Model Selection with Many More Variables than Observations

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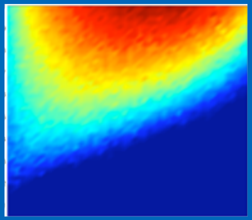

Microsoft Research Asia

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Classical Linear Regression Problem

- Given predictors $X_{n\times p}$ and response $y_{n\times 1}$,
- Linear model $y = X\beta + \varepsilon$, with $\varepsilon \sim N(0,\sigma^2)$
- Estimate β with $(X'X)^{-1}X'y$
- Widely used in a huge amount of empirical statistical research.

Developing Trend

- Classical model requires $p < n$, but recent developments have pushed people beyond the classical model, to $p \gg n$.

New Data Types

- **MicroArray Data**: p is number of genes, n is number of patients
- **Financial Data**: p is number of stocks, prices, etc, n is number of time points
- **Data Mining**: automated data collection can imply large numbers of variables
- **Texture Classification in Images** (eg. satellite): p is number of pixels, n is number of images

Estimating the model

> Can we find an estimate for β when $p \gg n$?

> George Box (1986) *Effect-Sparsity*: the vast majority of factors have zero effect, only a small fraction actually affect the reponse.

> $y = X\beta + \varepsilon$ can still be modeled but now β must be *sparse*, containing a few nonzero elements, the remaining elements zero.

Commonly Used Strategies for Sparse Modeling

1. All Subsets Regression
   - Fit all possible linear models for all levels of sparsity.

2. Forward Stepwise Regression
   - Greedy approach that chooses each variable in the model sequentially by significance level.

3. LASSO (Tibshirani 1994), LARS (Efron, Hastie, Johnstone, Tibshirani 2002)
   - ‘shrinks’ some coefficient estimates to zero.

LASSO and LARS: a quick tour

> LASSO solves: $\min_{\beta} \ \| y - X\beta \|_2^2 \ \text{ s.t. } \ \| \beta \|_1 \le t$ for a choice of t.

> LARS: a stepwise approximation to LASSO

- Advantage: guaranteed to stop in n steps

A New Perspective

- Up until now we've described the statistical view of the problem when $p \gg n$.
- Now we introduce ideas from Signal Processing and a new tool for understanding regression when $p > n$, in the case of n large.

- **Claim:** This will allow us to see that, for certain problems, statistical solutions such as LASSO, LARS, are just as good as all subsets regression.

Background from Signal Processing

> There exists a signal y, and several ortho-bases (eg. sinusoids, wavelets, gabor).

> Concatenation of several ortho-bases is a *dictionary*.

> Postulate that the signal is sparsely representable, i.e. made up from few components of the dictionary.

> Motivation:

- Image = Texture + Cartoon
- Signal = Sinusoids + Spikes
- Signal = CDMA + TDMA + FM + …

Overcomplete Dictionaries

$$\begin{pmatrix} 1 & 0 & \cdots & 0 & 0 \\ 0 & 1 & & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & & 1 & 0 \\ 0 & 0 & \cdots & 0 & 1 \end{pmatrix}$$

Canonical Basis

- n orthogonal columns

$$\begin{pmatrix} \vdots & \vdots \\ \vdots & \vdots \\ \phi_{(\omega,0)} & \phi_{(\omega,1)} \\ \vdots & \vdots \\ \vdots & \vdots \end{pmatrix}$$

Standard Fourier Basis

- where $\omega_k = 2\pi k,\ k = 0,\ldots,n/2$
- $0,1$ indicates cosine, sine
- n orthogonal columns

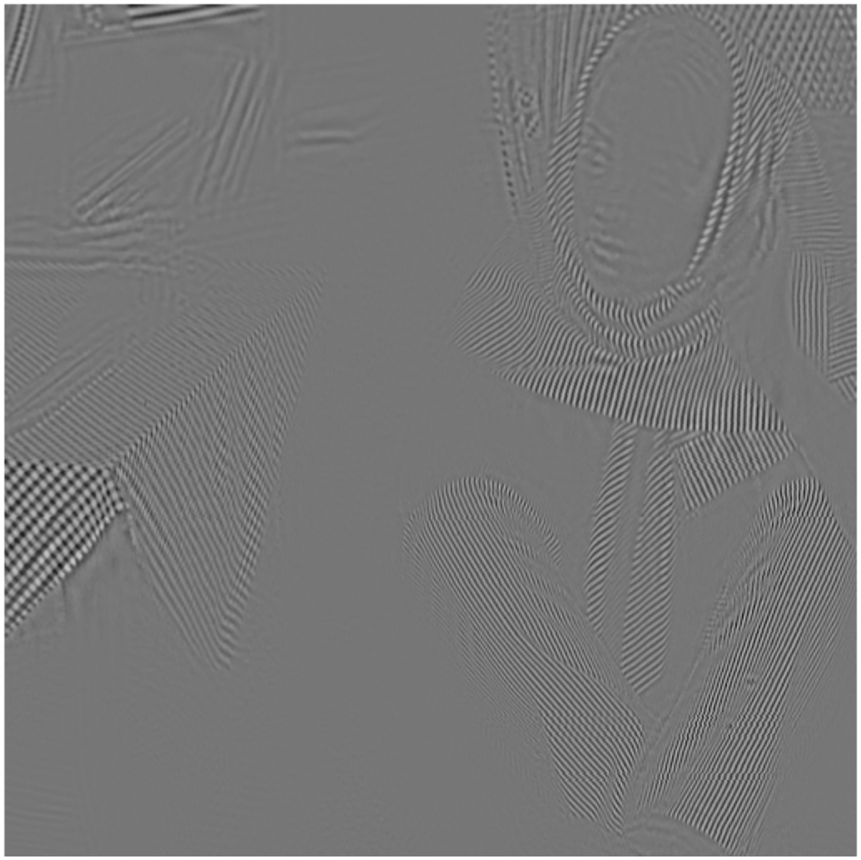
$A = [B_C \mid B_F]_{n\times 2n}$ is an *overcomplete dictionary*

