Sparse Modeling

Theory, Algorithms and Applications

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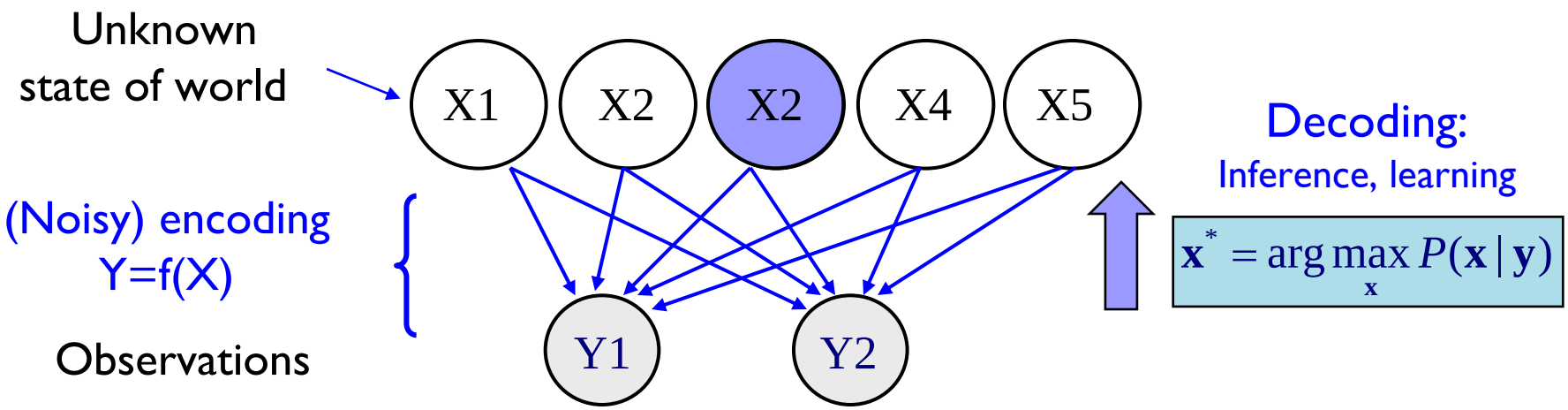
Outline

- Introduction
- Sparse Linear Regression: Lasso
- Sparse Signal Recovery and Lasso: Some Theory
- Sparse Modeling: Beyond Lasso
  - Consistency-improving extensions
  - Beyond l_1-regularization (l1/lq, Elastic Net, fused Lasso)
  - Beyond linear model (GLMs, MRFs)
  - Sparse Matrix Factorizations
  - Beyond variable-selection: variable construction
- Summary and Open Issues

Schedule

- 9:00-9:40
  - Introduction
  - Lasso
- 9:40-10:20
  - Sparse signal recovery and Lasso: Some Theory
- 10:20-10:30
  - Coffee Break
- 10:30-11:45
  - Sparse Modeling Beyond Lasso

A Common Problem



Can we recover a high-dimensional X from a low-dimensional Y?

Yes, if:

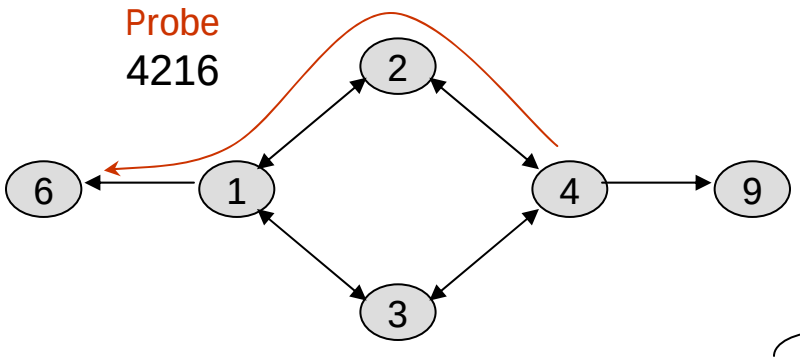
- X is structured; e.g., sparse (few $X_i \neq 0$) or compressible (few large X_i)
- encoding preserves information about X

Examples:

- **Sparse signal recovery** (compressed sensing, rare-event diagnosis)
- **Sparse model learning**

Example 1: Diagnosis in Computer Networks

(Beygelzimer, Kephart and Rish 2007)



N links (possible bottlenecks)

vector Y of end-to-end probe delays

vector X of (unknown) link delays

Routing matrix A

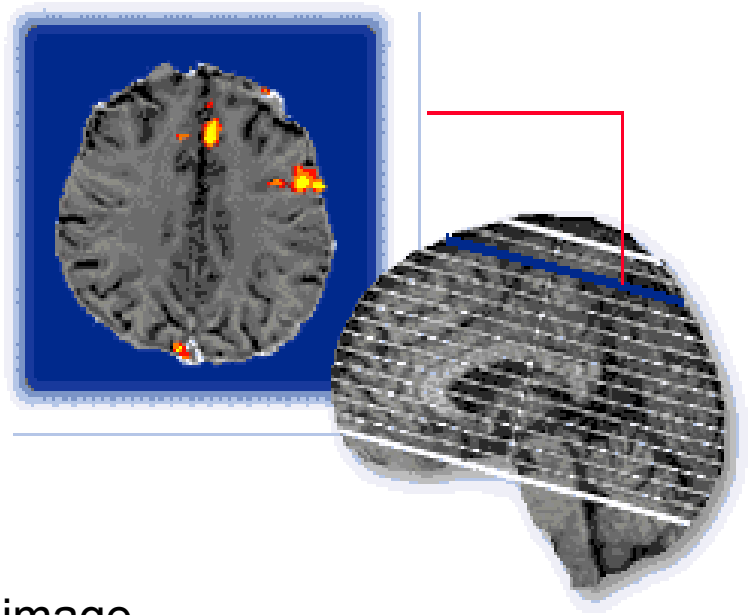
M probes

	X1	X2	X3	X4	X5	X6
	❶❷	❶❸	❶❻	❷❹	❸❹	❹❾
Y1 ❹❷❶❻	1	0	1	1	0	0
Y2 ❹❸❶❻	0	1	1	0	1	0
Y3 ❸❶❷	1	1	0	0	0	0
Y4 ❶❷❹❾	1	0	0	1	0	1

- **Model:** **y = Ax + noise**
- **Problem structure:** **X is nearly sparse - small number of large delays**
- **Task:** find bottlenecks (extremely slow links) using probes (M << N)

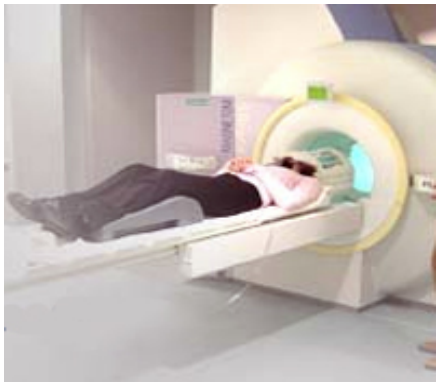
Recover sparse state (`signal') X from noisy linear observations

Example 2: Sparse Model Learning from fMRI Data



- Data: high-dimensional, small-sample
  - **10,000 - 100,000 variables** (voxels)
  - **100s of samples** (time points, or TRs)

- Task: given fMRI, predict mental states
  - emotional: angry, happy, anxious, etc.
  - cognitive: reading a sentence vs viewing an image
  - mental disorders (schizophrenia, autism, etc.)



- Issues:
  - **Overfitting:** can we learn a predictive model that generalizes well?
  - **Interpretability:** can we identify brain areas predictive of mental states?

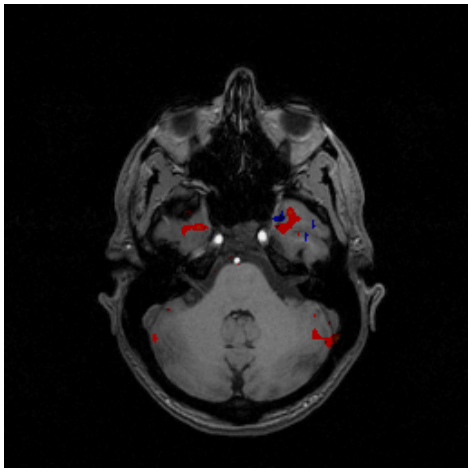
fMRI image courtesy of fMRI Research Center @ Columbia University

Sparse Statistical Models: Prediction + Interpretability

Data

x - fMRI voxels,

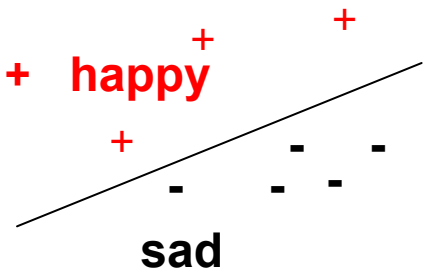
y - mental state



Small number of Predictive Variables ?

Predictive Model

y = f(**x**)



- Sparsity → variable selection → model interpretability
- Sparsity → regularization → less overfitting / better prediction

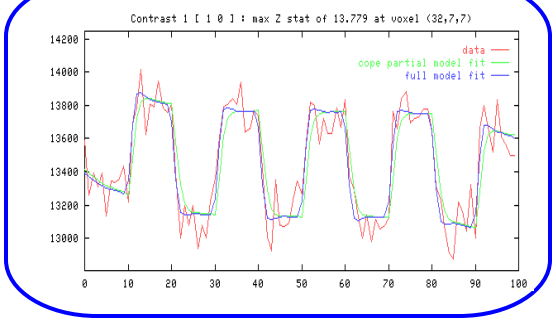
Sparse Linear Regression

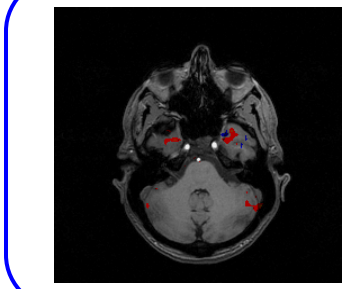
$$y = Ax + \text{noise}$$

Measurements:
mental states, behavior, tasks or stimuli

fMRI data ("encoding')
rows – samples (~500)
Columns – voxels (~30,000)

Unknown parameters ('signal')

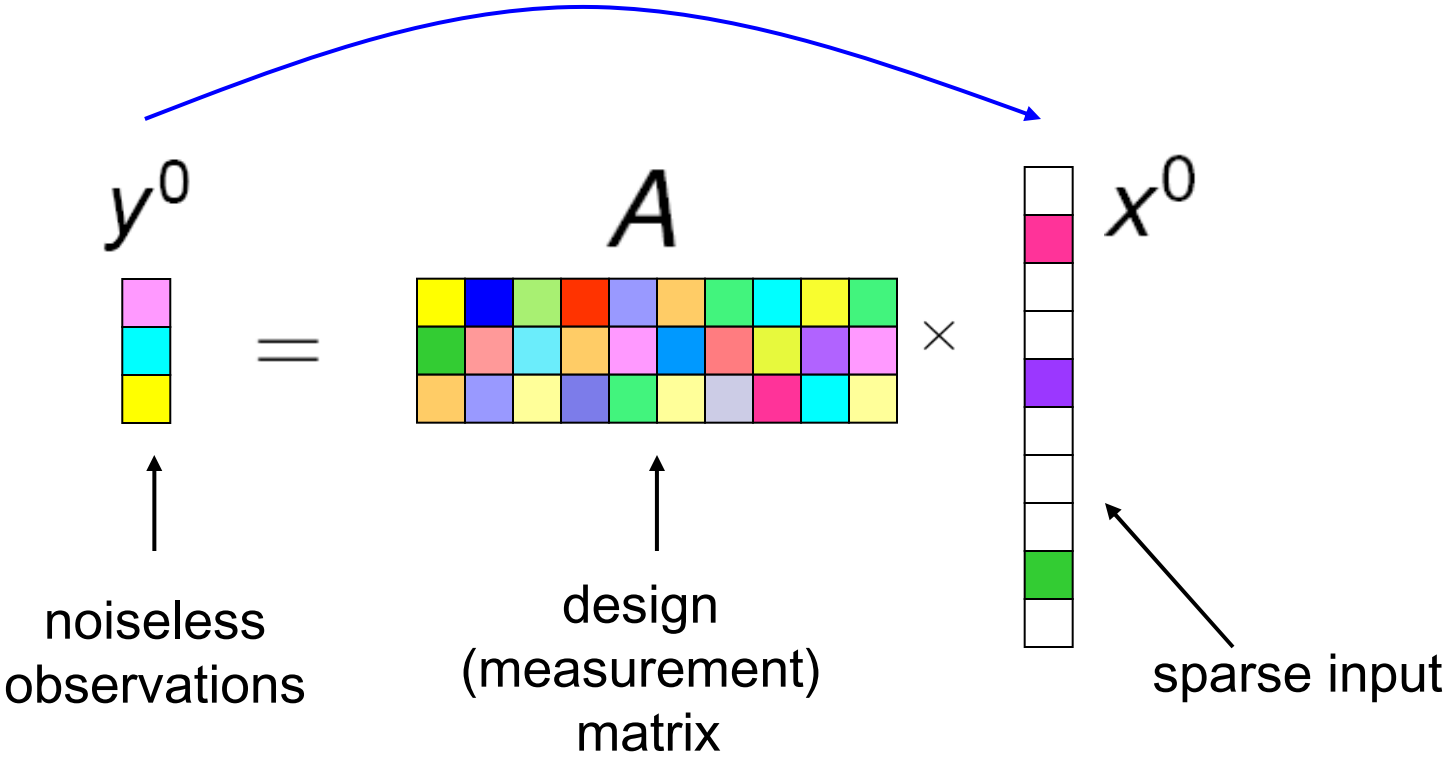




Find small number of most relevant voxels (brain areas)

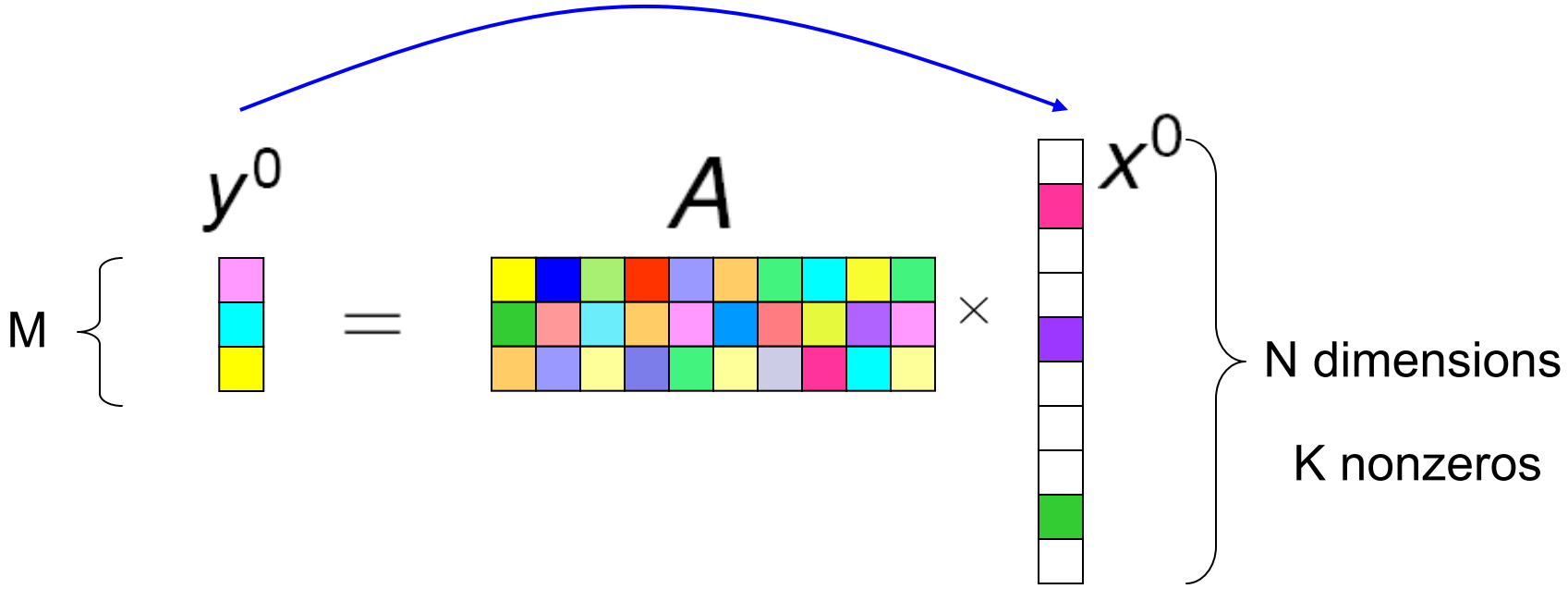
fMRI activation image and time-course courtesy of Steve Smith, FMRIB

Sparse Recovery in a Nutshell



Can we recover a sparse input efficiently from a small number of measurements?

Sparse Recovery in a Nutshell

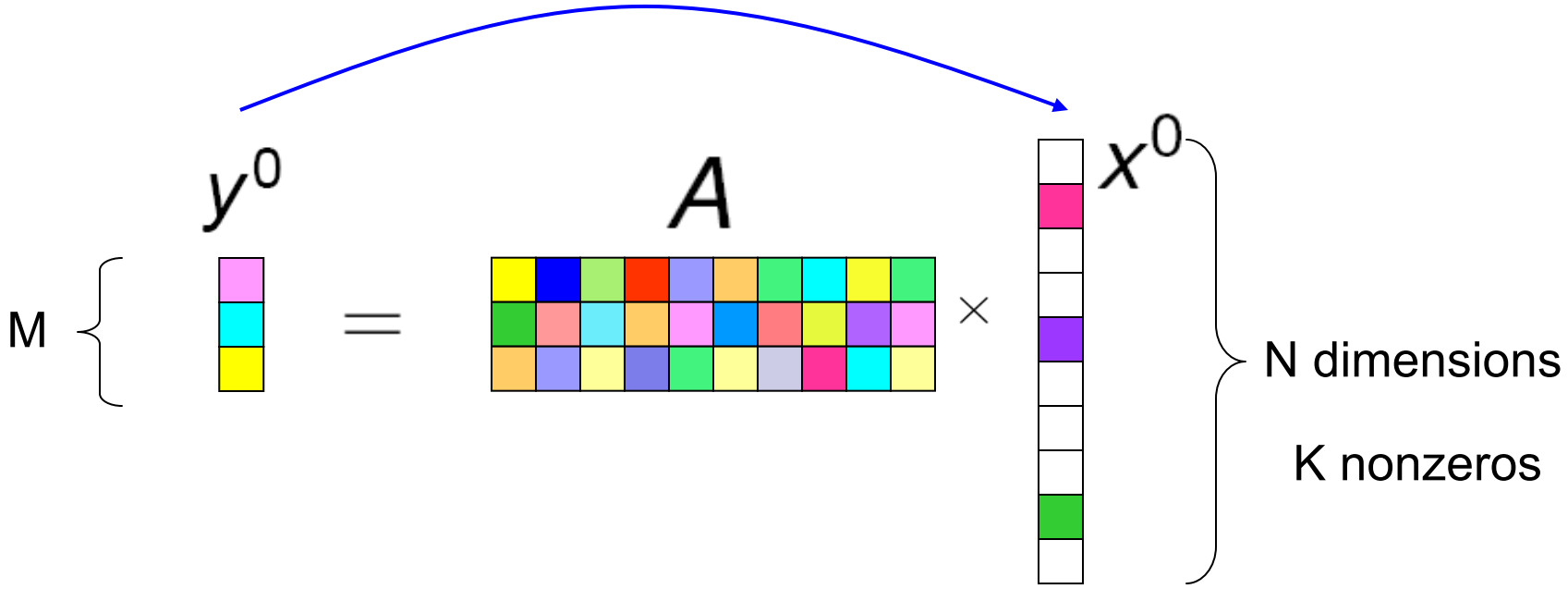


``Compressed Sensing Surprise'':

Given random A (i.i.d. Gaussian entries), x^0 can be reconstructed exactly (with high probability):

- from just $M = O(K \log(N/K))$ measurements
- efficiently - by solving convex problem $\min_x ||x||_1 \; s.t. \;\; y = Ax$ ($\Leftrightarrow$ linear program)

