resting-state brain networks.

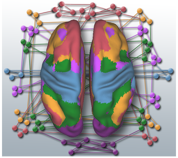


Image credit Simons Foundation

Section 3

The End

References

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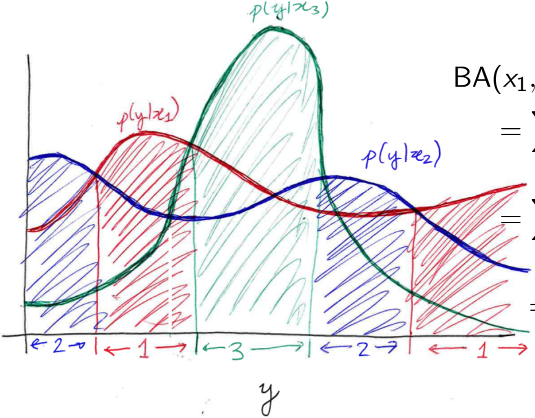
$$\text{BayesRisk}_k[p(x,y)] = 1 - \text{BA}_k[p(x,y)] = 1 - \mathbf{E}[\max_{i=1}^k p(Y|X_i)].$$



$$\begin{aligned}
&\text{BA}(x_1, x_2, x_3) \\
&= \sum_i \Pr[x_i] \Pr_{Y \sim p(y|x_i)}[Y \in \text{zone } i] \\
&= \sum_i \frac{1}{k} \text{Area under curve } i \text{ in zone } i \\
&= \frac{1}{k} \text{Area under } \max_{i=1}^k p(y|x_i)
\end{aligned}$$

Back to main