Example: Image = Texture + Cartoon
(Elad and Starck 2003)

Original Image

Example: Image = Texture + Cartoon
(Elad and Starck 2003)

Cartoon (Curvelets)



Texture (local sinusoids)

Formal Signal Processing Problem Description

Signal decomposition: $y = Ax$

With a noise term: $y = Ax + z, \quad z \sim N(0, \sigma^2)$

	Regression	Decomposition
Signal	y	y
Matrix	X	A
Coefficients	β	x
Noise	ε	z
n	observations	signal length
p	predictors	p/n = #bases

If #bases > 1, $\Rightarrow$ $\mathrm{p} > \mathrm{n}$.

Signal Processing Solutions

1. *Matching Pursuit* (Mallat, Zhang 1993)
   - Forward Stepwise Regression

2. *Basis Pursuit* (Chen, Donoho 1994)
   - Simple global optimization criteria:

$$(P_1) \qquad \min_x \ \|x\|_1 \ \text{ s.t. } y = Ax$$

3. Maximally Sparse Solution:
   - Intuitively most compelling but not feasible!

$$(P_0) \qquad \min_x \ \|x\|_0 \ \text{ s.t. } y = Ax$$

l_0 Problem Impossible!

> We can't hope to do an all subsets search, but we are lucky!

(P_1) is a convex problem, and it can sometimes solve (P_0).

(l_1, l_0) Equivalence

- Signal processing results show (P_1) solves (P_0) for certain problems.

- Donoho, Huo (IEEE IT, 2001)
- Donoho, Elad (PNAS, 2003)
- Tropp (IEEE IT, 2004)
- Gribonval (IEEE IT, 2004)
- Candès, Romberg, Tao (IEEE IT, to appear)