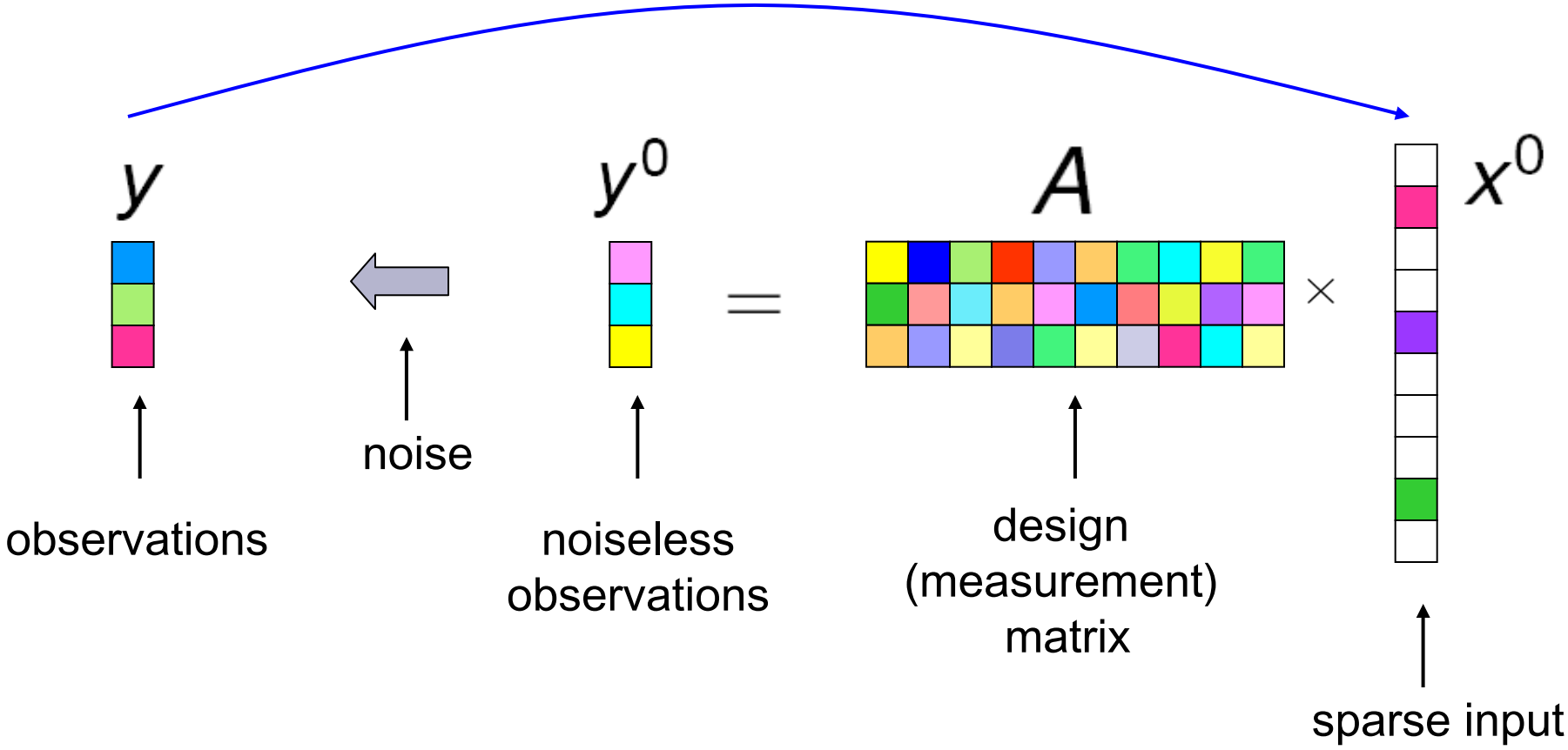
Sparse Recovery in a Nutshell



In general, if A is ``good'' (e.g., satisfies Restricted Isometry Property with a proper constant), sparse x^0 can be reconstructed with M <<N measurements by solving (linear program):

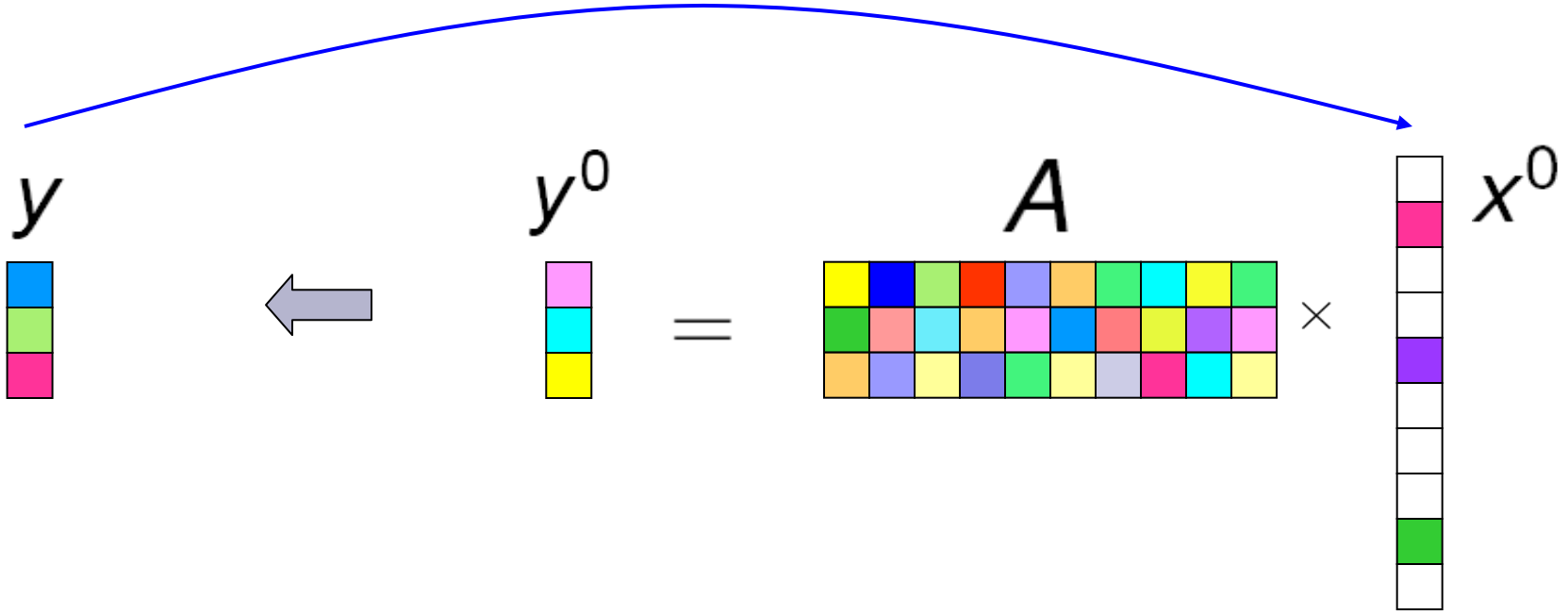
$$\min_x ||x||_1 \; s.t. \;\; y = Ax$$

Sparse Recovery in a Nutshell



And what if there is noise in observations?

Sparse Recovery in a Nutshell



Still, can reconstruct the input accurately (in l_2-sense), for A satisfying RIP; just solve a noisy version of our l_1-optimization:

$$\min_x ||x||_1 \ s.t. \ \ ||y - Ax||_2^2 \leq \epsilon$$

$$\Updownarrow$$

$$\min_x ||y - Ax||_2^2 \ s.t. \ \ ||x||_1 \leq t$$

(Basis Pursuit, aka Lasso)

Sparse Linear Regression vs Sparse Signal Recovery

- Both solve the same optimization problem
- Both share efficient algorithms and theoretical results
- However, sparse learning setting is more challenging:
  - We do not design the "design" matrix, but rather deal with the given data
  - Thus, nice matrix properties may not be satisfied (and they are hard to test on a given matrix, anyway)
  - We don't really know the ground truth (``signal") – but rather assume it is sparse (to interpret and to regularize)
- Sparse learning includes a wide range of problems beyond sparse linear regression (part 2 of this tutorial)

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Notation and Assumptions

- $X_1, \cdots, X_p$ - predictors, or features (e.g., voxel intensities)
- Y - response, or label (e.g., level of happiness)

- Data $Z = (\mathbf{X}, \mathbf{y})$, where $\mathbf{X}$ is $n \times p$ matrix and $\mathbf{y}$ is $n \times 1$ vector

  n samples-rows X^i, p predictors-columns X_p, n labels y^i

$$\mathbf{X} = \begin{pmatrix} x_1^1 & \cdots & x_p^1 \\ \cdots & \cdots & \cdots \\ x_1^n & \cdots & x_p^n \end{pmatrix} \qquad \mathbf{y} = \begin{pmatrix} y^1 \\ \cdots \\ y^n \end{pmatrix}$$

- Assumptions:

  - observations y^i are conditionally independent given $\mathbf{X}$

  - centered Y and standardized X_i: $\bar{Y} = 0$, $\bar{X}_i = 0$, $Var(X_i) = 1$

  - X has maximal rank

Motivation: Variable Selection

- Filter methods:
  rank each x_i (or a small subset of X) using a ranking function $r(i)$, such as correlation or mutual information with the response y.
  Fast but suboptimal - can miss multivariate predictive patterns.

- Wrapper methods:
  rank each x_i (or a small subset of X) by its predictive accuracy, i.e., train a separate model for each x_i and evaluate its accuracy.
  Wrappers yield better predictions, but are quite expensive.

- Embedded methods:
  variable selection is *embedded* in model learning.
  (E.g., via greedy methods or certain regularization techniques).

Model Selection as Regularized Optimization

Regularization constrains the model space to avoid overfitting:

$$\min_{\beta} L(Z, \beta) \quad s.t.\ R(\beta) \leq t$$

$$\Updownarrow$$

$$\min_{\beta} L(Z, \beta) + \lambda R(\beta)$$

- $Z = \{Z^1, ..., Z^n\}$ - data (e.g., $Z^i = (X_{(i,:)}, y_i)$)
- β - vector of model parameters
- $L(\cdot)$ - loss function (e.g., model's error on the data)
- $R(\cdot)$ - regularization penalty (e.g., model's complexity)
- λ - regularization parameter

Bayesian Interpretation: MAP Estimation

- Loss: negative log-likelihood
- Regularization: negative log-prior on model parameters
- Learning: maximum a posteriori (MAP) probability estimation

$$\arg\max_{\beta} \log P(Z|\beta)P(\beta|\lambda)$$

$$\Updownarrow$$

$$\arg\min_{\beta} -\log P(Z|\beta) - \log P(\beta|\lambda)$$

$$\Updownarrow$$

$$\arg\min_{\beta} L(Z,\beta) + R(\beta,\lambda)$$

Log-likelihood Losses: Examples

- linear regression: Gaussian noise with unit variance $P(y_i|X_{(i,:)}\beta) = N(\mu = X_{(i,:)}\beta, \sigma = 1)$:

$$L = -\log \sum_{i=1}^{n} P(y_i|X_{(i,:)}\beta) = ||y - X\beta||_2^2$$

- Generalized Linear Model (GLM) regression (logistic, Poisson, etc.): exponential-family noise $P(y_i|\Theta_i)$ with natural parameters $\Theta_i = X_{(i,:)}\beta$ and means $\mu_i(\Theta_i)$

$$L = -\log \sum_{i=1}^{n} P(y_i|\Theta_i) = \sum_{i=1}^{n} B(y_i, \mu_i)$$

- Gaussian Markov Network: multivariate Gaussian with the inverse covariance matrix C, $P(Z^i|C) = N(\mu = \mathbf{0}, \mathbf{C})$:

$$L = -\log \sum_{i=1}^{n} P(Z^i|C) = \mathrm{tr}(SC) - \log\det(C),$$

where S is the empirical covariance matrix

Regularization: l_q-norm, $0 \leq q$

- l_0-norm: $|\{i|\beta_i \neq 0\}|$ - number of non-zero parameters; used by AIC, BIC/MDL criteria
- (squared) l_2-norm $||\beta||_2^2 = \sum_{i=1}^{p} \beta_i^2$ - Gaussian prior; used in ridge regression (Hoerl and Kennard, 1988)
- l_1-norm $||\beta||_1 = \sum_{i=1}^{p} |\beta_i|$ - Laplace prior; Lasso regression (Tibshirani, 1996)
- more generally, l_q-norm $||\beta||_q^q = \sum_{i=1}^{p} |\beta_i|^q$ - bridge regression (Frank and Friedman, 1993; Fu, 1998)

$$p_{\lambda,q}(\beta) \sim C(\lambda, q) e^{\lambda ||\beta||_q^q}$$

- Extensions of l_1: block-penalties (l_1/l_q - e.g., l_1/l_2, l_1/l_∞), Elastic Net penalty (convex combination of l_1 and l_2)

Best Subset Selection

- find best subset of M predictors, i.e.

$$\min_{\beta} L(Z, \beta) \quad s.t. \ ||\beta||_0 \leq M$$

where l_0-norm $||\beta||_0$ is the number of nonzeros $|\{i|\beta_i \neq 0\}|$

- NP-hard problem!

- various approximations (mainly greedy):

forward stepwise regression $\Leftrightarrow$ Orthogonal Matching Pursuit (Mallat and Zhang, 1993)
stagewise OMP (StOMP) (Donoho et al., 2006)
regularized OMP (ROMP) (Needell and Vershynin, 2009)
subspace pursuits (Dai and Milenkovic, 2008)
CoSaMP (Needell and Tropp, 2008)
SAMP(Do et al., 2008)
GraDeS (Gradient Descent with Sparsification) (Garg and Khandekar, 2009), etc. etc.

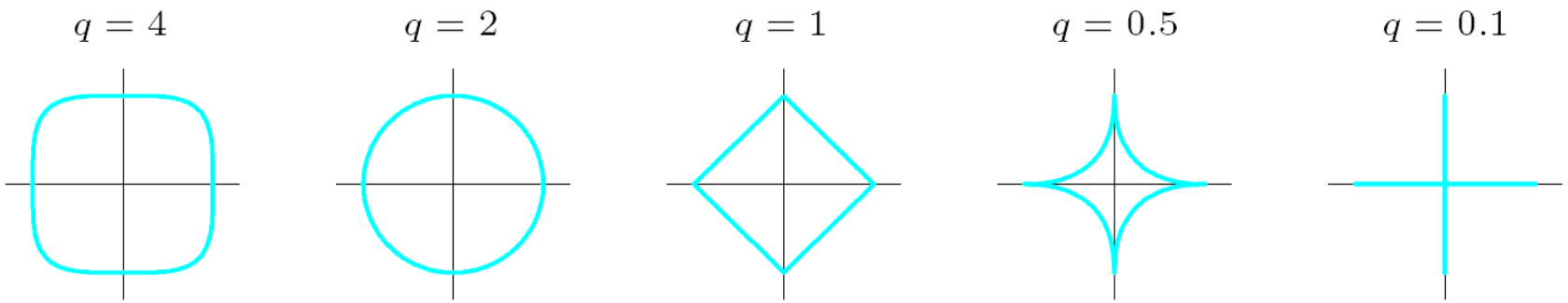
see more at http://dsp.rice.edu/cs (Compressive Sensing Resources)

- Alternative approach:

l_1-norm relaxations of l_0 (or, more generally, l_q-norms, $0 < q \leq 1$)

What is special about l_1-norm? Sparsity + Computational Efficiency

l_q-norm constraints for different values of q



Convexity $\Rightarrow$ efficient optimization methods

Sparsity $\Rightarrow$ variable selection

- $q < 1$: convexity, but no sparsity (no "sharp edges")
- $q > 1$: sparsity (sharp edges), but no convexity
- $q = 1$: sparsity and convexity

Image courtesy of [Hastie, Friedman and Tibshirani, 2009]

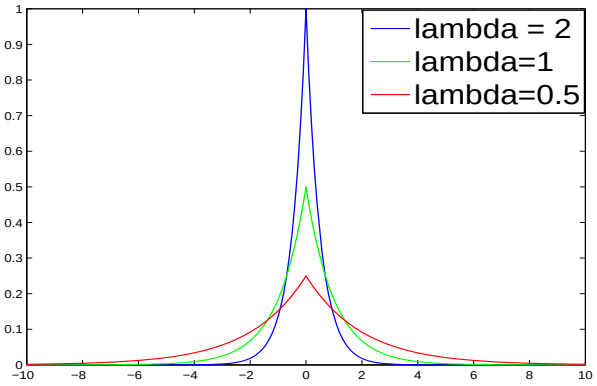
LASSO: Least Absolute Shrinkage and Selection Operator

$$\min_{\beta} ||y - X\beta||_2^2 + \lambda||\beta||_1$$

- First proposed by (Tibshirani, 1996)
- Known as Basis Pursuit (Chen et al., 1999) in signal processing
- Bayesian view: MAP estimation with:

  - independent Gaussian observations $y_i \sim e^{-\frac{1}{2}(y - X^i\beta)^2}$ and

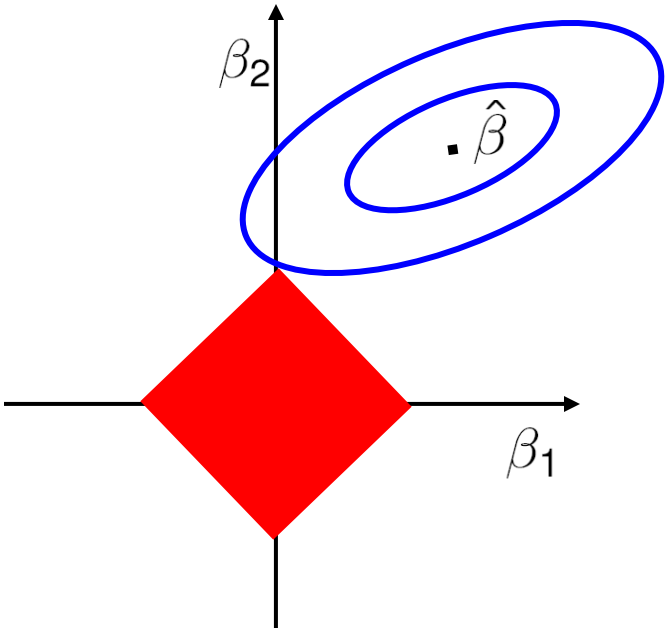
  - independent Laplace parameters $\beta_j \sim e^{-\lambda|\beta_j|}$

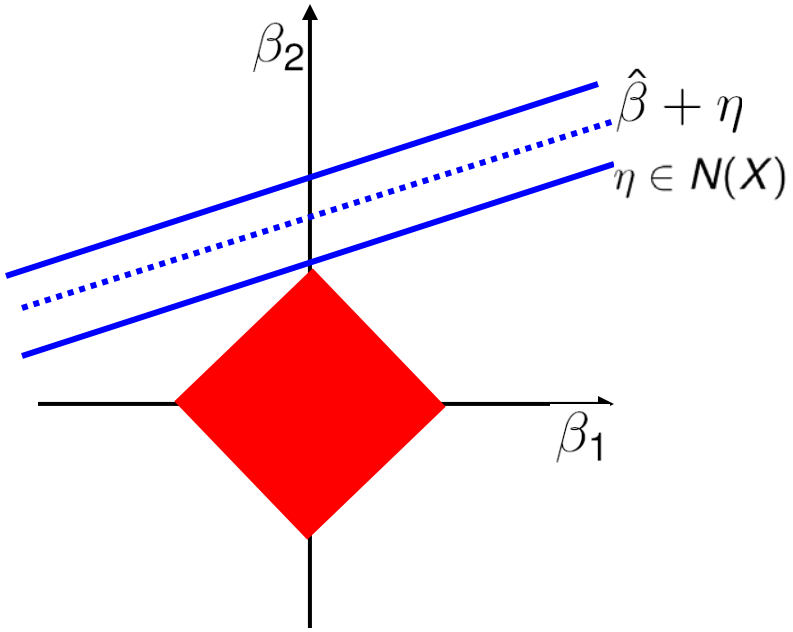


- Laplace prior enforces solution sparsity $\Longleftrightarrow$ variable selection

Equivalent Constrained Formulation: A Geometric View

$$\min_{\beta} ||y - X\beta||_2^2 \quad s.t. \ ||\beta||_1 \leq t$$





$p \leq n$

$p > n$

unique OLS solution

$\hat{\beta} = \arg\min_{\beta} ||y - X\beta||_2^2$

multiple OLS solutions $\hat{\beta} + \eta$:

$\forall \eta \in N(X)$ (null-space), $y = X(\hat{\beta} + \eta)$

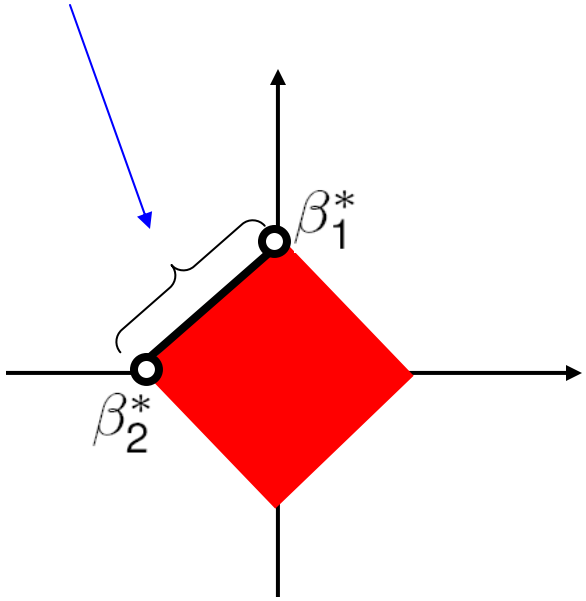
Properties of LASSO Solution(s)

Assume $t < t_0 = \min_{\eta \in N(X)} ||\hat{\beta} + \eta||_1$ (otherwise LASSO $\Leftrightarrow$ OLS).

Theorem (Osborne et al., 2000).

- If $p \leq n$, a *unique* LASSO solution β^* exists and $||\beta^*||_1 = t$.
- If $p > n$, a solution β^* exists, and $||\beta^*||_1 = t$ for any solution.

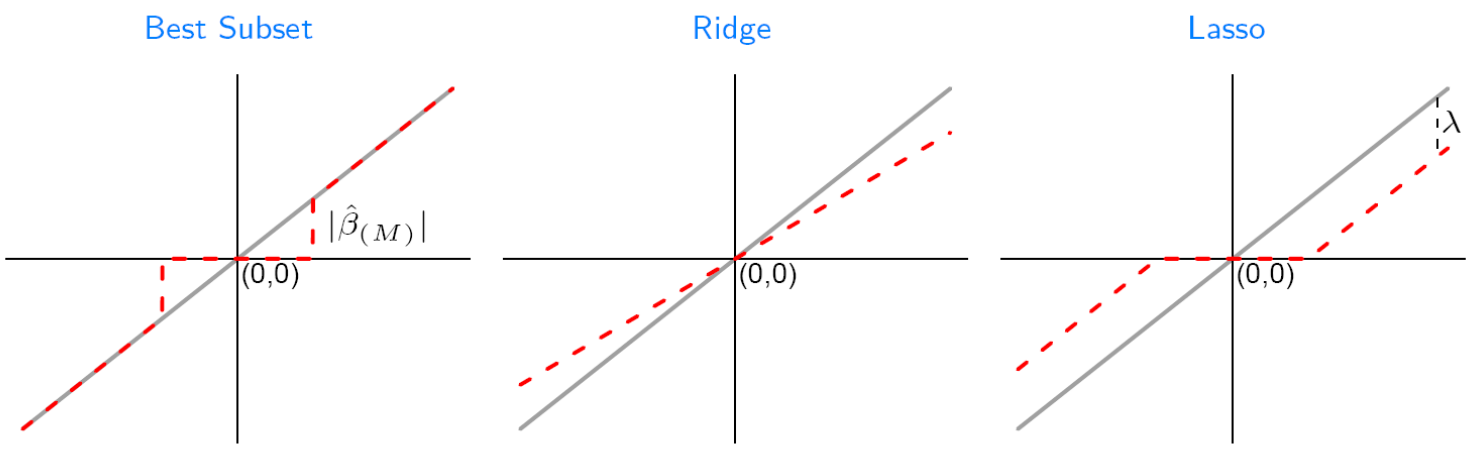
  If β_1^* and β_2^* are both LASSO solutions, then their convex combination $\alpha\beta_1^* + (1-\alpha)\beta_2^*$ is also a solution for any $0 \leq \alpha \leq 1$.



