Discussion of the Maximal Information Coefficient

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Outline

1. Defining MIC
2. Subtleties & technical issues
3. Simon & Tibshirani’s response
4. Broader concerns & lessons
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Motivation

- Have high-dimensional dataset
- 100s-1000s of variables; often fewer observations than variables
- **Goal**: find novel bivariate relationships
- General definition of relationships (not just nonlinear, even nonfunctional)
- “Equitable” wrt different types of relationships
- Alternative to manual search (according to authors)
Generality & equitability

Stated goals of the method (heuristic)

- **Generality:** ability to detect broad range of relationships
  - Includes nonfunctional
  - Also want “noncoexistence” and mixtures of functions

- **Equitability:** similar scoring of “equally noisy relationships of different types”
  - Harder to pin down; asymptotic?
  - How do nonfunctional fit?
  - Symmetry $\rightarrow$ complications; predictive distribution from sinusoid, e.g.
Technical definition

- Start from scatterplot
- Consider grid on scatterplot
- Define mutual information of empirical distribution on grid $I_G$
  - KL divergence of factored distribution from actual joint
  - Always $\geq 0$
  - Information-theoretic measure of dependence; compression interpretation

From Figure 1 of Reshef et al. 2011
Now, fix grid size \((x, y)\)

Maximize \(I_G\) over grid layouts

\[ \rightarrow I_G^* \]

Normalize to \(M_{x,y} = \frac{I_G^*}{\log \min\{x,y\}}\)

Maximize again over \((x, y)\) s.t. \(x, y < B(n) \rightarrow M^*\)

\(M^*\) is MIC for pair of variables

From Figure 1 of Reshef et al. 2011
Computation, briefly

Hard to do this maximization
- Approximate search methods needed
- Dynamic-programming based solution
- Quite fast
MIC, as defined:

- Symmetric (from MI symmetry)
- $\rightarrow 0$ iff variables independent (with $B(n)$ conditions)
- $\rightarrow 1$ for functionally related variables
- Lower bound linked to $R^2$ for noisy functional relationships
Initial statistical reaction

That sounds great
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But it can’t be a panacea
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- Must have lower power than, e.g., F-test for linear
- Nonfunctional $\rightarrow$ multimodal predictive distribution;
  harder than nonparametric regression
- Huge multiple comparisons problem
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And we have theorems
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There’s always a tuning parameter

Nonparametric techniques nearly always have smoothness parameters

- Kernel width, number of knots, penalty weight, etc.
- Require careful attention to ensure validity and efficiency
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Here, it’s grid size $B(n)$
- Large $B(n) \rightarrow$ overfitting; find structure in everything
- Small $B(n) \rightarrow$ oversmoothing; miss noisy/subtle structure
Showed that $B(n) = \Omega(n^{1+\varepsilon})$, $\varepsilon > 0 \implies M^* \to 1$ almost surely.

So, $B(n)$ too large does overfit.

If $B(n) = O(n^{1-\varepsilon})$, $\varepsilon > 0$, MIC converges to correct value.

In particular, this implies MIC $\to 0$ for independent RVs.
Choice of $B(n)$ — published method

Selected $B(n)$ via simulation in paper

- Showed $B(n) = n^{1-\varepsilon}$ had proper limits under independence
- Settled on $B(n) = n^{0.6}$
- Rationale not apparent; no power or predictive checks
What about the coefficient?

Usually need both rate and coefficient for smoothness parameters

- Standard to get both in nonparametric statistics
- Rates analytically, coefficient estimated/approximated
- Neither completely handled here
- Could compromise power
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Simulations

Simon and Tibshirani addressed power concerns directly:
- Simulated from range of relationships with Gaussian noise
- Varied noise scale over factor of 3
- Evaluated frequentist power at FPR of 0.05
- Compared to Pearson and Brownian distance correlation
Brownian distance correlation

- Published by Székely and Rizzo in AoAS (2009)
- Uses distances between points and Brownian process approx
- Tuning parameter is power on distance
- Easy to compute (energy R package)
Power comparisons

Alright for short-period sine wave and circular
Power comparisons, continued

Underpowered for linear and cubic, as expected
Power comparisons, continued

Surprisingly poor for $X^{1/4}$ and step functions
Power comparisons, continued

Alright, but not dominant, for long-period sine and quadratic
As expected, there’s no free lunch here

- Model-free method means less power for MIC
- Looking for extremely general forms of structure; inevitable tradeoffs
- Distance correlation is surprisingly good
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Pitfalls & potential of broader approach

Searching a vast amount of raw data for complex relationships can be problematic

- Often find mainly artifacts of the measurement process
- Conversely, using preprocessed data can show effects of processing rather than science
- Discovery is good goal, but is this too general?
  - Semi-supervised approaches
  - Hierarchical methods
Beyond bivariate

What types of complexity matter most?

- Increasing number of variables vs. increasing complexity
- Ideally both, but curse of dimensionality stings
- Often observe greater gains from covariates than complex low-dimensional structure
- Depends upon setting, of course
Independent detection vs. pooling information

Need to consider tradeoffs depending on richness of data per variable

- Little lost working independently with many data per variable
- With few observations per variable, pooling becomes more important
- Appears relevant even for some examples in paper (Spellman et al. data)
Example — Spellman data

Could benefit from hierarchical modeling

From Figure 5 of Reshef et al. 2011
Next steps with discovery-oriented analyses

Exploration and discovery, then?

- After exploration phase, want stronger scientific results
- Predictive models, mechanistic hypotheses, etc.
- Dangers of inference with detected variables
- Distinction between EDA and data reduction
- Keeping sight of core modeling challenges
Location and publication

Where should statistics research appear?
- Nature/Science vs. statistics journals
- MIC & power law papers (Science)
- Contrast with FDR development (Jeff Leek’s comments)