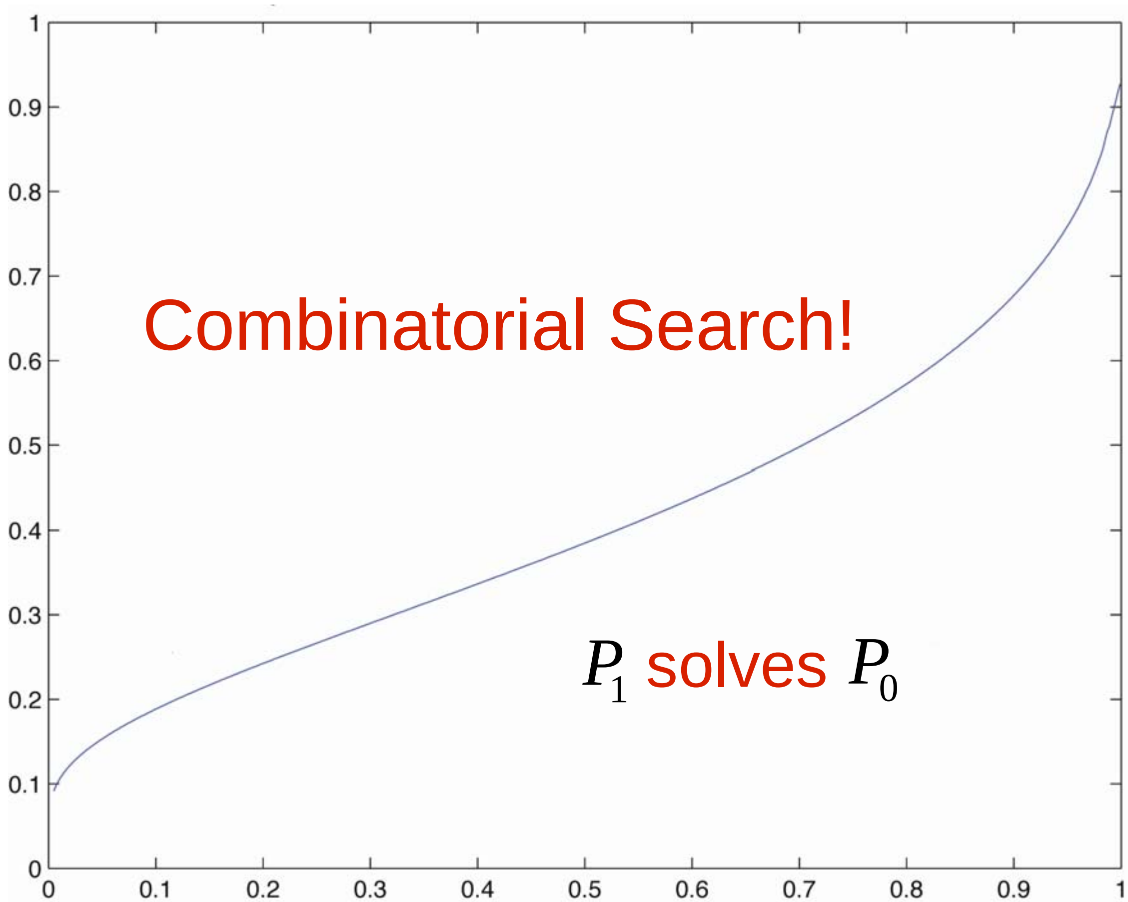
Phase Transition in Random Matrix Model

- > $A_{n \times p}, \quad A_{i,j} \sim N(0,1)$
- > $y = Ax$, where x has k random nonzeros, positions random.
- > Phase Plane (δ, ρ)
  - $\rho = k / n$: degree of sparsity
  - $\delta = n / p$: degree of underdetermination

Theorem (DLD 2005) There exists a critical $\rho_w(\delta)$ such that, for every $\rho < \rho_w$, for the overwhelming majority of (y, A) pairs, if $\rho < \rho_w$, (P_1) solves (P_0).

Phase Transition: (l_1, l_0) equivalence

$\rho = k / n$



$\delta = n / p$

Paradigm for study

- P is a property of an algorithm,
- (y, X) is a random ensemble,
- Find the Phase Transitions for property P.

Approach pioneered by Donoho, Drori, and Tsaig:

1. Generate $y = X\beta$, where β sparse.
2. Run full solution path to find solution $\hat{\beta}$,
3. Property $P: \dfrac{\|\hat{\beta} - \beta\|_2}{\|\beta\|_2} \leq \varepsilon$

This implies a statistics question!

- Could this paradigm be used for linear regression with noisy data?
- For example, when are LASSO, LARS, Forward Stepwise just as good as all subsets regression?
- Reformulate problems with Noise:

$$(P_{0,\lambda}) \qquad \min_{\beta} \; \| y - X\beta \|_2^2 + \lambda \| \beta \|_0$$

$$(P_{1,\lambda}) \qquad \min_{\beta} \; \| y - X\beta \|_2^2 + \lambda \| \beta \|_1$$

Experiment Setup

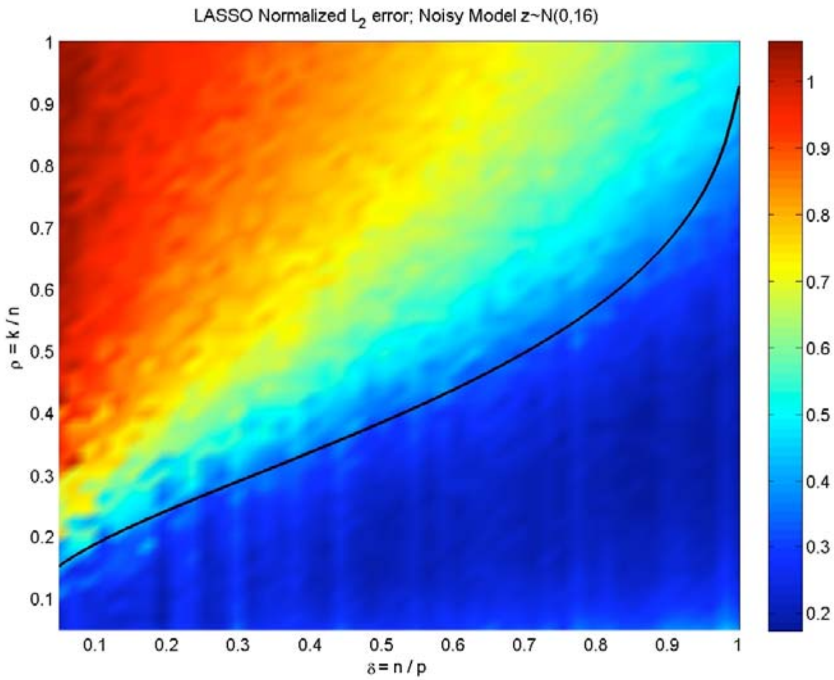
- $X_{n \times p}$, with random entries generated from $N(0,1)$, and normalized columns.
- β is a p-vector with the first k entries drawn from $U(0,100)$ remaining entries 0.
- $\varepsilon \sim N(0,16)$ n-vector.
- Create $y = X\beta + \varepsilon$
- We find the solution $\hat{\beta}$ using an algorithm (LASSO, LARS, Forward Stepwise) with y and X as inputs.