Lasso vs Ridge and Best-Subset in Case of Orthonormal Designs

For orthonormal X, explicit solutions are given by the following transformations, where $\hat{\beta} = (X^T X)^{-1} X^T y$ is an ordinary least-squares (OLS) solution:

Estimator	Formula
Best subset (size M)	$\hat{\beta}_j \cdot I[\text{rank}(\lvert\hat{\beta}_j\rvert \leq M)$
Ridge	$\hat{\beta}_j/(1+\lambda)$
Lasso	$\text{sign}(\hat{\beta}_j)(\lvert\hat{\beta}_j\rvert - \lambda)_+$



hard thresholding shrinkage soft thresholding

Image courtesy of [Hastie, Friedman and Tibshirani, 2009]

Algorithms

- Standard quadratic programming methods: too slow

- Least Angle Regression (LARS) (Efron et al., 2004):

  much faster; moreover, produces the entire solution path (all solutions for all values of the regularization parameter λ) at the cost of a single least-squares fit. Similar to homotopy (continuation) method of (Osborne et al., 2000b).

- Coordinate descent (Fu, 1998), (Daubechies et al., 2004), (Friedman et al., 2007a), (Wu and Lange, 2008):

  for fixed λ, optimizes each parameter at a time; using warm-starts, it can compute the solutions on a grid of λ values faster than LARS (however, the full path is NOT computed)

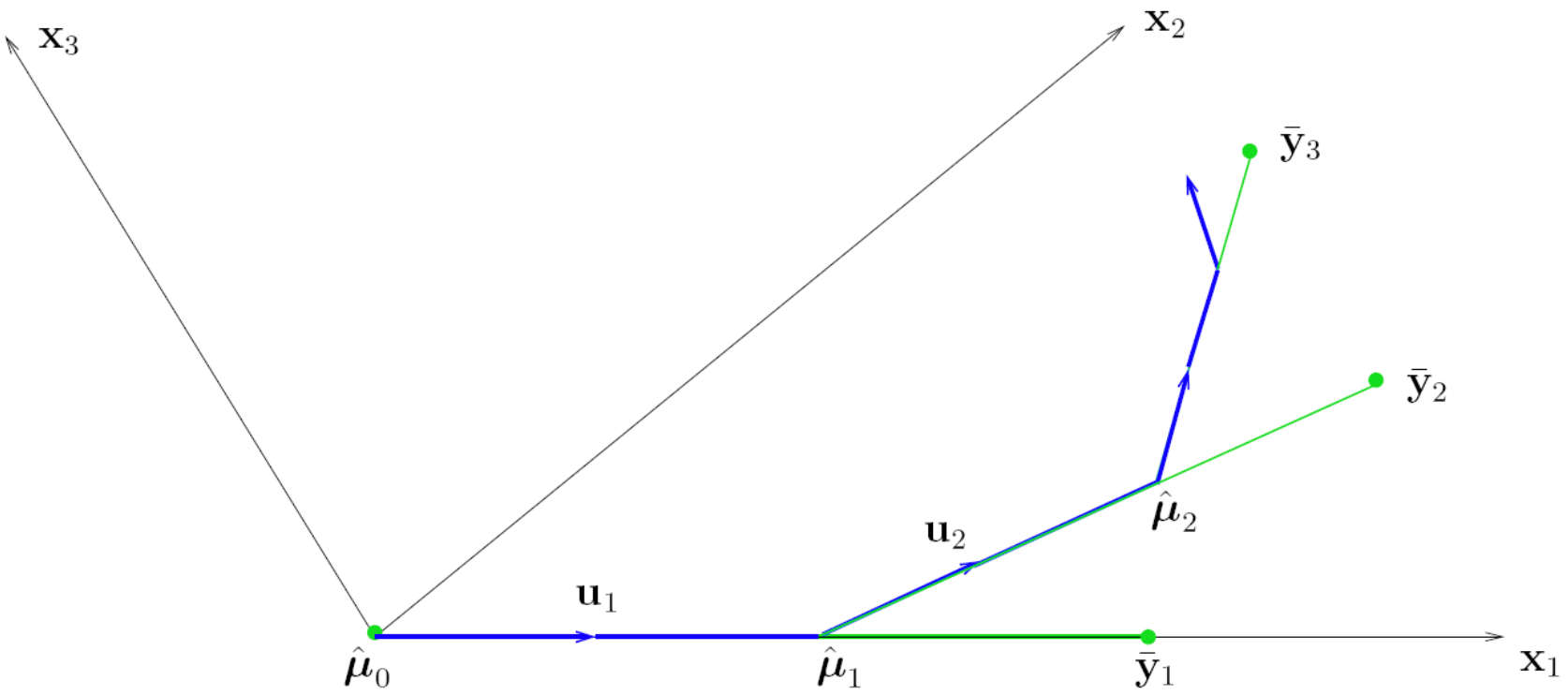
- Many other methods, including generalizations to other losses; various software packages, e.g., see http://dsp.rice.edu/cs

Least Angle Regression (LARS) (Efron et al., 2004)

Assume that y and all X_i have zero means), and all X_i have unit norm.

- *Initialize:* current residual $\mathbf{r} = \mathbf{y} - \bar{\mathbf{y}}$, coefficients $\beta_i = 0$, $i = 1, ..., p$
- Find X_i most correlated with $\mathbf{r}$, i.e. $X_i = \arg\max_j X_j \mathbf{r}$
- Move β_i towards $sign(X_j \mathbf{r})$, updating residual $\mathbf{r}$ along the way. Stop when some other predictor X_j has as much correlation with the current $\mathbf{r}$ as X_j has.
- Increase β_i and β_j in their joint least-squares direction $\mathbf{u}$ (equiangular between X_i and X_j), until some other predictor X_k has as much correlation with the current residual.
- Continue adding predictors for $\min(n-1, p)$ steps, until full OLS solution is obtained. If $p < n$, all predictors are now in the model.

Geometric View of LARS



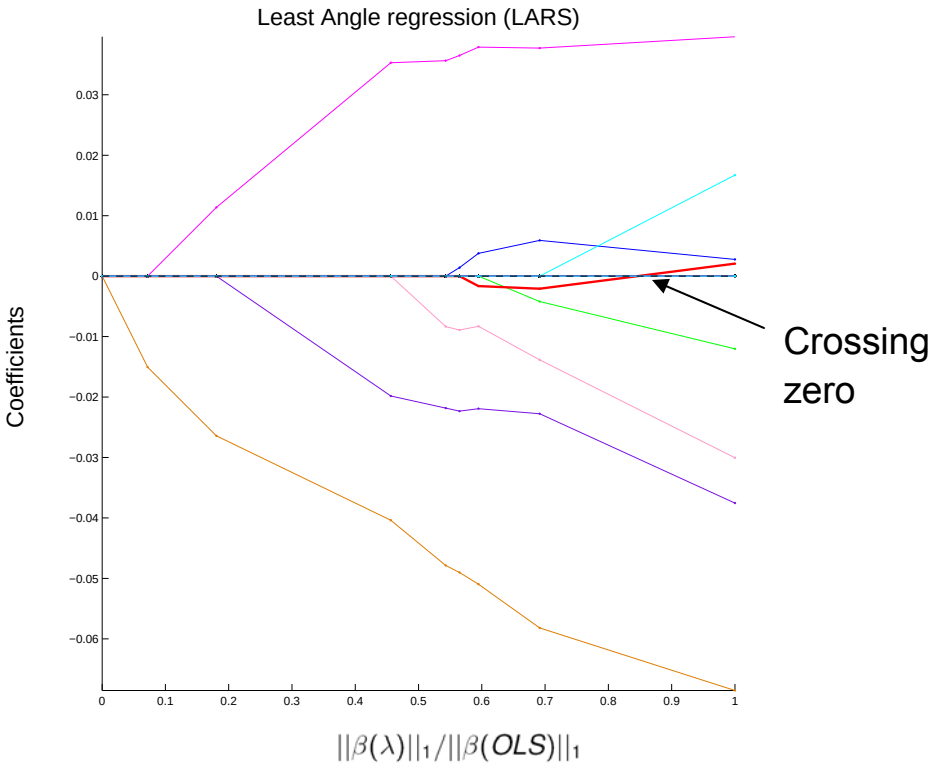
At step k, LARS estimate $\mu_{\mathbf{k}}$ moves towards the current OLS estimate $\bar{\mathbf{y}}_k$ in the direction $\mathbf{u_k}$ equiangular among the current predictors.

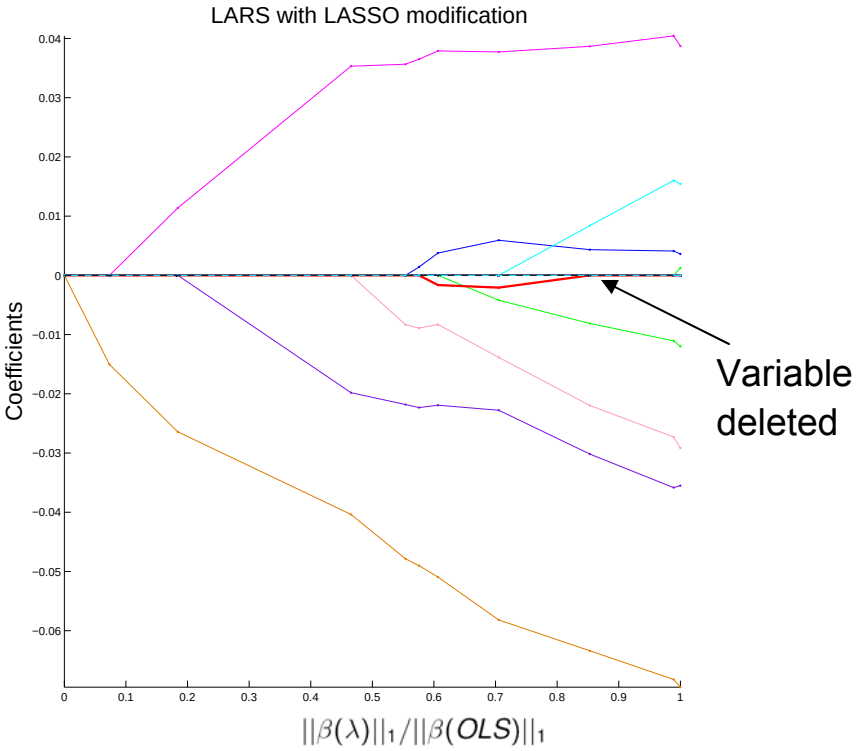
The direction changes before reaching $\bar{\mathbf{y}}_k$ when a new variable enters the active set.

Image courtesy of [Hastie, 2007]

Piecewise Linear Solution Path: LARS vs LASSO

LARS vs LASSO for pain perception prediction from fMRI data [Rish, Cecchi, Baliki, Apkarian, 2010]:
for illustration purposes, we use just n=9 (out of 120) samples, but p=4000 variables; LARS selects n-1=8 variables





Lasso modification

If non-zero β_k hits zero, delete X_k from the active set and recompute the current direction **u** and residual **r**.

LARS with Lasso modification produces the same solution path as Lasso

Predictive Performance

Three scenarios (Tibshirani, 1996):

	Best Subset	Ridge	Lasso
a few large β_j	best	worst	2nd
medium number of moderate β_j	worst	2nd	best
large number of small β_j	worst	best	2nd

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Plan

- Signal restoration with random Fourier projection (Candès et al., 2006)
  - Phenomenon
  - Signal restoration for random Fourier projection
  - Uncertainty principle
  - Examples for worst case, Dirac comb
  - Main techniques
  - Robustness and stability
- Compressed Sensing (Donoho, 2006a; Candès, 2006; Candès and Tao, 2006b; Candès and Romberg, 2007; Donoho et al., 2006; Candès and Tao, 2006a)
- Back to Lasso (Knight and Fu, 2000; Zhao and Yu, 2006; Bickel et al., 2009; Meinshausen and Yu, 2009; Wainwright, 2009; Juditsky and Nemirovski, 2008))

Phenomenon (Candès et al., 2006)

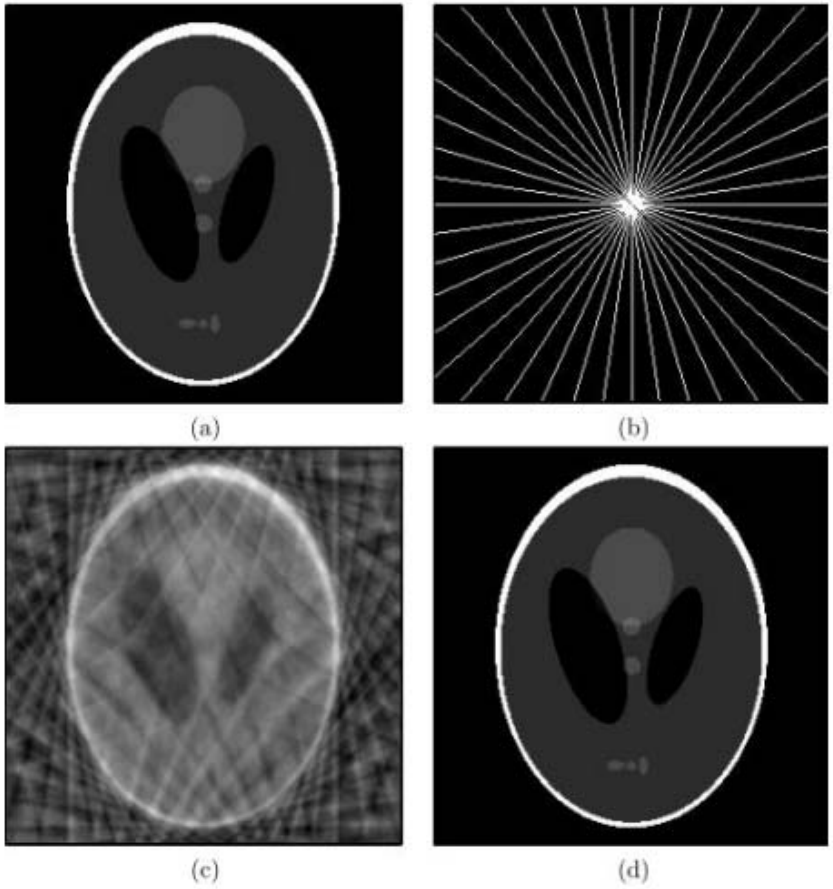

Figure: Example of a recovery problem(a) The Logan-Shepp phantom test image(b) Sampling domain O in the frequency plane (c) Minimum energy reconstruction by thresholding Fourier coefficients (d) Reconstruction by minimizing the variation (l_1 norm of a gradient)

Theorem (Nyquist-Shannon-Whittaker)

Let f be a function with a Fourier transform $\mathcal{F}[f(x)] = 0$ for $|x| > L$, then f is determined by values of f at $2L$ points spaced $\frac{1}{2L}$ apart.

Example (The Logan-Shepp phantom image (512x512))

In this example direct zeroing of the Fourier coefficients does not do much. Minimization of the variances allows to precisely restore data from 22 instead of 512 (5%) sample planes.

Notation

Denote by $\mathbb{Z}_N = 0, 1, \cdots, N-1$.

Definition (Discrete Fourier Transform)

For vector $x \in \mathbb{C}^N$ *discrete Fourier Transform (DFT)* $\mathcal{F}x = \hat{x} \in \mathbb{C}^N$ is:

$$\hat{x}_\omega = \sum_{\omega \in \mathbb{Z}_N} x_t e^{-2\pi i \omega t / N}, \ \omega \in \mathbb{Z}_N.$$

The vector x may be restored from $\hat{x}$ by *inverse DFT* ($\mathcal{F}^{-1} = \frac{1}{N}\mathcal{F}^*$):

$$x_t = \frac{1}{N} \sum_{\omega \in \mathbb{Z}_N} \hat{x}_\omega e^{2\pi i \omega t / N}, \ t \in \mathbb{Z}_N.$$

Let $T, \Omega \subset \mathbb{Z}_N$. Denote by $\mathcal{F}_{T,\Omega}$ operator mapping $\mathbb{C}^N \to \mathbb{C}^N$:

$$\mathcal{F}_{T,\Omega} x = (\mathcal{F}(x|_T))|_\Omega.$$

For vector $x \in \mathbb{C}^N$ denote by $supp(x) = \{i \in \mathbb{Z}_N | x_i \neq 0\}$.

Exact recovery for random Fourier projection

Definition (OPL1)

Let $\Omega \subset \mathbb{Z}_N$ and $x \in \mathbb{C}^N$. *Optimization problem L1 (OPL1)* is

$$min||u||_{l_1} := \sum_{t \in \mathbb{Z}_N} |u_t|, \text{ subject to } (\mathcal{F}u)_k = (\mathcal{F}x)_k, \text{ for } k \in \Omega$$

Theorem (Candès et al. (2006))

Let $x \in \mathbb{C}^N$ be a vector with $supp(x) = T \subset \mathbb{Z}_N$.
Let $\Omega \subset \mathbb{Z}_N$ be a uniformly at random set of size $|\Omega| = N_\omega$.
Fix $B > 0$ (accuracy).
With probability $p \geq 1 - O(N^{-B})$
the minimizer of the OPL1 restores x precisely when

$$|\Omega| \geq C'_B |T| \log N$$

Here $C'_B \asymp 23(B+1)$.

“Take-home message”

Theorem interpretation

- The theorem describes restoration behavior on probabilistically typical (random) DFT projection.
- The theorem claims that vector may be restored
  1. with high probability
  2. using OPL1
  3. given its DFT coefficients on the set of size proportional to its support size times log N.

The worse case restoration behavior relates to *Uncertainty Principle* (Donoho and Stark, 1989).

Uncertainty Principle (UP)

Classical uncertainty principle (Heisenberg) $\Delta t \cdot \Delta p > 1$.

Theorem (DS Uncertainty Principle, Donoho and Stark (1989))

If $h \in \mathbb{C}^N$, then

$$|supp(h)| \cdot |supp(\hat{h})| > N \text{ or } |supp(h)| + |supp(\hat{h})| \geq 2\sqrt{N}.$$

How UP relates to l_1 minimization?

If x^* is not unique solution of the OPL1, $h \neq 0$, $\hat{h}|_\Omega = 0$, $supp(x^*) = T \subset \mathbb{Z}_N$, then

$$\sum_{t \in \mathbb{Z}^N} |x_t^* + h_t| = \sum_{t \in T} |x_t^* + h_t| + \sum_{t \in T^c} |h_t| \geq \sum_{t \in T} |x_t^*| - |h_t| + \sum_{t \in T^c} |h_t|.$$

The $||x^* + h||_{l_1} = ||x^*||_{l_1}$ implies $\sum_{t \in T} |h_t| \geq \sum_{t \in T^c} |h_t|$, or h is *half-l_1 concentrated on T*.

Now uniqueness of OPL1 minimum obtained from the following.

Theorem (Concentration form of UP, Donoho and Stark (1989))

Let $h \in \mathbb{C}^N$ is half-l_1 concentrated on T, and $supp(\hat{h}) \subset \mathbb{Z}_N - \Omega$. Then $2|T| \cdot (N - |\Omega|) < N$ implies $h \equiv 0$.

Refinement of UP in Tao (2005): $|supp(h)| + |supp(\hat{h})| > N$ for prime N.

Example illustrating difference between worst case and typical case

Example (Dirac's comb)

Suppose that $N = k^2$, and $f = \{f_t = 1 \text{ for } t = jk;\ f_t = 0 \text{ for } t \neq jk; j \in \mathbb{Z}_k\}$.

The signal is invariant under the Fourier transform $f = \hat{f}$.

Let $T = \{jk | j \in \mathbb{Z}_k\}$, and let $\Omega = \mathbb{Z}_N - T$ be the set of all frequencies except for the multiples of $k = \sqrt{N}$.

The $\hat{f}|_\Omega \equiv 0$.

The OPL1 reconstruction of f from $\hat{f}|_\Omega$ is identical zero.

For sufficiently large N holds $|\Omega| = N - \sqrt{N} \geq C'_B |T| \log N = C'_B \sqrt{N} \log N$.

"Take-home message"

Reconstruction Theorem (Candès et al., 2006) does not work for all sets of proper sizes (Dirac comb).

Dirac's comb gives extreme sizes for uncertainty principles (Donoho and Stark, 1989).

Dirac's comb with $k = 2^m$ shows that *logN* is necessary.

Plan

- Signal restoration with random Fourier projection (Candès et al., 2006)
  - Phenomenon
  - Signal restoration for random Fourier projection
  - Uncertainty principle
  - Examples for worst case, Dirac comb
  - Main techniques
    - Type of randomness
    - Duality, convex optimization
    - Hilbert (energy) polynomial
  - Robustness and stability
- Compressed Sensing (Donoho, 2006a; Candès, 2006; Candès and Tao, 2006b; Candès and Romberg, 2007; Donoho et al., 2006; Candès and Tao, 2006a)
- Back to Lasso (Knight and Fu, 2000; Zhao and Yu, 2006; Bickel et al., 2009; Meinshausen and Yu, 2009; Wainwright, 2009; Juditsky and Nemirovski, 2008))

What type of randomness?