Questions

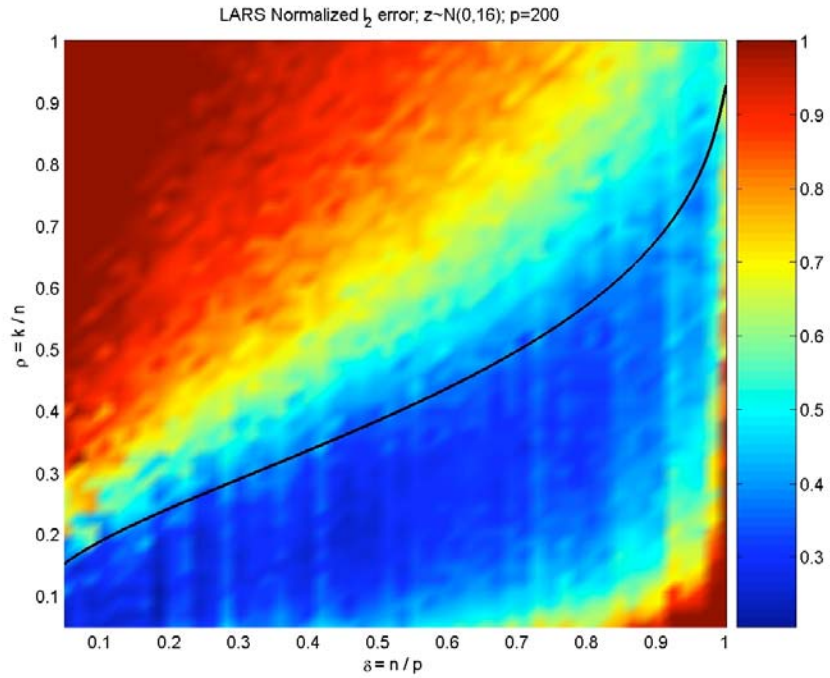
> Will there be any phase transition?

> Can we learn something about the properties of these algorithms from the Phase Diagram?

LASSO, LARS Phase Transitions for Noisy Model



LASSO, z~N(0,16)



LARS, z~N(0,16)

Aside: Stepwise Thresholding

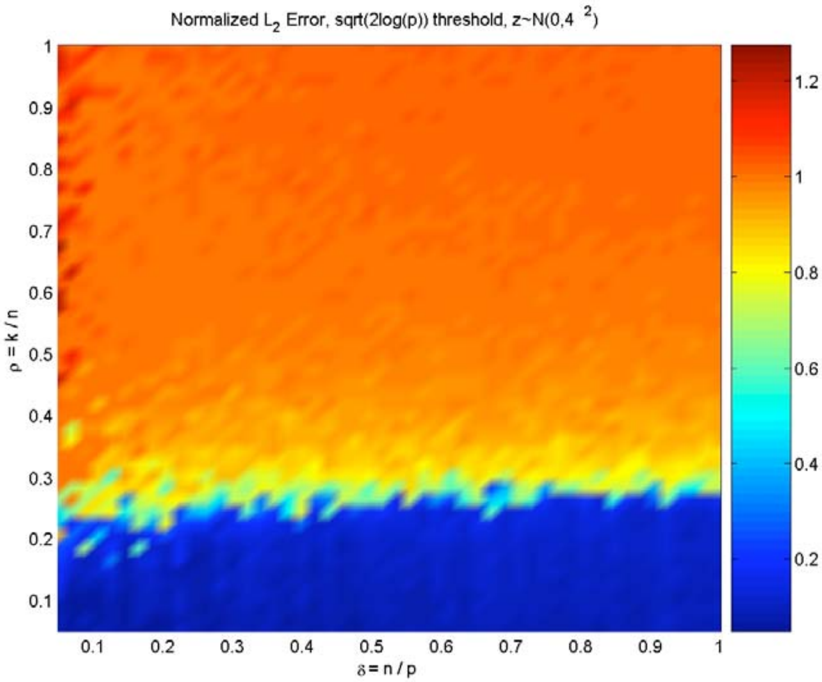
> Stepwise Algorithm – typical implementation:

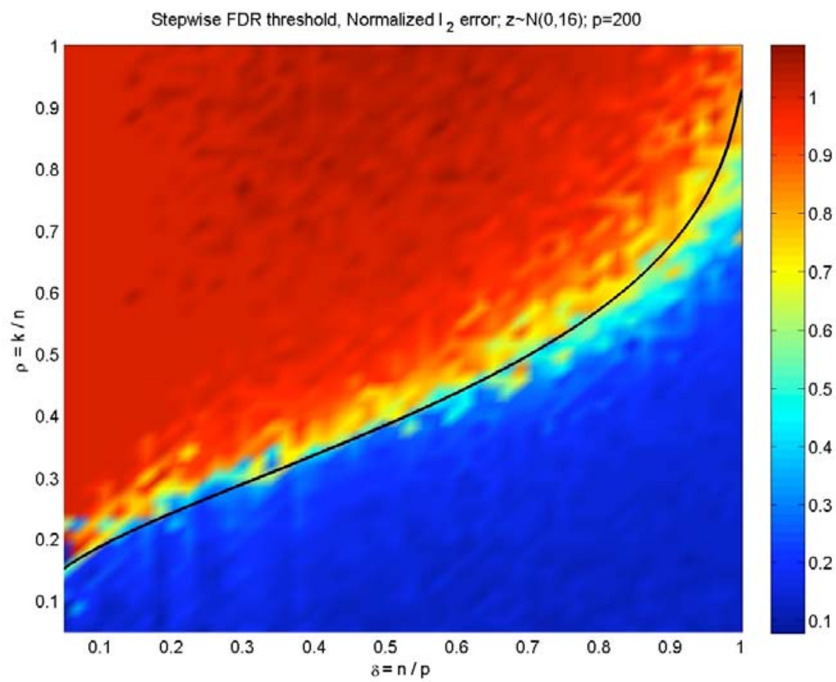
- Add the variable with the highest t-statistic to the model, if that t-statistic is greater than $\sqrt{2\log(p)}$, (Bonferroni).

> Stepwise Algorithm: False Discovery Rate (FDR) Threshold:

- Add the variable with the highest t-statistic to the model, if that t-statistic's p-value is less than the FDR statistic.
- $FDR_{stat} \equiv \dfrac{q*k}{p}$, where q is $E\dfrac{\{\#\text{falseDiscoveries}\}}{\{\#\text{totalDiscoveries}\}}$ (the FDR parameter), k is the number of variables in the current model, and p is the potential number of variables.

Stepwise Phase Transitions for Noisy Model





Stepwise $\sqrt{2\log(p)}$, z~N(0,16)

Stepwise FDR, z~N(0,16)

Phase Transition Surprises

> **Surprise**: LASSO finds underlying model, for $\rho < \rho_{LASSO}$

> **Hoped for**: LARS finds underlying model, for $\rho < \rho_{LARS}$.

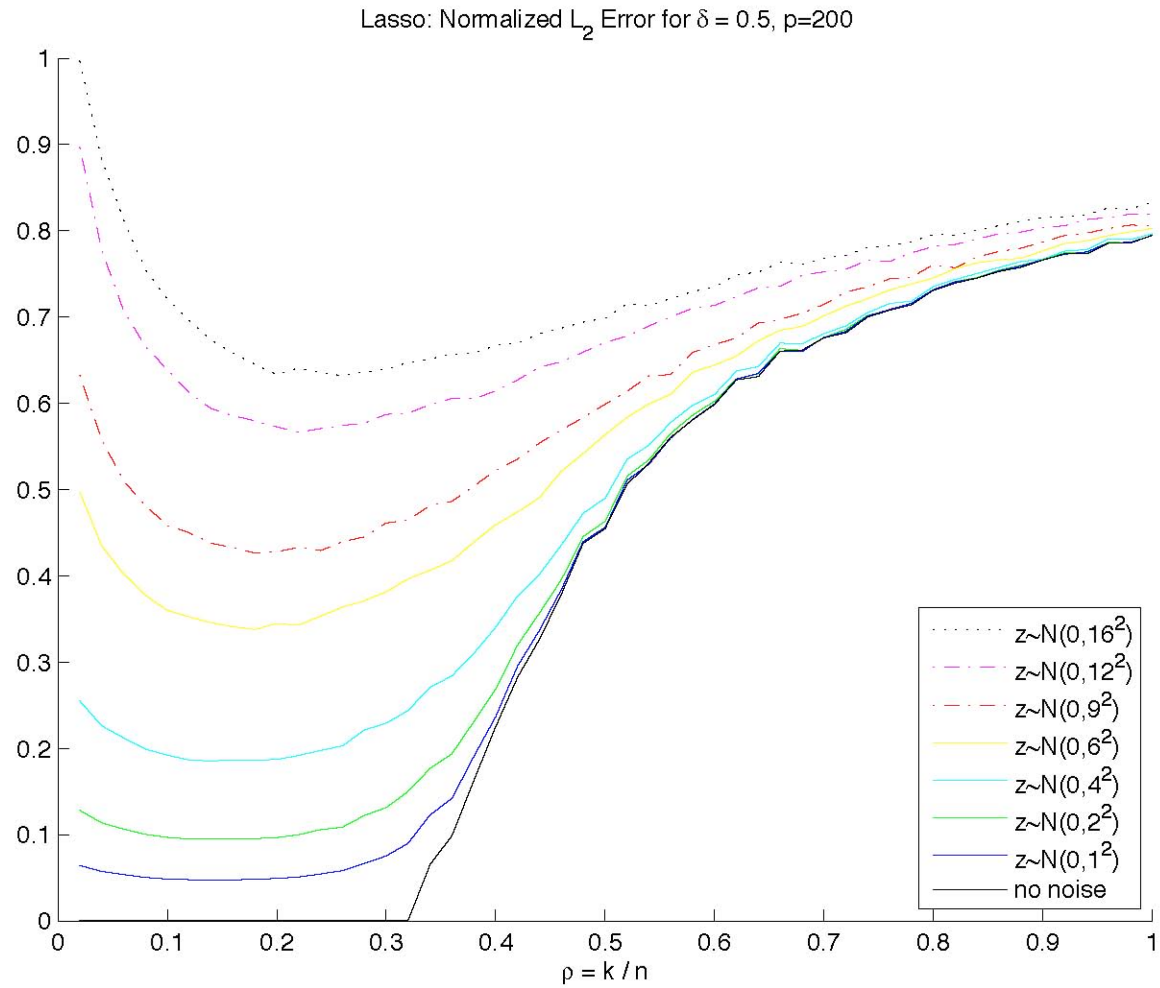
> **Surprise**: Stepwise only successful for $\rho \ll c \ll \rho_{LASSO}$.

Error Analysis

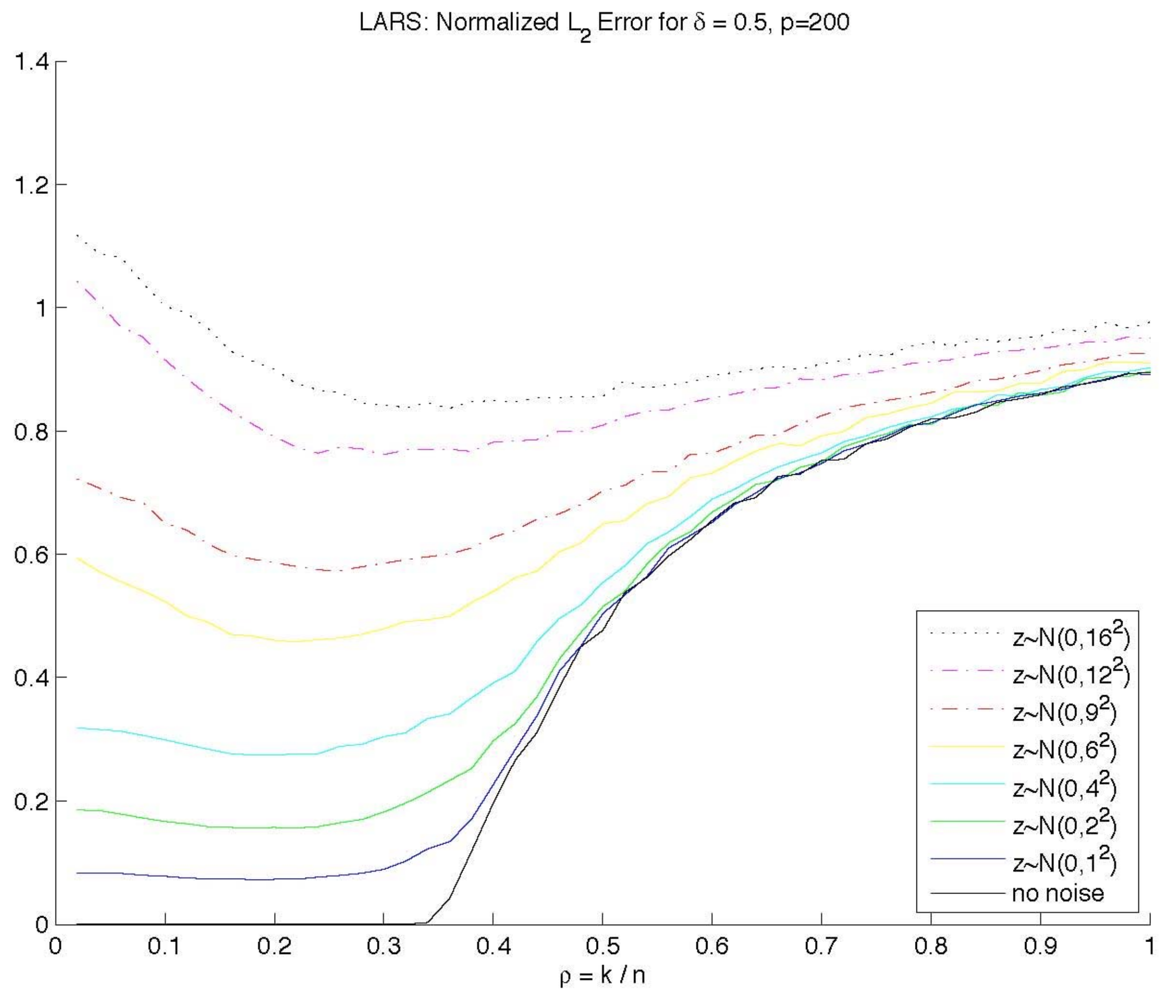
- With increased noise levels, at what sparsity levels does these algorithms continue to recover the correct underlying model, if at all?