Reconstruction Theorem (Candès et al., 2006) deals with uniform random projections.

Uniform distribution is difficult to work with.

Consider instead binomial random projections with sample size N and probability of success τ.

Probability of failure to exactly reconstruct for uniform and binomial random projections are equivalent.

Remark (Details)

Let Ω be a uniform random sample set (projection). Let $\Omega' = \{j \in \mathbb{Z}_N | P(j \in \Omega') = \tau\}$ for some $0 < \tau < 1$.

The $E(|\Omega'|) = \tau N$ and for large N, $|\Omega'|/N \approx \tau$ with high probability.

Let Failure($\Omega^{(')}$) be an event of not restoring vector with support in T. If $\Omega_1 \subset \Omega_2$ then Failure(Ω_2) $\subset$ Failure(Ω_1).

For $\tau \cdot N$ integer, median of $|\Omega'| = \tau \cdot N$ (Jogdeo and Samuels, 1968) since

$$P(|\Omega'| \leq \tau N - 1) < 1/2 < P(|\Omega'| \leq \tau N). \tag{1}$$

Then

$$P(\text{Failure}(\Omega')) = \sum_{k=0}^{N} P(\text{Failure}(\Omega_k)) \cdot P(|\Omega'| = k) \tag{2}$$

$$\geq \sum_{k=0}^{N_\omega} P(\text{Failure}(\Omega_k)) \cdot P(|\Omega'| = k) \geq P(\text{Failure}(\Omega)) \sum_{k=0}^{N_\omega} P(|\Omega'| = k) \geq \frac{1}{2} P(\text{Failure}(\Omega)). \tag{3}$$

How do we solve problems like bellow (OPL1)?

$$min||u||_{l_1} := \sum_{t \in \mathbb{Z}_N} |u_k|, \text{ subject to } (\mathcal{F}u)_k = (\mathcal{F}x)_k, \text{ for } k \in \Omega$$

Take a derivative, set it to zero, find solution.

But $||.||_{l_1}$ is not smooth, it has special points when one of the coordinates is zero. What to do?

Apply convex analysis!

Definition (Subgradient)

For convex space X, and it's Y and function $f : X \to \mathbb{R}$, subgradient of f is defined as

$$\partial f(x_0) = \{y \in Y | f(x) - f(x_0) \geq (x - x_0, y)\}$$

If function f is differentiable, then ∂f coincides with gradient ∇f.

Theorem (Fermat's like theorem)

The point u is an extremal point of function f iff $0 \in \partial f(u)$

Example (Case of l_1)

For $x \in \mathbb{C}^N$,

$$\partial(||.||_1)(x)_i = \begin{cases} sign(x_i) & \text{for } i \in supp(x), \\ [-1,1] & \text{for } i \notin supp(x). \end{cases}$$

Karush Kuhn Tucker Theorem with Slater conditions (Rockafellar, 1996; Nesterov, 2004; Boyd and Vandenberghe, 2004), see also (Fuchs, 2005) imply that

Observation

If $\mathcal{F}_{T,\Omega}$ is injective then u is unique solution of OPL1 iff

there exists u^* with

$$u_i^* = \begin{cases} sign(x_i) & \text{for } i \in supp(x); \\ |x_i| < 1 & \text{for } i \notin supp(x). \end{cases}$$

Stability and Robustness of recovery

To recover we can find support of the vector x by l_1 optimization (OPL1) and run regression to find coefficients.

Stability means small change in the conditions gives small change in the results.

Robustness means stability under noise.

Is regression stable?

Regression is given by formula:

$$x = (\mathcal{F}^*_{T,\Omega}\mathcal{F}_{T,\Omega})^{-1}\mathcal{F}^*_{T,\Omega}\hat{x}|_\Omega.$$

The proof of Reconstruction Theorem implies

$\mathcal{F}^*_{T,\Omega}\mathcal{F}_{T,\Omega} \geq \delta\,\mathbb{1}\!\mathbb{1}$ (with $\delta > 1/2$) with high probability,

hence for $|\Omega| > C'_B \cdot |T| \cdot \log N$ stability has place.

To deal with robustness (signal + noise) we need some generalization.

Plan

- Signal restoration with random Fourier projection (Candès et al., 2006)
- Compressed Sensing (Donoho, 2006a; Candès, 2006; Candès and Tao, 2006b; Candès and Romberg, 2007; Donoho et al., 2006; Candès and Tao, 2006a)
- Back to Lasso (Knight and Fu, 2000; Zhao and Yu, 2006; Bickel et al., 2009; Meinshausen and Yu, 2009; Wainwright, 2009; Juditsky and Nemirovski, 2008))

Compressed Sensing (CS)

Compressed/compressive sensing is a sampling based on 2 principles:

Sparsity is a low dimensionality in some sense,

Incoherence extends uncertainty principle.

Vector $x \in \mathbb{R}^N$ for the basis $\Psi = (\psi_1, \cdots, \psi_N)$, and $x_i = (x, \psi_i)$.
Vector x is S-sparse if $|supp(x)| \leq S$.

Definition (Coherence between orthonormal bases)

Given a pair of orthonormal bases Ψ, Φ,

$$\mu(\Psi, \Phi) = \sqrt{N} \cdot \max_{1 \leq k,j \leq N} |(\phi_k, \psi_j)|.$$

Note that $1 \leq \mu(\Psi, \Phi) \leq \sqrt{N}$.

Fourier bases:
for $\mathcal{F} = \Phi : \ \phi_k(\omega) = \sqrt{N} e^{i2\pi k\omega/N}$,[1]
for $\mathcal{F}^* = \Psi : \ \psi_k(\omega) = \sqrt{N} e^{-i2\pi k\omega/N}$.
In this case $\mu(\Psi, \Phi) = 1$ - *maximal incoherence*.

[1] Different normalization

Under sampling and Sparse recovery

If we measure all N coefficients, but observe only $M << N$, can we reconstruct signal?

Theorem (Candès and Romberg (2007))

Fix $\delta > 0$ and $x \in \mathbb{R}^N$ and suppose that x is S-sparse. Choose Ω measurements uniformly at random. If

$$|\Omega| \geq C \cdot \mu^2(\Phi, \Psi) \cdot S \cdot \log N/\delta$$

then solution of the convex optimization problem

$$\arg\min_{\bar{x} \in \mathbb{R}^N} ||\bar{x}||_{l_1} : (x, \phi_k) = (\phi_k, \Psi\bar{x}), k \in \Omega \quad (OPL1B)$$

recover x with probability at least $1 - \delta$.

"Take-home message"

To restore signal in the two orthonormal basis case, one needs *sparsity* times *log correction* times *mutual coherence*.

Unfortunately mutual coherence runs up to $\sqrt{N}$.

Robust signal recovery from noisy data

What happened if signal is nearly sparse and noisy?
Consider now recovery $x \in \mathbb{R}^N$ with

$$y = Ax + z,$$

here A is $M \times N$ *sensing* matrix, z is small in some sense noise.
In previous cases we had $A = (\Phi\Psi)|_\Omega$.

Restricted Isometry

Let $S \leq N$. Matrix A is S-restricted isometry (RI) if matrix A satisfies

$$(1 - \delta_S)||x||_{l_2} \leq ||Ax||_{l_2} \leq (1 + \delta_S)||x||_{l_2},$$

for x with support $|supp(x)| < S$ and some $0 < \delta_S < 1$.

Theorem (Robust recovery from noisy data, Candès et al. (2006))

Let y as above, and let matrix A is RI with $\delta_{2S} < \sqrt{2} - 1$. Then solution x^* of the

$$\arg\min_{\bar{x} \in \mathbb{R}^N} ||\bar{x}||_{l_1} \ : \ ||Ax - y||_{l_2} \leq \varepsilon \quad (OPL1N)$$

satisfies

$$||x^* - x||_{l_2} \leq C_0 \cdot ||x - x_S||_{l_1} / \sqrt{S} + C_1 \cdot \varepsilon.$$

Sources of RIP matrices Candès and Tao (2006c); Donoho (2006a); Rudelson and Vershynin (2006)

Matrices satisfying RIP are generated by randomization Baraniuk et al. (2008); Mendelson et al. (2008).

Tree main random constructions:

- **Random matrices with i.i.d. entries.** Candès and Tao (2006c); Donoho (2006b); Rudelson and Vershynin (2006)

  Let matrix **A**'s entries are i.i.d. for a sub-gaussian distribution with $\mu = 0$ and $\sigma = 1$. Then , $\hat{\mathbf{A}} = \frac{1}{\sqrt{M}} A$ satisfies RIP with $\delta_S \leq \delta$ when $M \geq \text{const}(\varepsilon, \delta) \cdot S \cdot \log(2N/S)$ with probability $p > 1 - \varepsilon$.

  Distribution examples: Gaussian, Bernoulli

- **Fourier ensemble.** Candès and Tao (2006c); Rudelson and Vershynin (2006) Let $\hat{\mathbf{A}} = \frac{1}{\sqrt{M}} A$ with A being M randomly selected rows from an $N \times N$ DFT matrix. Then $\hat{\mathbf{A}}$ satisfies RIP with $\delta_S \leq \delta$ providing $M \geq \text{const}(\varepsilon, \delta) \cdot S \cdot log^4(2N)$. with probability $p > 1 - \varepsilon$.

- **General orthogonal ensembles.** Candès and Tao (2006c) Let $\dot{A}$ is M randomly selected rows from an $N \times N$ orthonormal matrix U with re-normalized columns. Then (OPL1B) S-sparse recover x with high probability when $M \geq const \cdot \mathcal{M}^2(U) \cdot S \cdot log^6 N$

Modeling: Dantzig Selector, consistency

Let $y = Ax + z$, x is parameters vector, A is design matrix, $z \sim N(0, \sigma^2 I_M)$. We are interested in estimating $||\hat{x}_D - x^*||_{l_2}$, where x^* is actual parameter, and $\hat{x}_D$ is a solution of the Dantzig Selector:

$$\hat{x}_D = \arg\min_{\overline{x} \in \mathbb{R}^N} (||\overline{x}||_{l_1} \ : ||A^*(y - A\overline{x})||_{l_\infty} \leq \lambda_N \cdot \sigma) \ , \lambda_N := (1 + t^{-1})\sqrt{2logN}.$$

For the ideal case suppose A is identity matrix and $y \sim N(x, \sigma^2 \cdot I_M)$. Oracle knowing x^*, choses $\hat{x}$ as x_i^* with $|x_i^*| > \sigma$ and σ otherwise. Then $E||x^* - \hat{x}||_{l_2}^2 = \sum_{i=1}^N min^2(x_i^*, \sigma)$ is a MSE.
Thresholding with level $\sqrt{2 \log N} \cdot \sigma$ achieves this with factor of $\log N$ (Donoho and Johnstone, 1994).

Theorem (DS estimate)

For S with $\delta_{2S} + \delta_{3S} < 1 - t$, DS estimator with high probability obeys

$$||\hat{x}_D - x^*||_{l_2}^2 \leq C_2 \lambda_N^2 (\sigma^2 + \sum_{i=1}^N min^2(x_i^*, \sigma)),$$

DS is log factor far from oracle choice of parameter.

Plan

- Signal restoration with random Fourier projection (Candès et al., 2006)
  - Robustness and stability
- Compressed Sensing (Donoho, 2006a; Candès, 2006; Candès and Tao, 2006b; Candès and Romberg, 2007; Donoho et al., 2006; Candès and Tao, 2006a)
- Back to Lasso (Knight and Fu, 2000; Zhao and Yu, 2006; Bickel et al., 2009; Meinshausen and Yu, 2009; Wainwright, 2009; Juditsky and Nemirovski, 2008))

Back to LASSO: Lasso consistency

Remind: Lasso estimates

$$\hat{x}(\lambda) = \arg\min_{x \in \mathbb{R}^N}(||y - Ax||_2^2 + \lambda||x||_1)$$

Types of LASSO consistency

Consistency Estimator converges to actual parameter in p- norm:

$$||\hat{x} - x||_p \to 0$$

Model (Support) Signed Consistency Signed support of estimator converges to signed support of actual parameter

Back to LASSO: Irrepresentability, Support (Signed) Recovery

Let $y^M = A_M x^M + \varepsilon_M$, M is an *index of experiment*, A_M is an $M \times N$ *design matrix*, x^M is *vector of parameters* in M-th experiment, ε_M is *noise*, an i.i.d. random variables with $\mu = 0$ and $var = \sigma^2$.
Remind: Lasso estimates $\hat{x}^M(\lambda) = \arg\min_{x \in \mathbb{R}^N}(||y^M - A_M x||_2^2 + \lambda||x||_1)$

For fixed N: $\hat{x}^M(\lambda_M) \xrightarrow{p} x$ and estimates are asymptotically normal (for $\lambda_M = o(M)$) (Knight and Fu, 2000).

Definition (Strongly Sign consistency)

Lasso is **strongly sign consistent** if for some $\lambda_M = f(M)$ holds $\lim_{M\to\infty} P(\hat{x}^M(\lambda_M) =_s x^M) = 1$

Let $supp(x^M) \subset I \subset \mathbb{Z}_N$. Let $Q^M = (A^M)^* A^M$ be a scale of covariance matrix.

Definition (Strong Irrepresentable Condition (SIC))

Matrix A satisfies Strong Irrepresentable Condition if $|1/M(Q^M|_{I,I^c}(Q^M|_{I,I})^{-1}| \leq \mathbb{1}_{N-|I|} - \eta$, for some fixed positive vector η.

Theorem (Strongly Sign Consistency for Lasso, Zhao and Yu (2006))

Lasso is strongly sign consistent if A^M satisfies SIC and $1/M \cdot Q^M \to 0$.

Lasso is not model selection consistent (Fuchs, 2005; Lv and Fan, 2009).

Restricted eigenvalue, Lasso persistency

Definition (Restricted eigenvalue assumption)

For integer $S \in \mathbb{Z}_N$ and positive c_0, matrix A satisfies **restricted eigenvalue** assumption ($RE(S, c_0)$) if for $Q = A^*A$

$$k^2(S, c_0) := \min_{\substack{J_0 \subset \mathbb{Z}_N, \\ |J_0| \le S}} \min_{\substack{x \in \mathbb{R}^N, x \neq 0, \\ ||x|_{J_0^c}||_1 \le c_0 ||x|_{J_0}||_1}} \frac{(Qx, x)}{M \cdot (x|_{J_0}, x|_{J_0})} > 0.$$

Let $\phi_{max}(S) = \max_{x \in \mathbb{R}^N, |supp(x)| \le S} \frac{(Qx,x)}{(x,x)}$.

Lasso (model) persistency

Theorem (Lasso persistency, (Bickel et al., 2009))

Under general condition for DS, let for some integer $|supp(x^*)| \leq S$ *and assume* $RE(S,3)$ *is satisfied. Let* $\lambda = C\sigma\sqrt{\frac{\log N}{M}}$ *and* $C^2 > 8$. *Then with probability at least* $1 - N^{1-C^2/8}$

$$||\hat{x}_L - x^*||_{l_1} \leq \frac{16C}{k^2(S,3)}\sigma S\sqrt{\frac{\log N}{M}} \tag{4}$$

$$||A(\hat{x}_L - x^*)||_{l_2}^2 \leq \frac{16C}{k^2(S,3)}\sigma^2 S \log N \tag{5}$$

$$|supp(\hat{x}_L)| \leq \frac{64\phi_{max}(S)}{k^2(S,3)}S. \tag{6}$$

Lasso consistency under Incoherent Design Meinshausen and Yu (2009)

Definition (m_M-Incoherent design)

Let m_M be a sequence with $m_M = o(M)$. Design matrix is incoherent for m_M if

$$\liminf_{M\to\infty} \phi_{min}(m_M) > 0, \text{ here } \phi_{min}(m_M) = \min_{x\in\mathbb{R}^N, |supp(x)|\le m_M} \frac{(Qx,x)}{(x,x)}.$$

We usually consider $S_M \log M$ *-incoherent design* (S_M is sparsity).

Theorem (Meinshausen and Yu (2009))

Suppose that design matrix satisfies m_M*-Incoherent design for* $m_M = S_M \log M$, $\lambda_M \approx \sigma m_M \sqrt{M \cdot logN_M}$. *Then*

$$||x^* - \hat{x_L}(\lambda_M)||_{l_2}^2 \le O_N(\frac{logN_M}{M} \frac{m_{\lambda_M}}{\phi_{min}^2(m_{\lambda_M})}) + O(\frac{S_M}{m_{\lambda_M}}).$$

Lasso consistence under Incoherent Design (Meinshausen and Yu, 2009)

Corollary (Lasso's l_2 consistency, (Meinshausen and Yu, 2009))

Under condition of the theorem, Lasso is l_2 consistent if

$$S_M \log N_M \cdot \frac{logM}{M} \to 0 \text{ when } M \to \infty.$$

'Sharp' thresholds for Lasso support consistency Wainwright (2009)

Let S be a sparsity set.

Definition (Incoherence and Eigenvalues (I&E))

Incoherence condition:

$$|||Q_{S,S^c}(Q_{S,S})^{-1}|||_{\infty,\infty} \leq (1-\nu) \text{ for some } 0 < \nu < 1 \ (Q = A^*A).$$

Eigenvalues Condition:

$$\phi_{min}(1/M \cdot Q_{S,S}) \geq C_{min}, \ C_{min} > 0.$$

Theorem (Lasso support inconsistency, Wainwright (2009))

Probability of sign support equality is less than $1/2$ *if either*

- *expression in Incoherence condition* $> 1 + \nu > 1$, *or*
- *minimum non-zero value in* $|x^*|$ *less than right side of above inequality.*

Lasso's l_∞ consistency, Wainwright (2009)

Theorem (Lasso's l_∞ consistency, Wainwright (2009))

Under general DS and I&E condition, let $\lambda_M > \frac{2}{\nu}\sqrt{\frac{2\sigma^2 \log N}{M}}$. *Then for some* $c_1 > 0$ *with probability greater than* $1 - 4e^{-c_1 M \lambda_M^2} \to 1$*:*

a) *The lasso has a unique solution* $\hat{x}$ *with* $supp(\hat{x}) \subset supp(x^*)$ *and satisfying* l_∞ *bound:*

$$||\hat{x_L} - x^*||_\infty \leq \lambda_M(||(A_S^* A_S/M||_\infty + \frac{4\sigma}{\sqrt{C_{min}}}).$$

b) *If in addition minimum non-zero value in absolute value of* x^* *greater than right side of above inequality, then* $\hat{x_L}$ *has proper signs.*

Efficient condition for RIP verification

Mutual coherence property is easily verifiable.

RI type properties are complex to verify, since they include min over all subspaces of given dimensions.

The following papers apply either linear programming or semidefinite programming to extend RIP verification beyond Random matrices.

- (Juditsky and Nemirovski, 2008), (Juditsky et al., 2009)
- (D'Aspremont and Ghaoui, 2008)

Summary

- Signal restoration with random Fourier projection
- Compressed Sensing
- Lasso consistency
- Efficient restoration and consistency conditions

Outline

- Introduction
- Sparse Linear Regression: Lasso
- Sparse Signal Recovery and Lasso: Some Theory
- Sparse Modeling: Beyond Lasso
  - Consistency-improving extensions
  - Beyond l_1-regularization (l1/lq, Elastic Net, fused Lasso)
  - Beyond linear model (GLMs, MRFs)
  - Sparse Matrix Factorizations
  - Beyond variable-selection: variable construction
- Summary and Open Issues

Model Selection Consistency of LASSO

- Let X_S be the columns of the nonzero variables in the true model (support), and let X_{S^C} be the remaining columns (complement)

- (Strong) Irrepresentability condition for model selection (Zhao and Yu, 2006a; Yuan and Lin, 2007b; Zou, 2006; Wainwright, 2009b)

$$||(X_S^T X_S)^{-1} X_S^T X_{S^C}||_\infty \leq 1 - \epsilon, \quad \text{for some } 0 < \epsilon \leq 1$$

  states that the least-squares regression coefficients (i.e., correlations) for the non-essential variables (X_{S^C} columns) on support variables in X_S must not be large.

- Relaxing the consistency conditions via Lasso modifications:

- bootstrap Lasso (BOLASSO) Bach (2008a) and stability-selection (Meinshausen and Buehlmann, 2008) use bootstrap approach: learn multiple Lasso models on data subsets, and then include the intersection of nonzeros (Bach, 2008a) or only frequent-enough nonzeros (Meinshausen and Buehlmann, 2008). This gets rid of "unstable" variables and improves the model-selection consistency and stability to the choice of λ parameter.