- We fix $\delta = .5$ and examine a “slice” of the phase transition diagram.

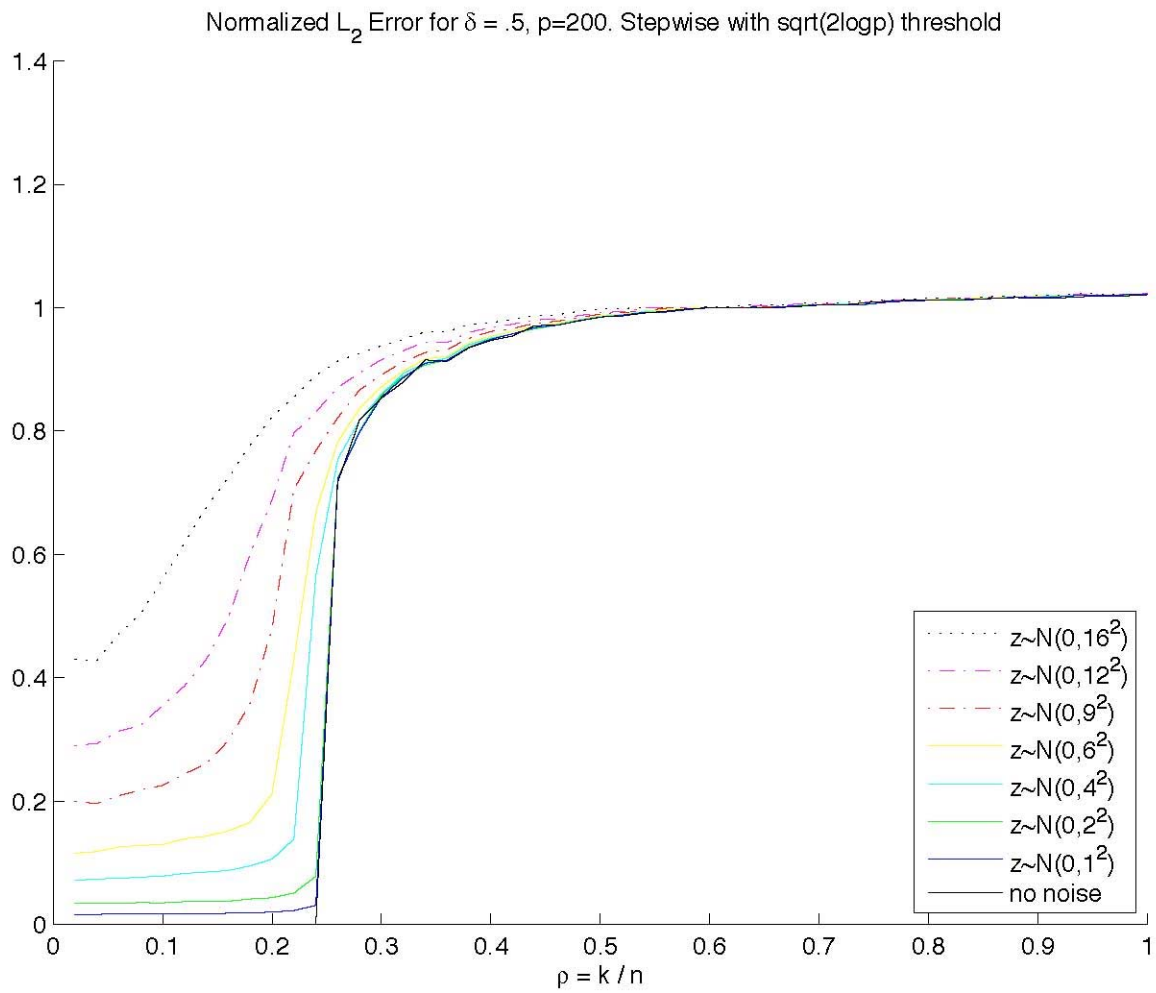
Lasso Normalized L_2 Error



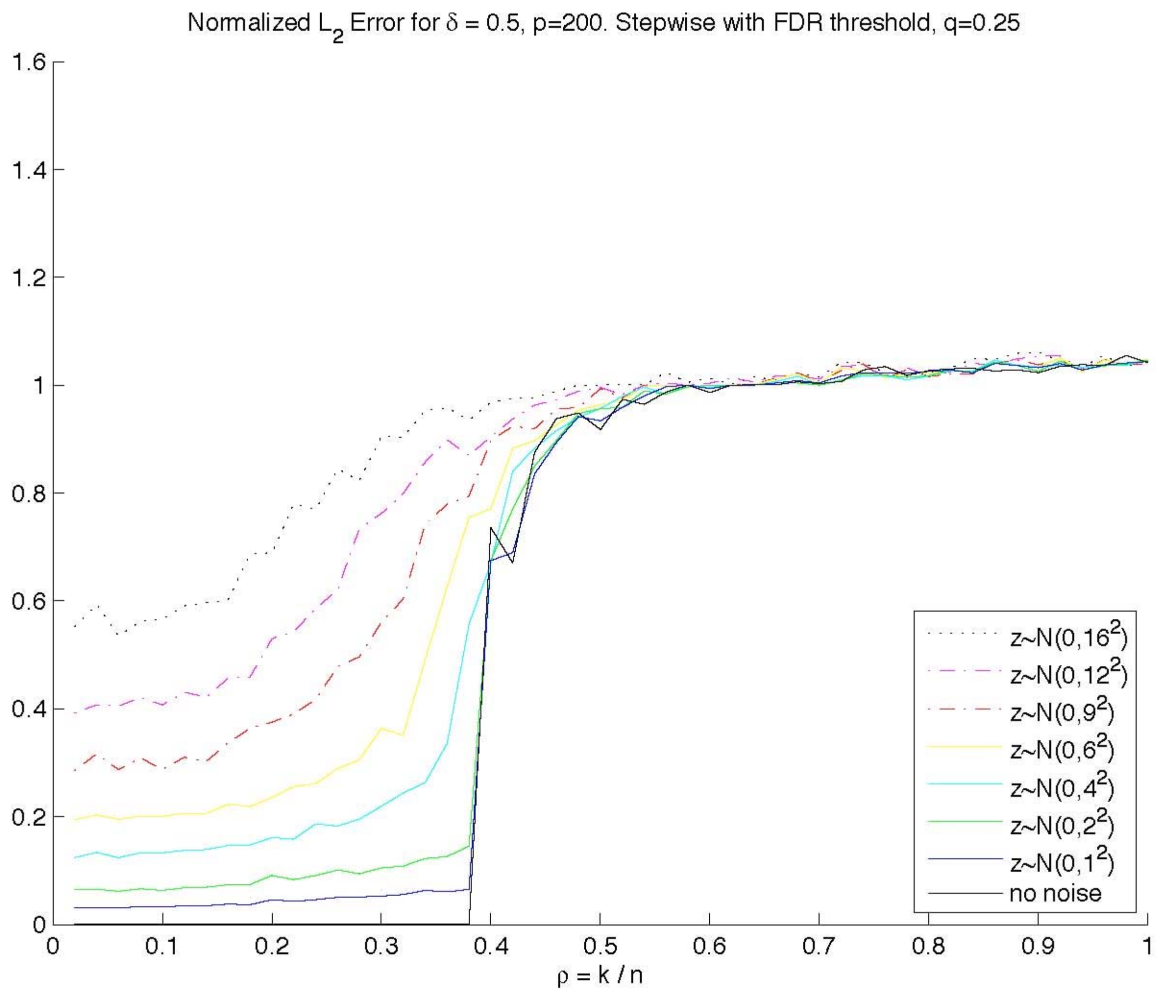
LARS Normalized L_2 Error



Forward Stepwise Normalized L_2 Error



FDR Stepwise Normalized L_2 Error



Experiences with Noisy Case

- Phase Diagrams revealing, stimulating.
- Stepwise Regression falls apart at a critical sparsity level (why?)
- LARS in same cases works very well!
- Suggests other interesting properties to study.
- Other algorithms: Forward Stagewise, Backward Elimination, Stochastic Search Variable Selection, ...

Introducing SparseLab!

http://sparselab.stanford.edu

> Matlab toolbox that makes software solutions for sparse systems available.

> Growing research on sparsity, variable selection issues – could advance the research community if they have standard tools.

> SparseLab is a system to do this.

SparseLab in Depth

> Reproducible Research: SparseLab makes available the code to reproduce figures in published papers.

> Some papers currently included:

- “Model Selection When the Number of Variables Exceeds the Number of Observations” (Donoho, Stodden 2006)
- “Extensions of Compressed Sensing” (Tsaig, Donoho 2005)
- “Neighborliness of Randomly-Projected Simplices in High Dimensions” (Donoho, Tanner 2005)
- “High-Dimensional Centrally-Symmetric Polytopes With Neighborliness Proportional to Dimension” (Donoho 2005)

> All open source!

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