Parameter-Estimation Consistency

- due to shrinkage, Lasso produces biases parameter estimation, and is in general inconsistent

- relaxed Lasso (Meinshausen, 2007) solves Lasso twice: first, to choose a subset of variables, and second (with less competition among the variables and thus smaller CV-selected λ) to fit the parameters; smaller $\lambda \Rightarrow$ less shrinkage (less bias)

- alternative - modifying Lasso penalty to shrink large coefficients less severely: SCAD penalty (Fan and Li, 2005); however, SCAD is non-convex

- adaptive Lasso (Zou, 2006) approximates SCAD using data-dependent weighted penalties, but retains convexity; results into consistent estimates

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Beyond LASSO

$$Loss(\mathbf{x}) + \lambda ||\mathbf{x}||_1$$

Other likelihoods (loss functions)

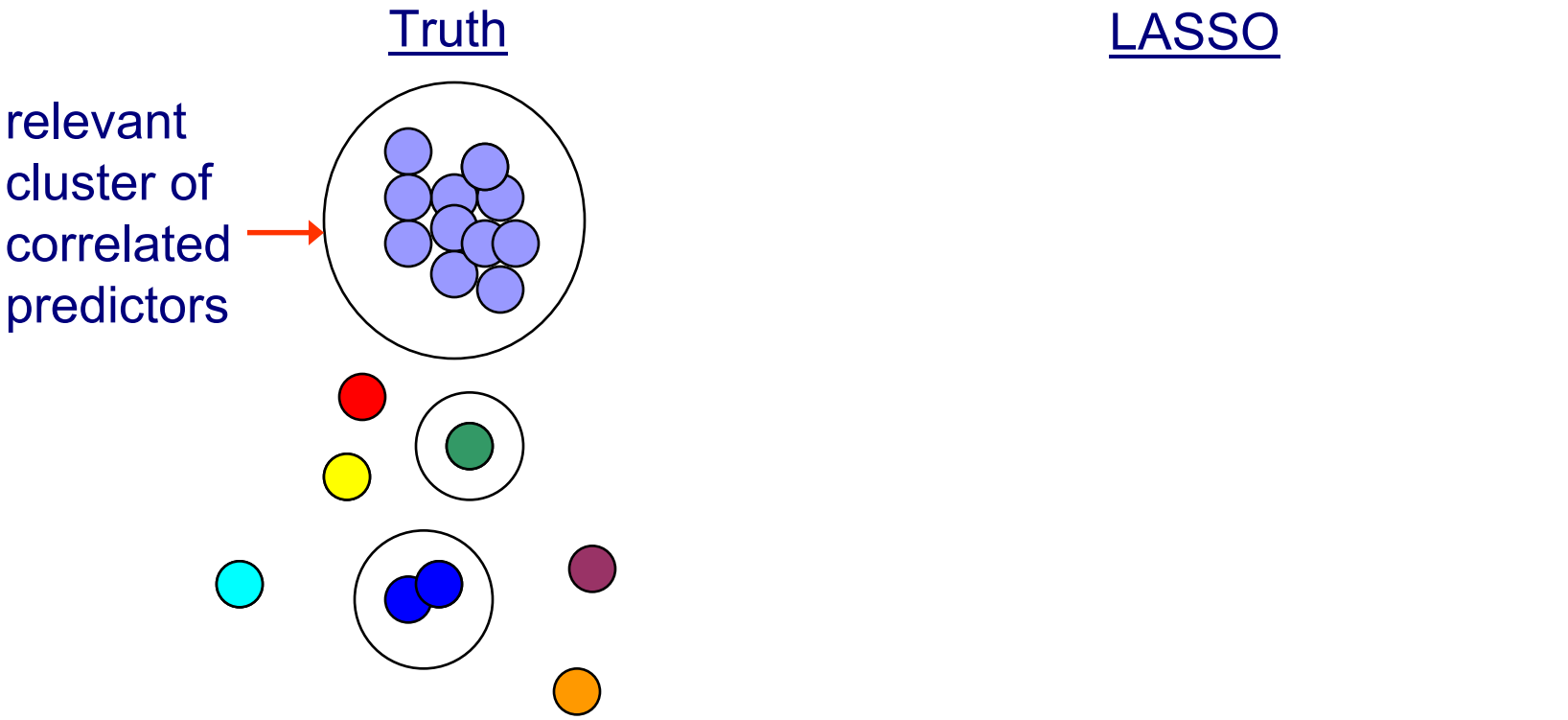
- Generalized Linear Models (exponential family noise)
- Multivariate Gaussians (Gaussian MRFs)

Adding structure beyond sparsity

- Elastic Net
- Fused Lasso
- Block l_1-l_q norms:
  - group Lasso
  - simultaneous Lasso

Some Limitations of LASSO

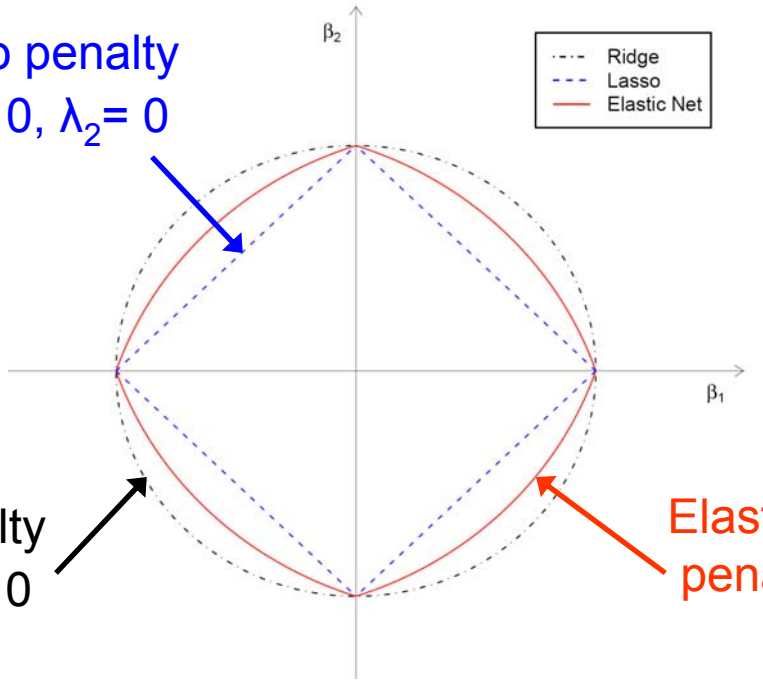
- selects at most n variables when $p > n$ (Osborne et al., 2000)
  (but what if more predictors are relevant?)
- does not group correlated variables (Zou and Hastie, 2005):
  - even if $X_i = X_j$, has many solutions with $\beta_i \neq \beta_j$
  - tends to select one variable out of a group of correlated ones



Elastic Net (Zou and Hastie, 2005)

$$\hat{\beta} = \arg\min_{\beta} ||y - X\beta||_2^2 + \lambda_1||\beta||_1 + \lambda_2||\beta||_2^2$$

lasso penalty
$\lambda_1 > 0$, $\lambda_2 = 0$



ridge penalty
$\lambda_1 = 0$, $\lambda_2 > 0$

Elastic Net penalty

Elastic Net penalty:

$$\alpha||\beta||_2^2 + (1-\alpha)||\beta||_1,$$

where $\alpha = \dfrac{\lambda_2}{\lambda_2 + \lambda_1}$

- l_1 keeps singularities at vertices $\Rightarrow$ sparsity
- l_2 enforces strictly convex edges $\Rightarrow$ grouping effect
- l_2 removes the limitation on the number of selected variables

NOTE: to eliminate "double-shrinkage", Elastic Net computes a re-scaled version $(1+\lambda_2)\hat{\beta}$ of the above *naive EN* estimate $\hat{\beta}$

Grouping Effect

- strictly convex penalty guarantees $\hat{\beta}_i = \hat{\beta}_j$ if $X_i = X_j$

- λ_2 controls grouping effect: highly correlated variables have similar coefficients (and thus are included/excluded together):

$$|\hat{\beta}_i - \hat{\beta}_j| \leq \frac{||y||_1}{\lambda_2}\sqrt{1(1-\rho)}$$

where $\rho = {X^i}^T X_j$ is the sample correlation (we also assume same-sign coefficients $\hat{\beta}_i \hat{\beta}_j > 0$).

- When $\lambda_2 \to \infty$, Elastic Net becomes equivalent to univariate soft thresholding:

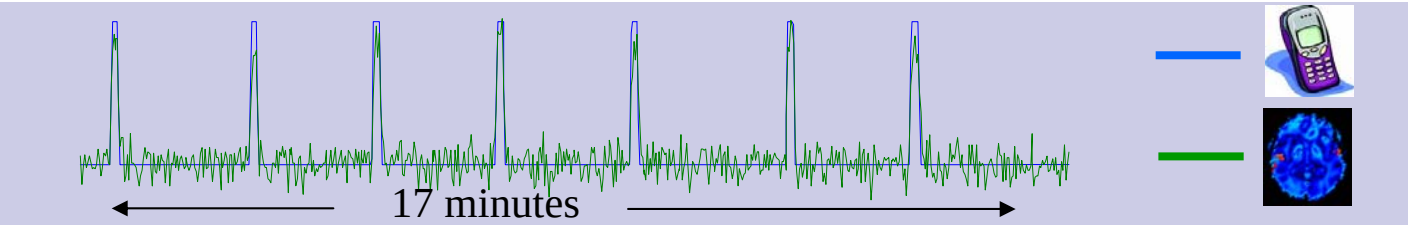
$$\hat{\beta}(\infty)_i = (|y^T X^i| - \frac{\lambda_1}{2})_+ sign(y^T X^i), \quad i = 1, ..., p.$$

Example: Application to fMRI Analysis

Pittsburgh Brain Activity Interpretation Competition (PBAIC-07):

- subjects playing a videogame in a scanner
- 24 continuous response variables, e.g.
  - Annoyance
  - Sadness
  - Anxiety
  - Dog
  - Faces
  - Instructions
  - Correct hits

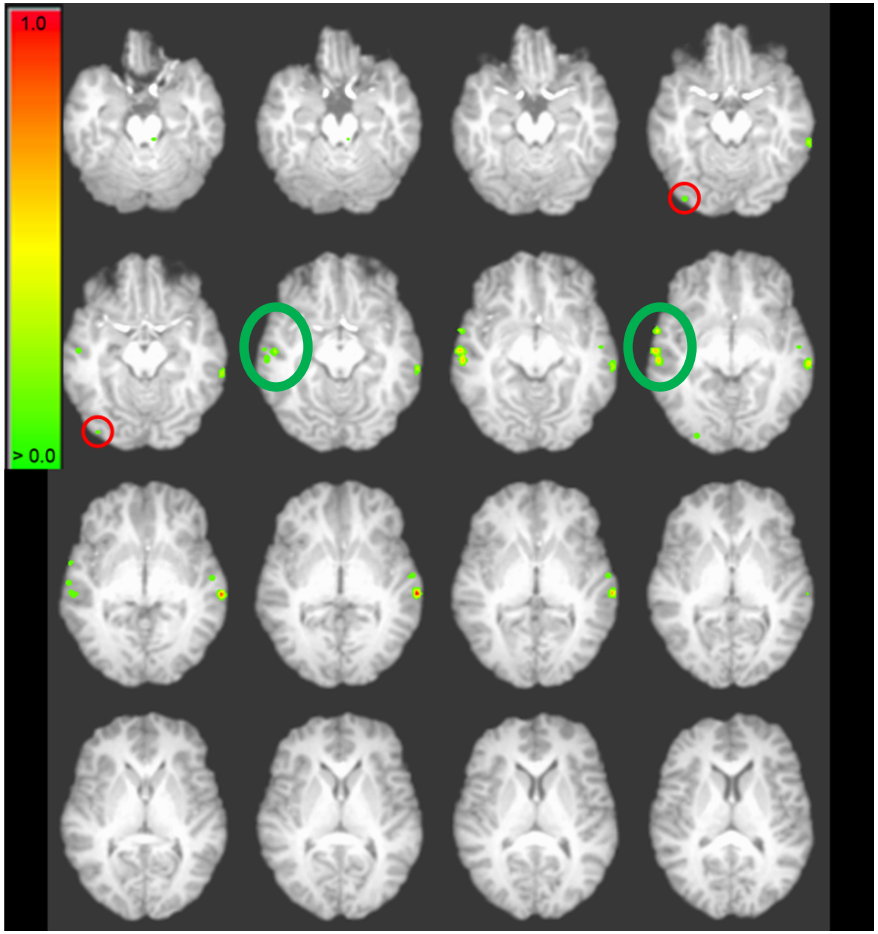
Goal: predict responses from fMRI data



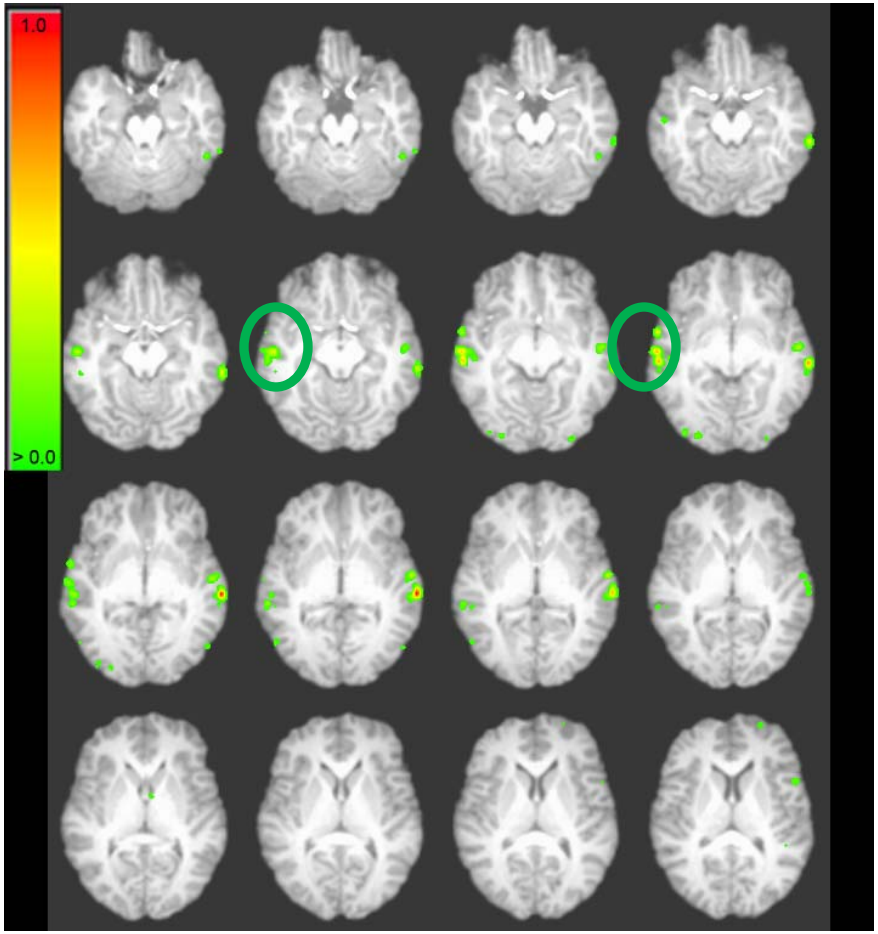
Grouping Effect on PBAIC data

(Carroll, Cecchi, Rish, Garg, Rao 2009)

Predicting 'Instructions' (auditory stimulus)



Small grouping effect: $\lambda_2 = 0.1$



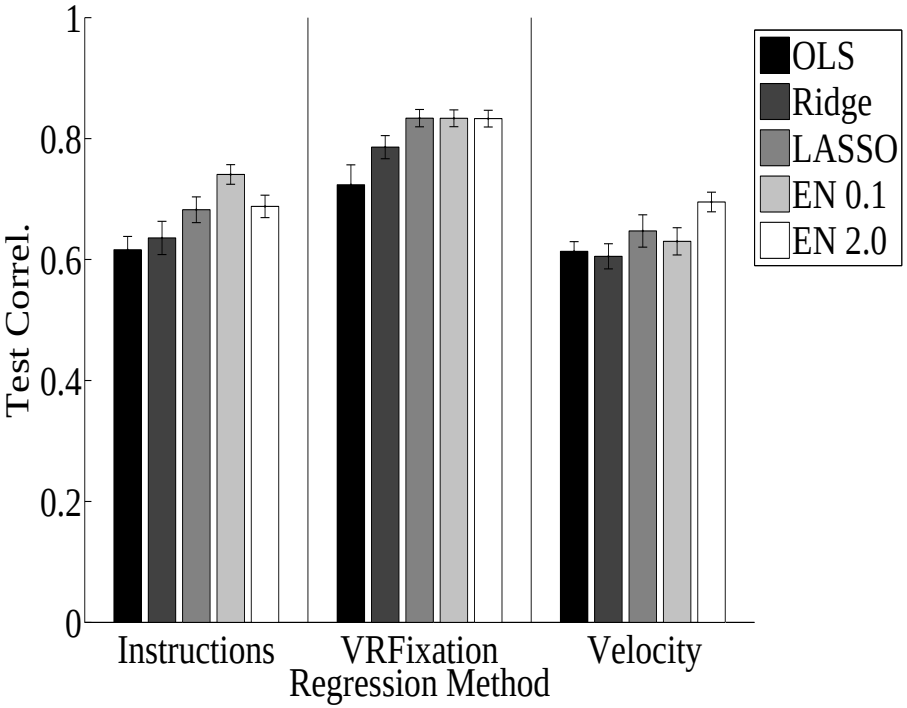
Larger grouping effect: $\lambda_2 = 2.0$

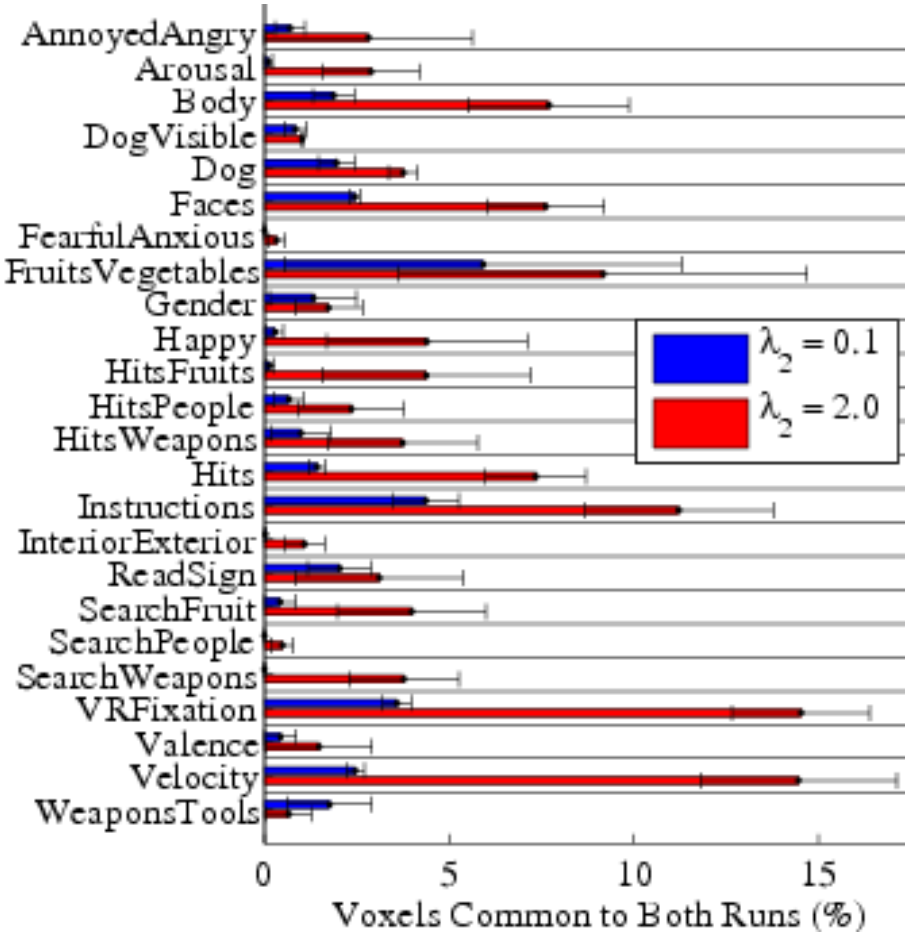
Higher λ_2→ selection of more voxels from correlated clusters →
larger, more spatially coherent clusters

Grouping Tends to Improve Model Stability

(Carroll, Cecchi, Rish, Garg, Rao 2009)

Stability is measured here by average % overlap between models for 2 runs by same subject



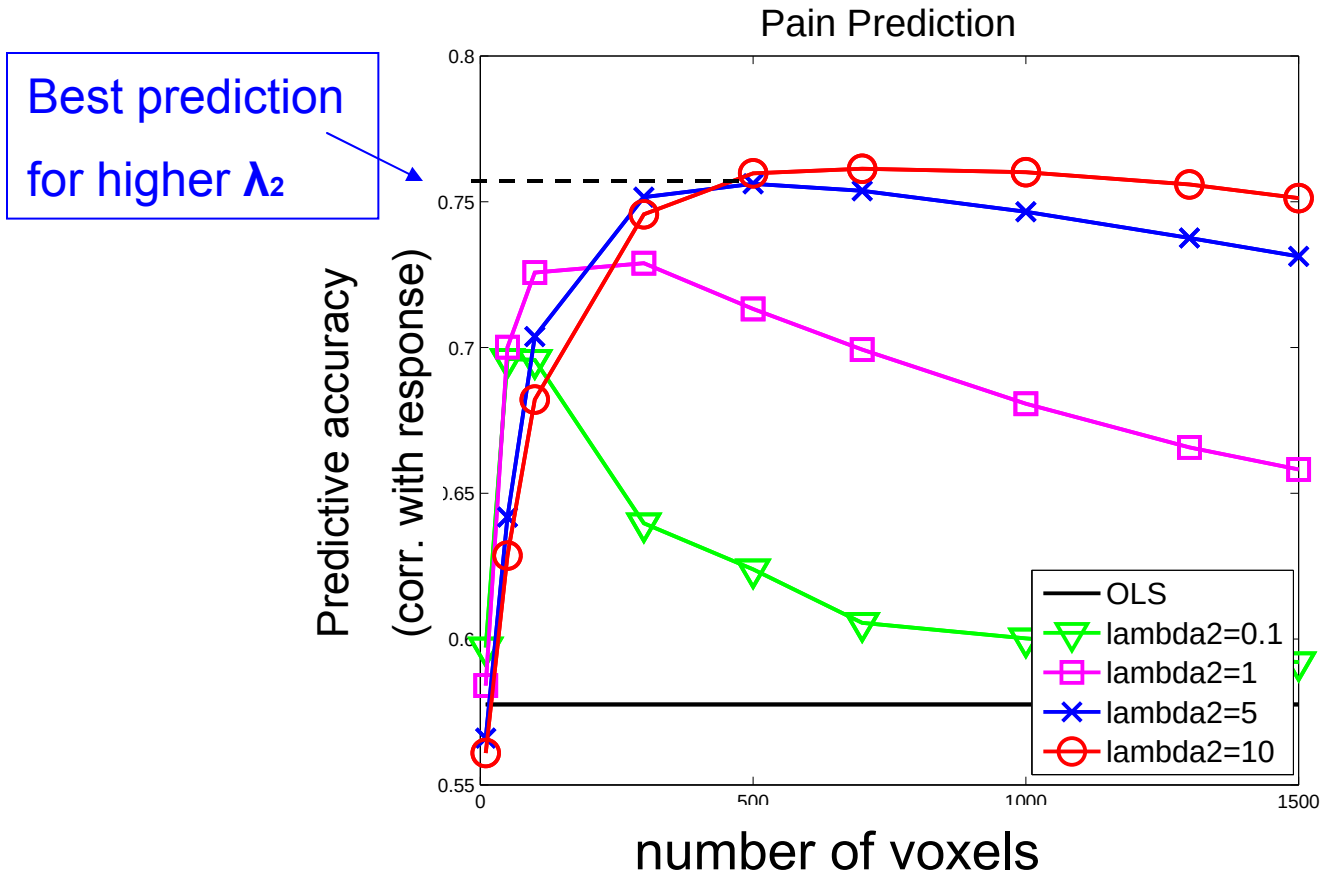


Among almost equally predictive models,

increasing λ_2 can significantly improve model stability

Another Application: Sparse Models of Pain Perception from fMRI

Predicting pain ratings from fMRI in presence of thermal pain stimulus
(Rish, Cecchi, Baliki, Apkarian, BI-2010)



Including more correlated voxels (increasing λ_2) often improves the prediction accuracy as well

Fused Lasso (Tibshirani et al., 2005)

- EN smoothes coefficients uniformly
- But what if there is a natural ordering of the predictors?
- Fused Lasso encourages smoothness along such ordering (besides sparsity):

$$\min_{\beta} ||y - X\beta||_2^2 + \lambda_1 ||\beta||_1 + \lambda_2 \sum^{p-1} |\beta_{i+1} - \beta_i|$$

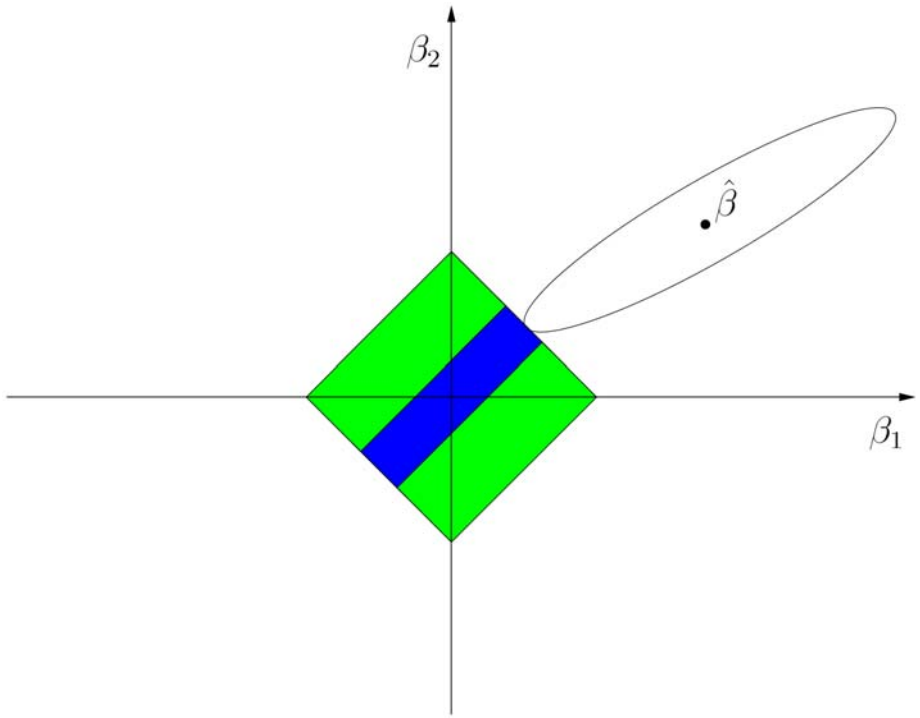


Image courtesy of [Tibshirani et al, 2005]

Group Lasso (Yuan and Lin, 2006)

- What if there is a natural group structure among the variables?
  - functional clusters of genes, or brain voxels
  - categorical variables encoded by groups of indicator variables
  - multi-task learning: parameters for same feature across all tasks

- Block l_1-l_2 penalty selects groups of variables from $G = \bigcup_{i=1}^{K} G_i$, a partition of $\{1, ..., p\}$:

  l_1 promotes sparsity between the groups,
  l_2 discourages sparsity within the groups:

$$\min_{\beta} ||y - X\beta||_2^2 + \lambda \sum_{i=1}^{K} ||\beta_{G_i}||_2$$

Group Lasso: Examples

- Generalized additive models (Bakin, 1999): groups $\Leftrightarrow$ basis expansion coefficients for each component function f_i:

$$g(E(Y)) = \sum_i f_i(X_i), \qquad f_i(x) = \sum_k \alpha_{ik} h_k(x)$$

- Multiple kernel learning (Lanckriet et al., 2004; Bach et al., 2004): groups $\Leftrightarrow$ kernels $\Leftrightarrow$ weights of multi-dimensional features:

$$K(x, x') = \sum_{i=1}^{m} \alpha_i K_i(x, x'), \quad K_i(x, x') = \Phi_i^T(x)\Phi_i(x'), \ \Phi_i(x) \in R^{n_i}$$

$$\text{predictor: } \sum_{i=1}^{m} w_i^T \Phi_i(x), \quad \text{penalty: } \sum_{i=1}^{m} ||w_i||_2$$

- Sparse vector-autoregressive models: groups $\Leftrightarrow$ time-lagged variables of the same time-series (Lozano et al., 2009a)

More on Group Lasso

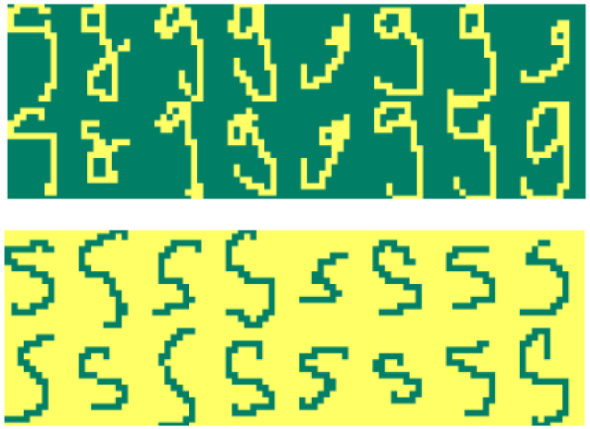
- Extensions to logistic regression (Meier et al., 2008) and generalized linear models (Roth and Fischer, 2008)
- Extensions to overlapping groups (Jacob et al., 2009)
- Consistency analysis Bach (2008b)
- Algorithms:
  - block-coordinate descent (Yuan and Lin, 2006)
  - active set approach (Roth and Fischer, 2008; Obozinski et al., 2010)
  - Nesterov's method (Liu et al., 2009b)
  - greedy approach (group OMP) Lozano et al. (2009b)

Multi-Task (Simultaneous) Variable Selection

- Select a common subset of variables for k problems
- Example: joint feature selection for character-recognition problems for multiple writers (Obozinski et al., 2010); variables: pixels or strokes

The letter '*a*' *written by 40 different people*

Samples of the letters *s and g for one writer*



- Group-Lasso approach: groups $\Leftrightarrow$ same-variable coefficients across tasks (Obozinski et al., 2010, 2009; Liu et al., 2009b)

Multi-Task (Simultaneous) Variable Selection

- Alternative: l_1-l_∞ penalty (Turlach et al., 2005; Tropp, 2006):

$$\min_{\beta} \sum_{j=1}^{k} L(y(j), X, \beta(j)) + \lambda \sum_{j=1}^{k} ||\beta(j)||_\infty$$

where $L(\cdot)$ is a loss function, $y(j)$ and $\beta(j)$ are the response and parameters for the j-th subproblem, respectively, and $||\beta(j)||_\infty = \max\{\beta_1(j), ..., \beta_p(j)\}$.

- In general, composite penalties l_1-l_q, $1 \leq q \leq \infty$, enforce more variable sharing among tasks as $q \Rightarrow \infty$: from none ($q = 1$) to full ($q = \infty$)

- Hierarchical variable selection with l_1-l_q (Zhao et al., 2009)

- Efficient algorithms for l_1-l_∞: blockwise coordinate descent (Liu et al., 2009a), projected gradient (Quattoni et al., 2009)

Outline

- Introduction
- Sparse Linear Regression: Lasso
- Sparse Signal Recovery and Lasso: Some Theory
- Sparse Modeling: Beyond Lasso
  - Consistency-improving extensions
  - Beyond l_1-regularization (l1/lq, Elastic Net, fused Lasso)
  - Beyond linear model (GLMs, MRFs)
  - Sparse Matrix Factorizations
  - Beyond variable-selection: variable construction
- Summary and Open Issues

Beyond Lasso: General Log-likelihood Losses

$$Loss(\mathbf{x}) + \lambda ||\mathbf{x}||_1$$

$$\downarrow$$

$$-\log P(y|\mathbf{x}) + \lambda ||\mathbf{x}||_1$$

$$\downarrow$$

1. Gaussian $\Leftrightarrow$ Lasso
2. Bernoulli $\Leftrightarrow$ logistic regression
3. Exponential-family $\Leftrightarrow$ Generalized Linear Models (includes 1 and 2)
4. Multivariate Gaussian $\Leftrightarrow$ Gaussian MRFs

l_1-regularized M-estimators

Beyond LASSO

$$Loss(\mathbf{x}) + \lambda ||\mathbf{x}||_1$$

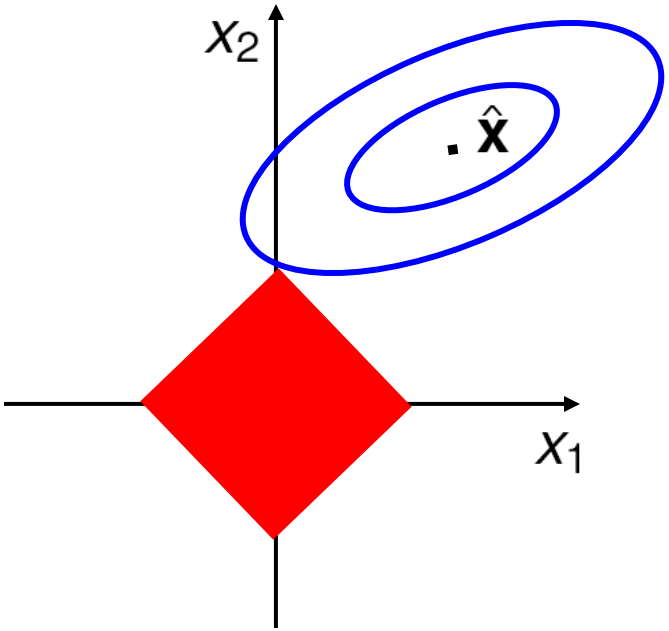
Other likelihoods (loss functions)

- Generalized Linear Models (exponential family noise)
- Multivariate Gaussians (Gaussian MRFs)

Adding structure beyond sparsity

- Elastic Net
- Fused Lasso
- Block l_1-l_q norms:
  - group Lasso
  - simultaneous Lasso

Sparse Signal Recovery with M-estimators

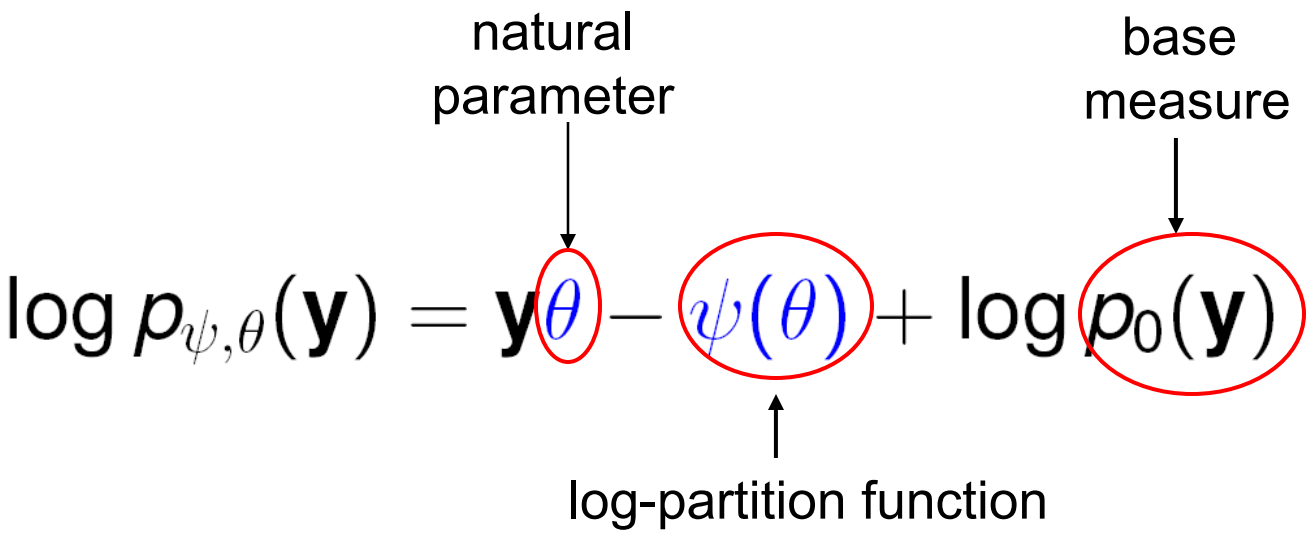


- Can l_1-regularization accurately recover sparse signals given **general log P(y|x) losses**?

- **Yes!**
  (under proper conditions)

- risk consistency of generalized linear models (Van de Geer, 2008)
- model-selection consistency of Gaussian MRFs (Ravikumar et al, 2008a)
- generalized linear models: recovery in l_2-norm (non-asymptotic regime) for exponential-family noise and standard RIP conditions on the design matrix (Rish and Grabarnik, 2009)
- Asymptotic consistency of general losses satisfying restricted strong convexity, with decomposable regularizers (Negahban et al., 2009)

Exponential Family Distributions



$\psi(\theta)$ is strictly convex and differentiable

$\psi(\theta)$ uniquely determines the member distribution of the family

Examples: Gaussian, exponential, Bernoulli, multinomial, gamma, chi-square, beta, Weibull, Dirichlet, Poisson, etc.

Generalized Linear Models (GLMs)

$$E_{p_{\psi,\theta}}(\mathbf{y}) = f^{-1}(\mathbf{Ax})$$

$E_{p_{\psi,\theta}}(\mathbf{y}) = \mu(\theta)$ - *expectation parameter*
Corresponds to the natural parameter $\theta = \mathbf{Ax}$

$f(\theta)$ - *link function*, where $f^{-1}(\theta) = \nabla\psi(\theta)$

1. Gaussian noise - *identity* function $f(\mu) = \mu$ (linear regression):

$$E(\mathbf{y}) = \mathbf{Ax}$$

2. Bernoulli noise - *logit* function $f(\mu) = \log \frac{\mu}{1-\mu}$ (logistic regression)

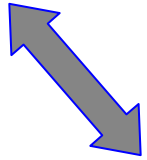
$$E(\mathbf{y}) = \frac{1}{1 + e^{-\mathbf{Ax}}}$$

Summary: Exponential Family, GLMs, and Bregman Divergences

Exponential-Family Distributions

$$\log p_{\psi,\theta}(\mathbf{y}) = \mathbf{y}\theta - \psi(\theta) + \log p_0(\mathbf{y})$$

$\theta = \mathbf{Ax}$
$f^{-1}(\theta) = \nabla\psi(\theta)$



Legendre duality:
$\psi(\theta) \Leftrightarrow \phi(\mu)$

Generalized Linear Models

$$E(\mathbf{y}) = f^{-1}(\mathbf{Ax})$$

Bregman Divergences

$$d_\phi(\mathbf{x},\mathbf{y}) = \phi(\mathbf{x}) - \phi(\mathbf{y}) - \\ - < (\mathbf{x}-\mathbf{y}), \nabla\phi(\mathbf{y}) >$$

Bijection Theorem (Banerjee et al, 2005):

$$p_{\psi,\theta}(\mathbf{y}) = e^{-d_\phi(\mathbf{y},\mu(\theta))} f_\phi(\mathbf{y})$$

Domain	Distribution	Divergence
$\mathbb{R}$	1*D* Gaussian	square loss
$\{0,1\}$	Bernoulli	logistic loss
R_{++}	Exponential	Itakura-Saito distance
n-simplex	*nD* Multinomial	KL-divergence
$\mathbb{R}^n$	*nD* Sph. Gaussian	squared Euclidean distance
$\mathbb{R}^n$	*nD* Gaussian	Mahalanobis distance

Fitting GLM $\Leftrightarrow$ maximizing exp-family likelihood $\Leftrightarrow$
$\Leftrightarrow$ minimizing Bregman divergence

Sparse Signal Recovery from Noisy Observations

Euclidean distance (Candes, Romberg and Tao, 2006):

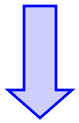
If

- small observation noise: $||y - Ax^0||_{l_2} \leq \epsilon$
- A satisfies the restricted isometry property (RIP)

Then the solution to the sparse linear regression problem

$$x^* = \arg\min_x ||x||_{l_1} \quad s.t. \; ||y - Ax||_{l_2} \leq \epsilon$$

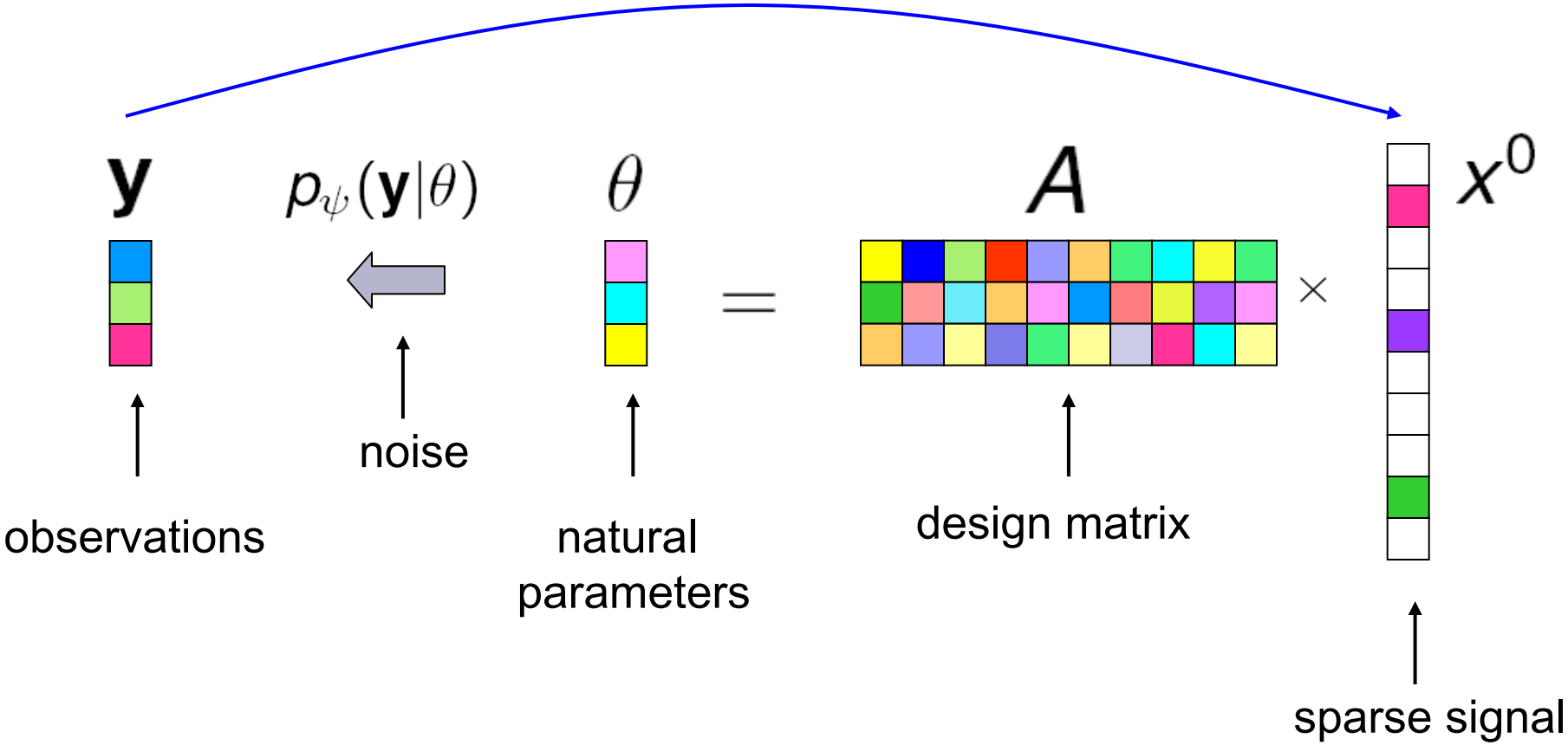
is a good approximation of x^0, i.e. $||x^* - x^0||_{l_2} \leq C_S \cdot \epsilon$.



Generalized Linear Models:

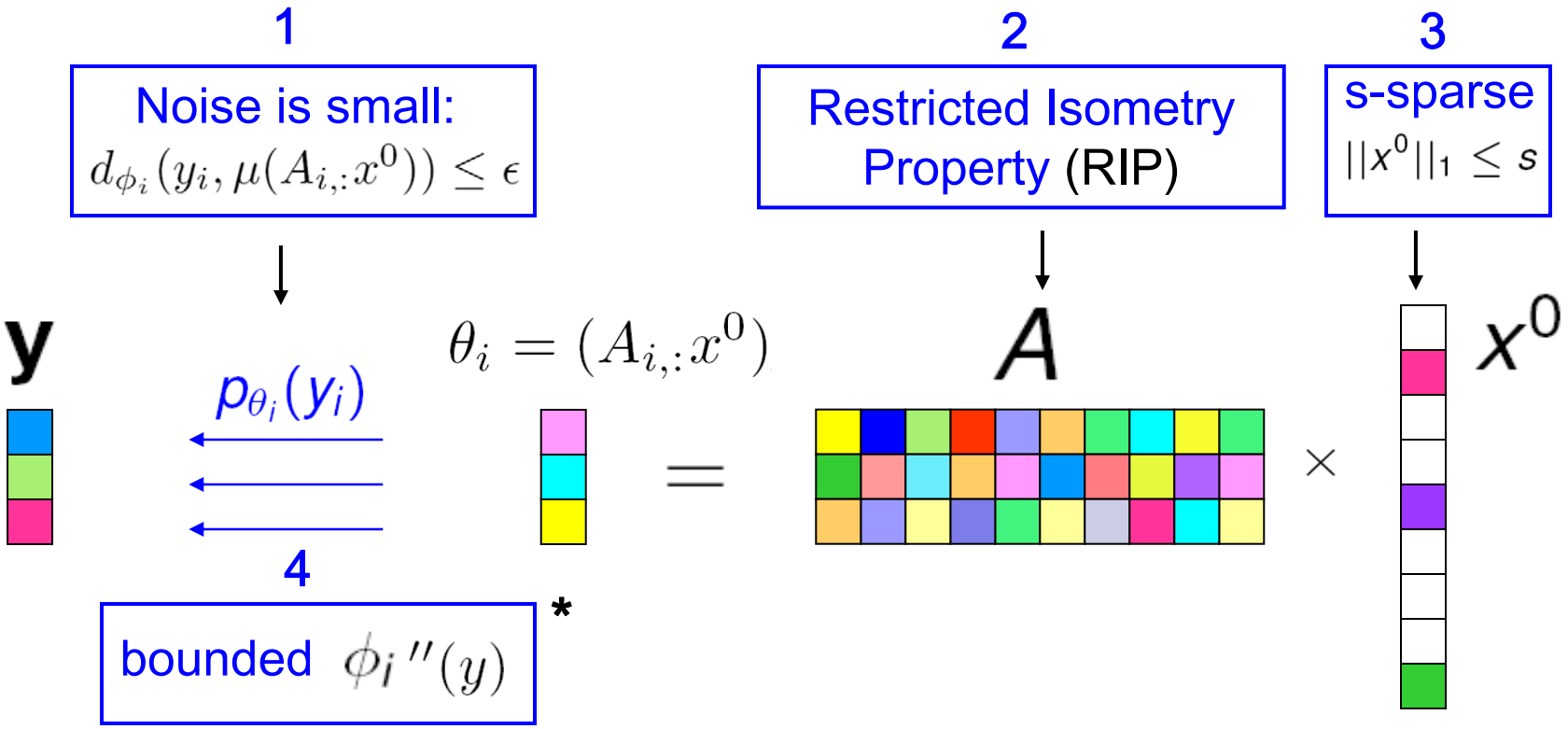
replace Euclidean distances $||y - Ax^0||_{l_2}$ and $||y - Ax||_{l_2}$ by the corresponding Bregman divergences $d(y, \mu(Ax^0))$ and $d(y, \mu(Ax))$.

Sparse Signal Recovery with Exponential-Family Noise



Can we recover a sparse signal
from a small number of noisy observations?

Sufficient Conditions



Then the solution x^* to the sparse GLM regression problem

$$min||x||_1 \quad subject\ to \quad \sum_i d(y_i, \mu(A_i x)) \leq \epsilon$$

is a good approximation of x^0, i.e. $||x^* - x^0||_{l_2} \leq C_S \cdot \delta(\epsilon)$

$\delta(\epsilon)$ - continuous monotone increasing function, and $\delta(0) = 0$ (i.e. $\delta(\epsilon)$ is small when ϵ is small).

*otherwise, different proofs for some specific cases (e.g., Bernoulli, exponential, etc.)

Summary

- sparse signal recovery (Candes, Romberg & Tao, 2006) can be extended from linear to generalized linear models (*exponential-family* observation noise)
- signal recovery requires solving an l_1-regularized *Generalized Linear Model (GLM)* regression problem
- recovery conditions include, besides standard RIP for design matrix:
  (1) small noise (Bregman divergence) $d_\phi(y_i, \mu(A_{i,:}x^0)) \leq \epsilon$
  (2) certain conditions on ϕ
- results also hold for compressible (rather than sparse) signals

Beyond LASSO

$$Loss(\mathbf{x}) + \lambda ||\mathbf{x}||_1$$

Other likelihoods (loss functions)

- Generalized Linear Models (exponential family noise)
- Multivariate Gaussians (Gaussian MRFs)

Adding structure beyond sparsity

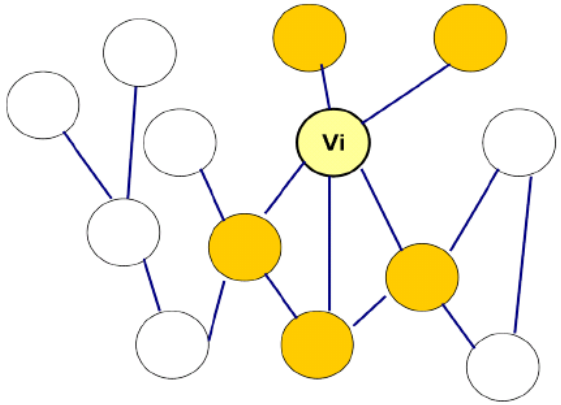
- Elastic Net
- Fused Lasso
- Block l_1-l_q norms:
  - group Lasso
  - simultaneous Lasso

Markov Networks (Markov Random Fields)

$X = \{X_1, ..., X_p\}, \quad G = (V, E)$

$$P(\boldsymbol{X}) = \frac{1}{Z} \prod_{C \in Cliques} \Phi_C(\boldsymbol{X}_C)$$

Lack of edge $(i, j) \rightarrow$
conditional independence $X_i \perp X_j | rest$

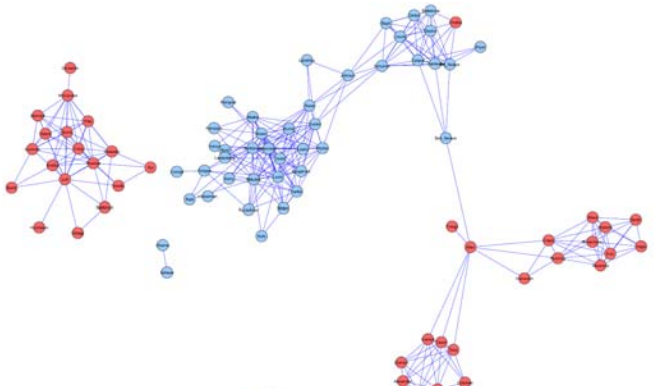


Gaussian Markov Networks (GMRFs):

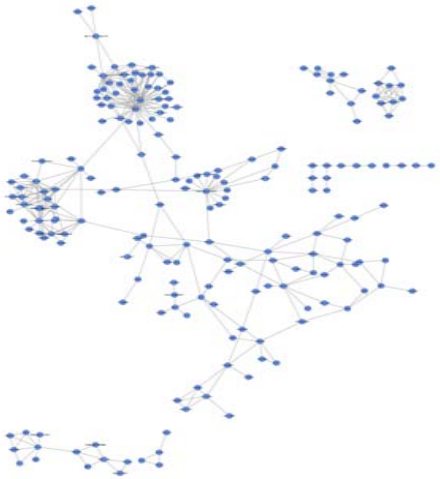
- $P(\mathbf{x}) = (2\pi)^{-\frac{P}{2}} \det(\Sigma)^{-\frac{1}{2}} \exp\left(-\frac{1}{2}(\boldsymbol{x} - \boldsymbol{\mu})^T \Sigma^{-1} (\boldsymbol{x} - \boldsymbol{\mu})\right)$
- Σ - covariance matrix, Σ^{-1} - precision (concentration) matrix
- Zeros in Σ: marginal independence
- Zeros in $\Sigma^{-1} \Leftrightarrow$ conditional independence $\Leftrightarrow$ lack of edge (Lauritzen, 1996)
- Sparse $\Sigma^{-1} \Leftrightarrow$ sparse Markov network

Sparse Markov Networks in Practical Applications

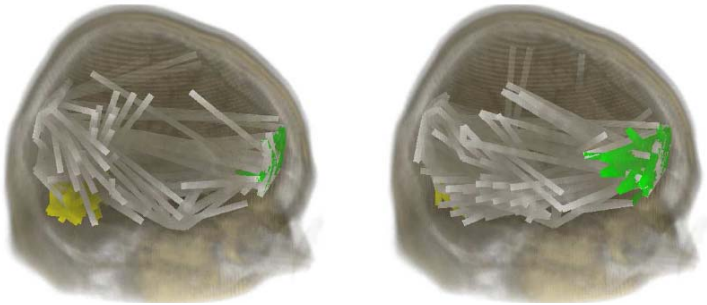
- Social Networks
  - US senate voting data (Banerjee et al, 2008): democrats (blue) and republicans (red)



- Genetic Networks
  - Rosetta Inpharmatics Compendium of gene expression profiles (Banerjee et al, 2008)



- Brain Networks from fMRI
  - Monetary reward task (Honorio et al., 2009)
  - Drug addicts more connections in cerebellum (yellow) vs control subjects (more connections in prefrontal cortex – green)



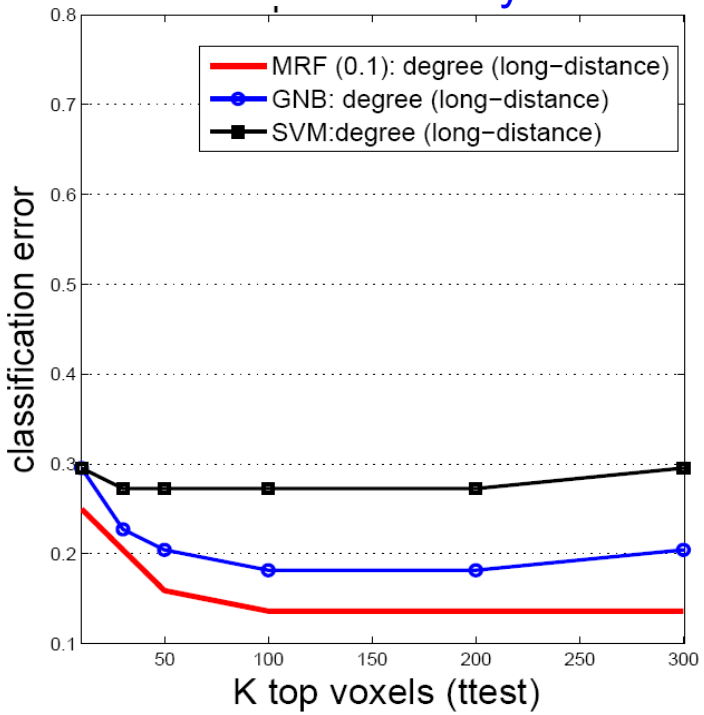
(a) Drug addicts (b) controls

Sparse MRFs Can Predict Well

Classifying Schizophrenia

(Cecchi et al., 2009)

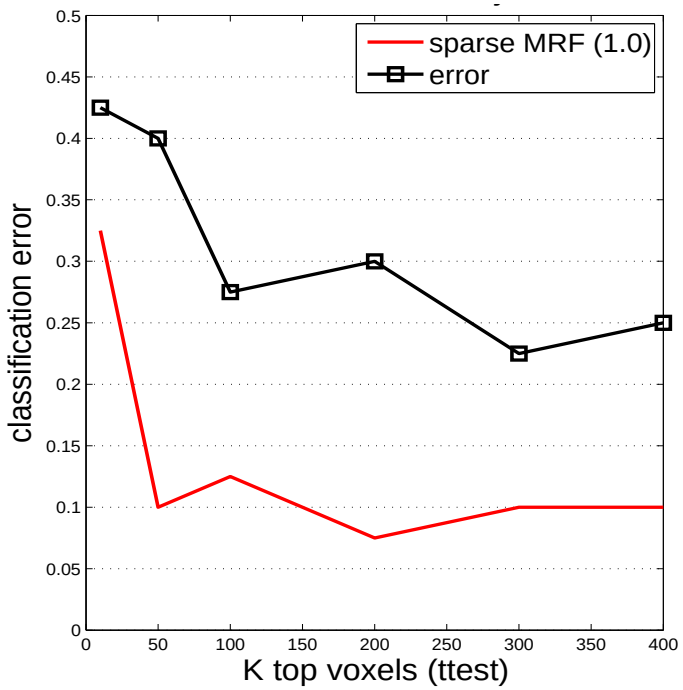
86% accuracy



Mental state prediction (sentence vs picture)*:

(Scheinberg and Rish, submitted)

90% accuracy



MRF classifiers can often exploit informative interactions among variables and often outperform state-of-art linear classifiers (e.g., SVM)

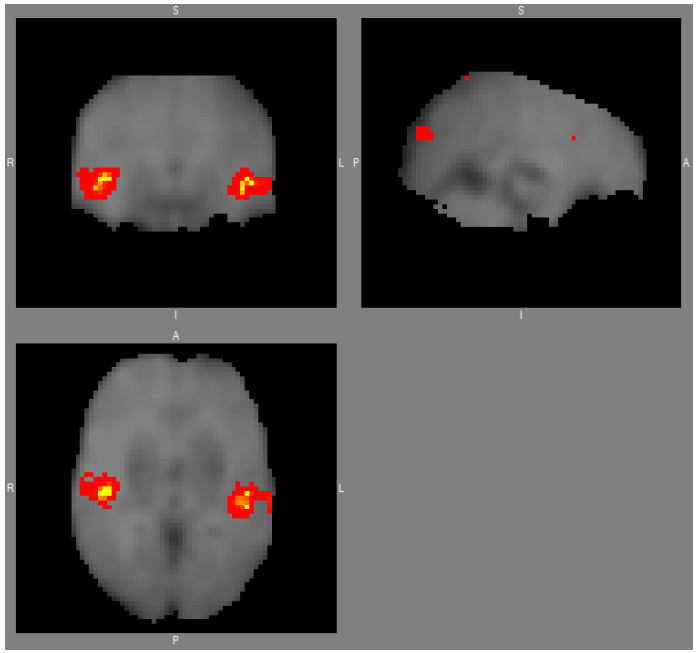
*Data @ www.cs.cmu.edu/afs/cs.cmu.edu/project/theo-81/www/ from T. Mitchell et al., *Learning to Decode Cognitive States from Brain Images,* Machine Learning, 2004.

Network Properties as BioMarkers (Predictive Features)

Discriminative Network Models of Schizophrenia (Cecchi et al., 2009)

- Voxel degrees in *functional networks* (thresholded *covariance* matrices) are statistically significantly different in schizophrenic patients that appear to lack "hubs" in auditory/language areas

FDR-corrected Degree Maps



2-sample t-test performed for each voxel in degree maps, followed by FDR correction

Red/yellow: Normal subjects have *higher* values than Schizophrenics

Also, abnormal MRF connectivity observed in Alzheimer's patients (Huang 2009), in drug addicts (Honorio 2009), etc.

Sparse Inverse Covariance Selection Problem

- First introduced in (Dempster, 1972)
  - maximum-likelihood (MLE) with bounded number of $\Sigma^{-1}_{ij} \neq 0$
  - intractable for large p; also, MLE may not even exist for $n > p$
- Most recent approaches exploit l_1-regularization
  - tractable up to thousands of variables
  - handle $n > p$ cases
  - enforce zeros in Σ^{-1} explicitly, while MLE does not
- Neighborhood selection via Lasso (Meinshausen and Buhlmann, 2006):
  - very simple and scalable approach
  - (1) fits Lasso to each X_i given the rest of the nodes; (2) includes link (i, j) if both X_i and X_j models include it (or, use OR-rule);
  - consistently estimates the *network structure* (zero-pattern of Σ^{-1})
  - but not the actual parameters! (may violate symmetry and posdef constraints on Σ^{-1})
  - can be viewed as an approximation to the l_1-regularized (joint) maximum-likelihood problem

Maximum Likelihood Estimation

Assume the data $\mathbf{X}$ are centered to have zero mean. Then:

$$\hat{\Sigma}^{-1} = \arg\max_{C \succ 0} \log p(C|\mathbf{X}) = \arg\max_{C \succ 0} \log p(\mathbf{X}, C) =$$

$$\boxed{= \arg\max_{C \succ 0} \log\det(C) - \mathrm{tr}(SC)}$$

where $S = \frac{1}{N}\sum_{i=1}^{N} x_i^T x_i$ is the empirical covariance matrix (MLE of Σ)

Why not just use $\hat{\Sigma}^{-1} = S^{-1}$?

- in small-sample case ($n < p$), S may not be even invertible
- even if it is, S^{-1} almost never contains exact zeros
- l_1-regularization takes care of both issues!

l_1-Regularized Maximum Likelihood Problem

Primal:

$$\hat{\Sigma}^{-1} = \arg\max_{C \succ 0} \log\det(C) - \mathrm{tr}(SC) - \lambda ||C||_1 \qquad (1)$$

Convex problem; unique optimum for any $\lambda > 0$ (Banerjee et al., 2008)

Dual:

$$\hat{\Sigma} = \{\arg\max_{W} \log\det(W) : ||W - S||_\infty \leq \lambda\} \qquad (2)$$

The dual estimates the covariance $\hat{\Sigma}$, rather than its inverse

The constraint $W \succ 0$ is implicit since $\log\det(W) = -\infty$ when $W \not\succ 0$

Smooth and convex problem; can be solved by an interior-point method

However, the complexity is $O(p^6 \log(1/\epsilon))$ (where ϵ is a solution accuracy)

Not scalable for more than a few hundred nodes

Block-Coordinate Descent on the Dual Problem

Initialize: $W \leftarrow S + \lambda I$

Iterate over columns of W until convergence:

1. swap the $j-th$ column (row) with the last column (row) in W and S:

$$W = \begin{pmatrix} W_{11} & w_{12} \\ w_{12}^T & w_{22} \end{pmatrix} \qquad S = \begin{pmatrix} S_{11} & s_{12} \\ s_{12}^T & s_{22} \end{pmatrix}$$

2. Solve a box-constrained quadratic program (QP):

$$\hat{w}_{12} = \arg\min_y \{ y^T W_{11}^{-1} y : ||y - s_{12}||_\infty \leq \lambda \} \qquad (3)$$

3. Update W using the new estimate $\hat{w}_{12}$

COVSEL (Banerjee et al., 2006):
solves (3) using an interior-method approach; overall time is $O(Tp^4)$
where T is the number of sweeps through all columns

GLASSO (Friedman et al., 2007):
solves the dual of (3) (Lasso problem), using coordinate descent;
about $O(Tp^3)$ complexity, much faster than COVSEL empirically

Projected Gradient on the Dual Problem

$$\min_x f(x)$$

$$x \in S \quad (S \text{ is convex})$$

Iteratively update x until convergence:

1. $x \leftarrow x + \alpha \nabla f(x)$ (step of size α in the direction of gradient)
2. $x \leftarrow \Pi_S(x) = \arg\min_z \{||x - z||_2 : z \in S\}$ (project onto S)

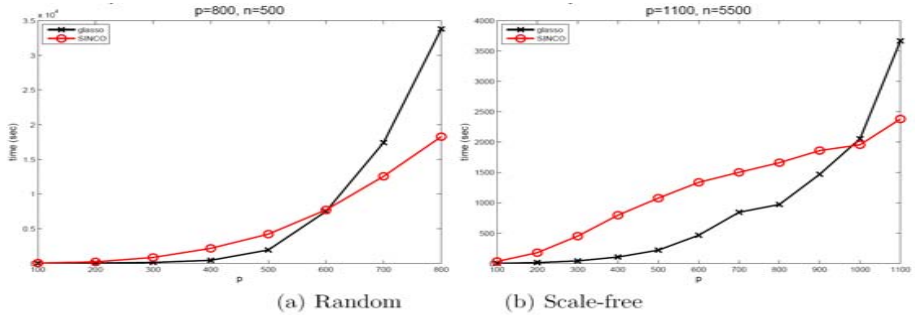
(Duchi et al., 2008) applies the PG approach to the dual problem (2)
S is defined by the box-constraint in (2)

$O(p^3)$ complexity - similar to *glasso*, but twice as fast empirically

Alternatives: Solving Primal Problem Directly

1. Greedy coordinate ascent approach: SINCO (Scheinberg et al., 2009)

   - updates one diagonal or two (symmetric) off-diagonal elements of C at each step
   - evaluating each C_{ij} takes constant time (solving quadratic equation), thus each step takes $O(p^2)$ time and can be easily parallelized
   - naturally preserves the sparsity of a solution; can reduce false-positive error by not including "weak" edges not contributing much to the objective
   - Speedwise, comparable to glasso; outperforms glasso on large-scale problems



(a) Random (b) Scale-free

CPU time comparison: SINCO vs *glasso* on (a) random networks ($N = 500$, fixed range of λ) and (b) scale-free networks (density 21%, N and λ scaled by the same factor with p, $N = 500$ for $p = 100$).

2. (Honorio et al., 2009) also solve the primal problem:

   - Optimize over each column (node) at a time
   - Exploit "local constancy" structure adding a regularizer similar to fused Lasso

Additional Related Work

- (Yuan and Lin, 2007) solve the primal problem (1) using interior-point method for the maxdet problem (Vandenberghe et al., 1998)
- (Lee et al., 2007) learn MRFs using clique selection heuristic and approximate inference
- (Wainwright et al., 2007) extend the approach of (Meinshausen and Buhlmann, 2006) to binary MRFs Ising models, applying sparse logistic regression at each node, and derive asymptotic consistency results
- (Schmidt et al., 2007) apply l_1-regularization to structure learning in Bayesian networks
- (Huang et al., 2009) prove the monotone property of (1) under decreasing λ (i.e., connected nodes stay connected with decreasing sparsity levels)
- (Lin et al., 2009) propose an alternative approach based on ensemble-of-trees that is shown to sometimes outperform l_1-regularization approaches of (Banerjee et al., 2008) and (Wainwright et al., 2007)
- (Schmidt and Murphy, 2010) learn log-linear models with higher-order (beyond pairwise) potentials; use group-l_1 regularization with overlapping groups to enforce hierarchical structure over potentials

Selecting the Proper Regularization Parameter

"…the general issue of selecting a proper amount of regularization for getting a right-sized structure or model has largely remained a problem with unsatisfactory solutions" (Meinshausen and Buehlmann , 2008)

"asymptotic considerations give little advice on how to choose a specific penalty parameter for a given problem" (Meinshausen and Buehlmann , 2006)

- Bayesian Approach (N.Bani Asadi, K. Scheinberg and I. Rish, 2009)
  - Assume a Bayesian prior on the regularization parameter
  - Find maximum a posteriory probability (MAP) solution

- Result:
  - more ``balanced'' solution (False Positive vs False Negative error) than
    - *cross-validation* - too dense, and
    - *theoretical* (Meinshausen & Buehlmann 2006, Banerjee et al 2008) - too sparse
  - Does not require solving multiple optimization problems over data subsets as compared to the *stability selection* approach (Meinshausen and Buehlmann 2008)

Existing Approaches

1. Cross-validation based on predictive accuracy:
   - Aims at the prediction rather than the structure reconstruction accuracy!
   - CV-estimate approximates the prediction-oracle λ, that does not lead to consistent model-selection due to possible inclusion of noisy edges (Meinshausen and Buhlmann, 2006)
   - Indeed, empirically, CV-estimate yields too high false-positive rate

2. Theoretical approach (Banerjee et al., 2008):

   guarantees consistent reconstruction of connected components for each node (i.e., rows in covariances matrix, rather than its inverse):

$$\lambda(\alpha) = (\max_{i>j} \sigma_i \sigma_j) \frac{t_{n-2}(\alpha/p^2)}{\sqrt{n-2+t^2_{n-2}(\alpha/p^2)}}$$

   guarantees that

$$P(\exists k \in \{1, ..., p\} : \hat{C}_k^{\lambda} \not\subseteq C_k) \leq \alpha,$$

   where $\hat{C}_k^{\lambda}$ is an estimate of the connectivity component of node k, and C_k is its "true" component.

   - Controls the false positive error in $\hat{\Sigma}$, rather than $\hat{\Sigma}^{-1}$
   - Too conservative, empirically: misses many edges

Being Bayesian about λ

- λ as a random variable: learn its distribution
- Maximize the joint log likelihood

$$\Sigma^{-1}, \widehat{\lambda} = \max_{C \succ 0, \lambda} \ln p(\mathbf{X}, C, \lambda)$$

$p(X, C, \lambda) = p(X|C)p(C|\lambda)p(\lambda)$

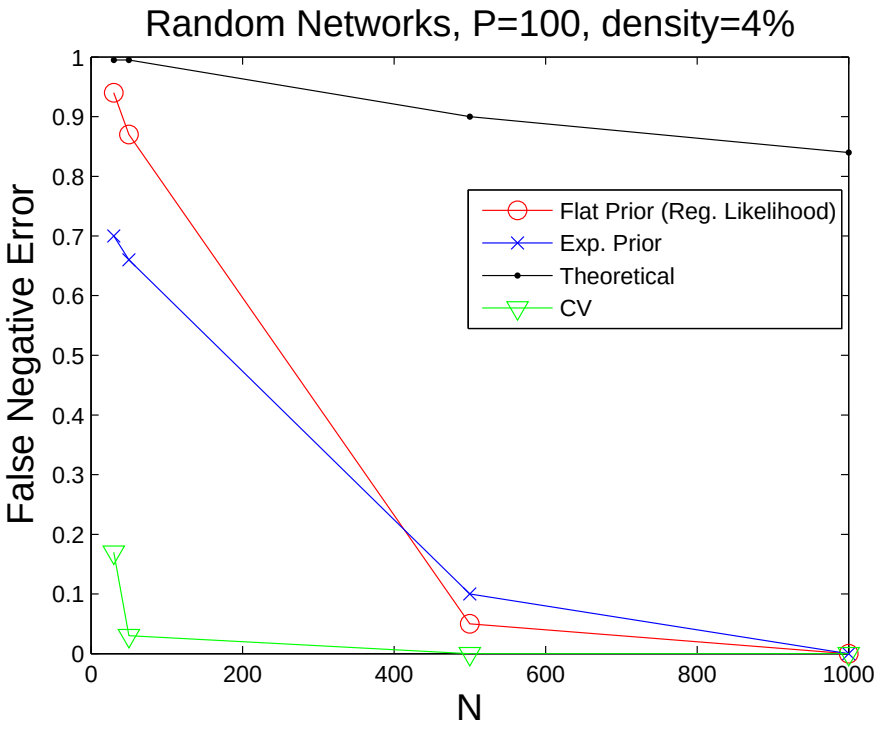
- Thus, we need to solve:

$$\max_{\lambda, C \succ 0} \frac{N}{2}[\ln \det(C) - \mathrm{tr}(SC)] + P^2 \ln \frac{\lambda}{2} - \lambda ||C||_1 + \ln p(\lambda).$$

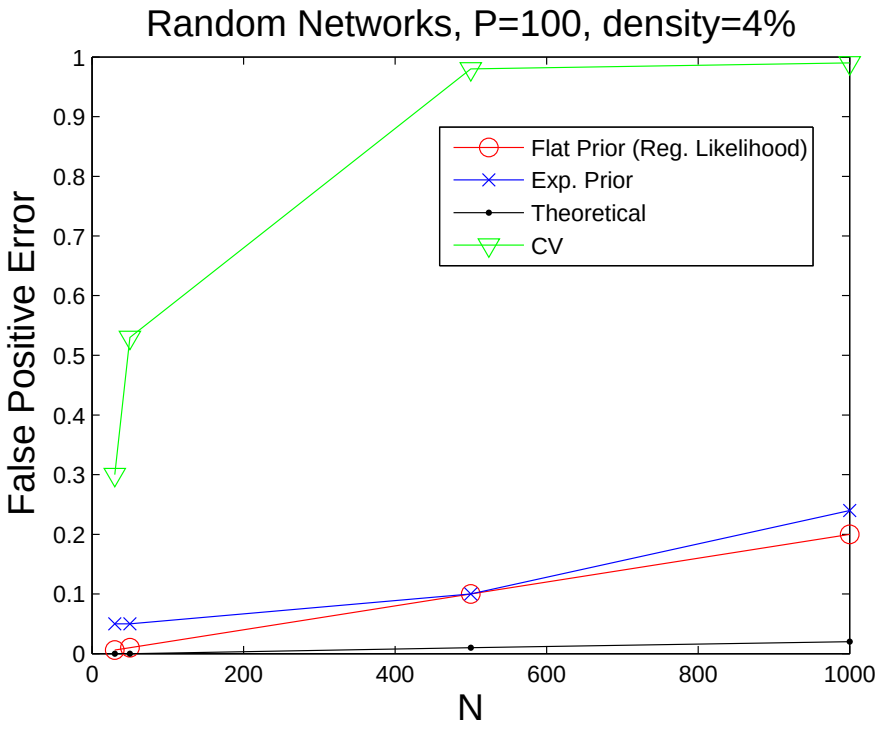
- The choice of P(λ): flat? exponential? Gaussian? etc.

Results on Random Networks

False Negatives: Missed Links



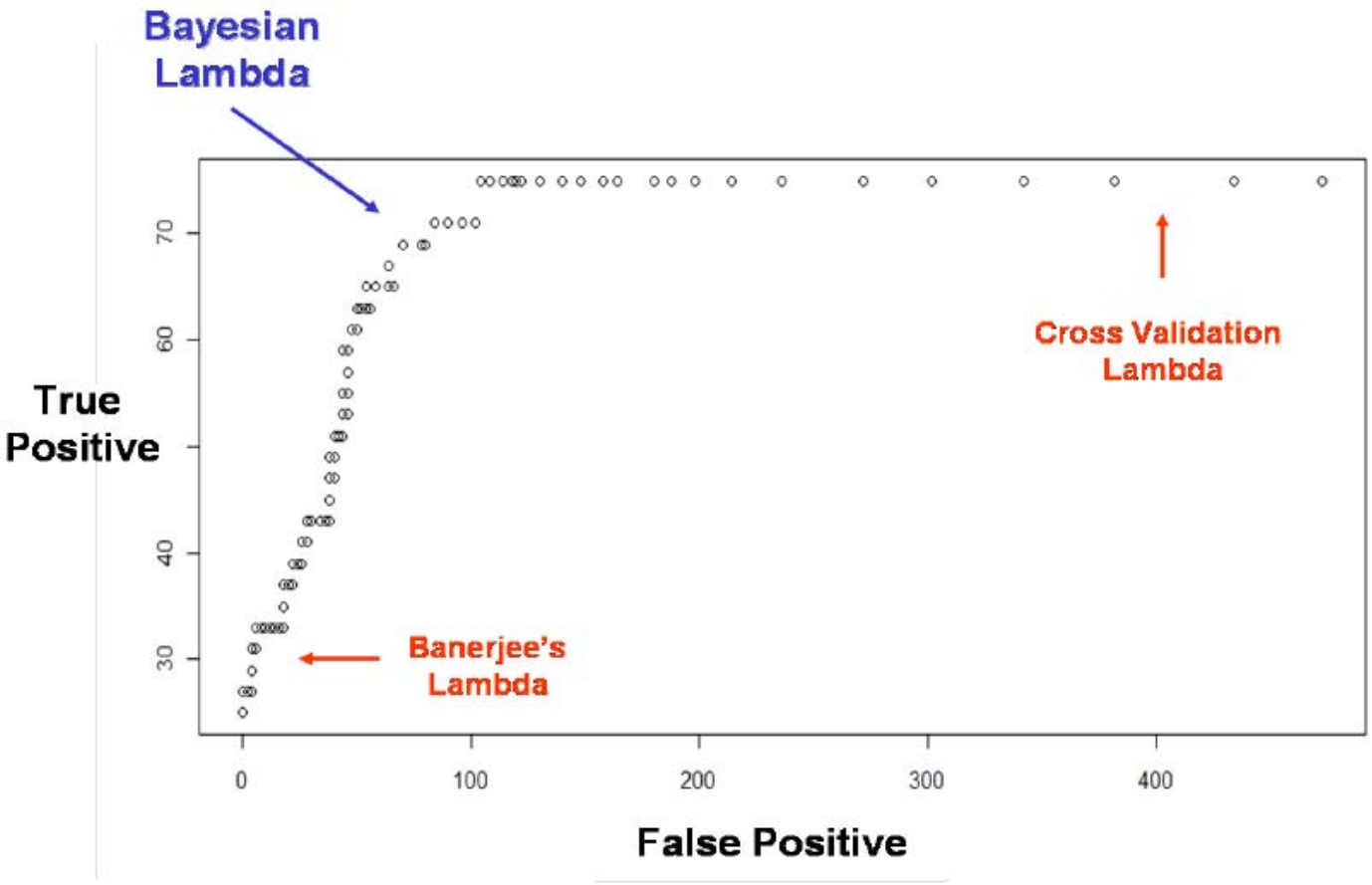
False Positives: 'Noisy' Links



- Cross-validation (**green**) overfits drastically, producing almost complete C matrix
- Theoretical (**black**) is too conservative: misses too many edges (near-diagonal C)
- Prior-based approaches (**red** and **blue**) are much more 'balanced': low FP and FN

The Bayesian λ

ROC Curve



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  - Consistency-improving extensions
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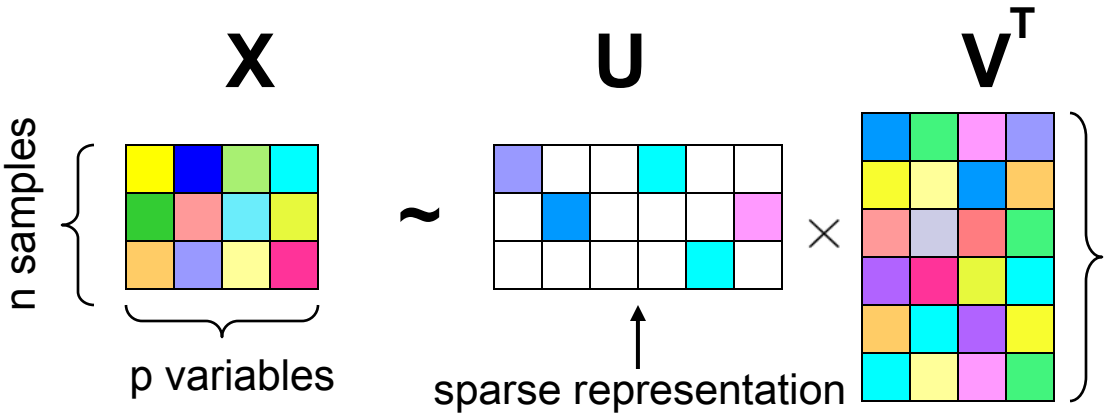
  - Beyond variable-selection: variable construction
- Summary and Open Issues

Sparse Matrix Factorization

- Dictionary learning
  (Elad and Aharon, 2006; Raina et al., 2007; Mairal et al., 2009):



$$\min_{U,V} ||X - UV^T||^2 + \lambda \sum_{i=1}^{n} ||U(i,:)||_1$$

$$\forall j = 1, ..., m, \ ||V(:,j)||_2 \leq 1$$

sparse $U(i,:) \Leftrightarrow$ sparse representation in dictionary V

- Sparse PCA (Zou et al., 2006; d'Aspremont et al., 2007):
  sparse $V(:,j)$ (loadings/coordinates of components) $\rightarrow$ interpretability

- other sparse matrix factorization methods:
  sparse CCA (Sriperumbudur et al., 2009; Hardoon and Shawe-Taylor, 2008), sparse NMF (Hoyer, 2004), with applications to blind-source separation and diagnosis (Chandalia and Rish, 2007)

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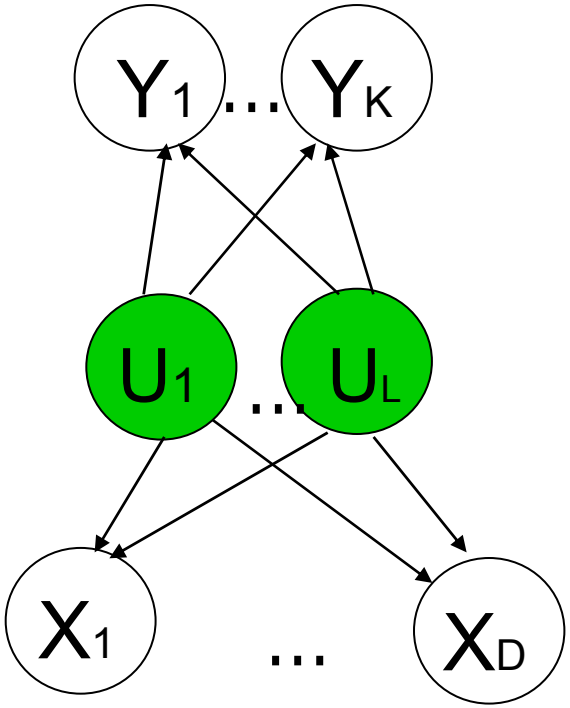
Supervised Dimensionality Reduction (SDR):



- Assume there is an inherent low-dimensional structure in the data that is predictive about the target Y
- Learn a predictor (mapping from U to Y) simultaneously with dimensionality reduction
- Idea: dimensionality reduction (DR) guided by the class label may result into better predictive features than the unsupervised DR

Particular Mappings X → U and U → Y

1. F. Pereira and G. Gordon. *The Support Vector Decomposition Machine*, ICML-06.
   Real-valued X, discrete Y (linear map from X to U, SVM for Y(U))

2. E. Xing, A. Ng, M. Jordan, and S. Russell. *Distance metric learning with application to clustering with side information*, NIPS-02.
3. K. Weinberger, J. Blitzer and L. Saul. *Distance Metric Learning for Large Margin Nearest Neighbor Classification*, NIPS-05.
   Real-valued X, discrete Y (linear map from X to U, nearest-neighbor Y(U))

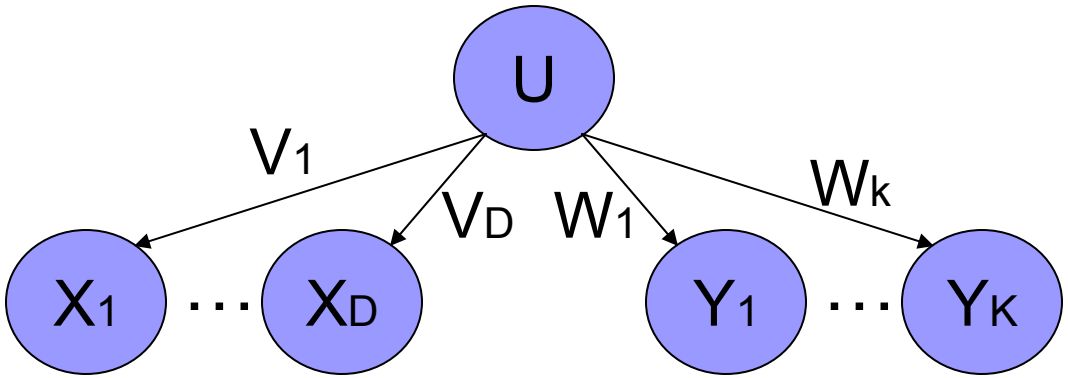
4. K. Weinberger and G. Tesauro. *Metric Learning for Kernel Regression*, AISTATS-07.
   Real-valued X, real-valued Y (linear map from X to U, kernel regression Y(U))

5. Sajama and A. Orlitsky. *Supervised Dimensionality Reduction using Mixture Models*, ICML-05.
   Multi-type X (exp.family), discrete Y (modeled as mixture of exp-family distributions)

6. M. Collins, S. Dasgupta and R. Schapire. *A generalization of PCA to the exponential family*, NIPS-01.
7. A. Schein, L. Saul and L. Ungar. *A generalized linear model for PCA of binary data, AISTATS-03*
   Unsupervised dimensionality reduction beyond Gaussian data (nonlinear GLM mappings)

8. I. Rish, G. Grabarnik, G. Cecchi, F. Pereira and G. Gordon. *Closed-form Supervised Dimensionality Reduction with Generalized Linear Models, ICML-08*

Example: SDR with Generalized Linear Models (Rish et al., 2008)



Generalized Linear Models (GLMs)

$$E(\mathbf{X}_d) = f_d^{-1}(\mathbf{UV_d})$$

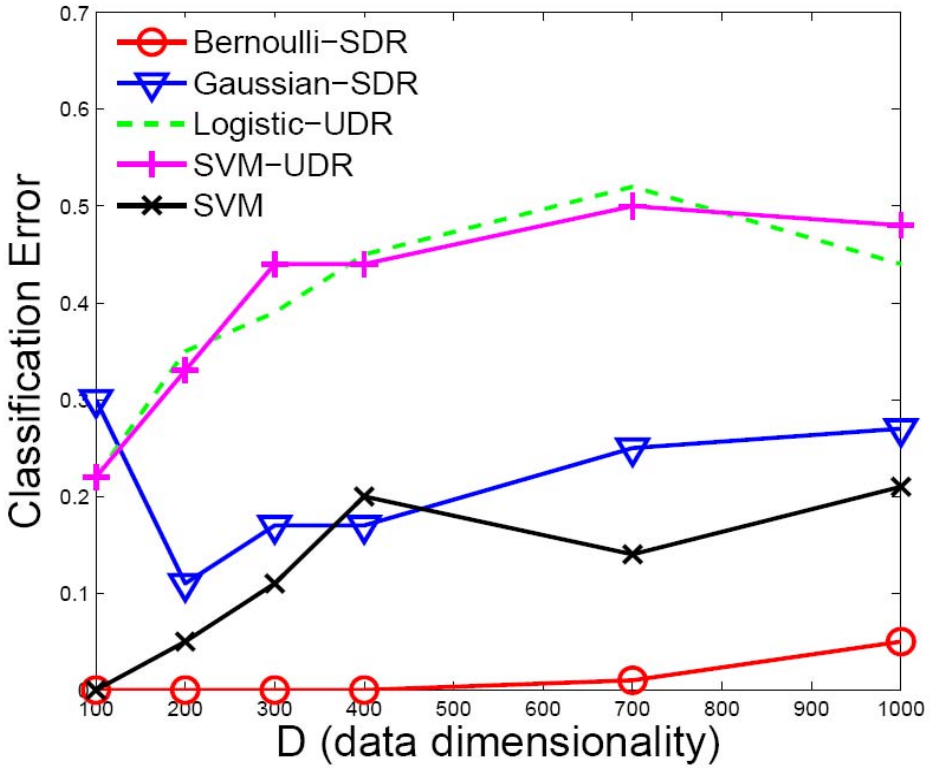
$$E(\mathbf{Y}_k) = f_k^{-1}(\mathbf{UW_k})$$

E.g., in linear case, we have:

X ~ U V and Y ~ U V

Supervised DR Outperforms Unsupervised DR on Simulated Data

- Generate a separable 2-D dataset U
- Blow-up in D dimensional data X by adding exponential-family noise (e.g., Bernoulli)
- Compare SDR w/ different noise models (Gaussian, Bernoulli) vs. unsupervised DR (UDR) followed by SVM or logistic regression



- SDR outperforms unsupervised DR by 20-45%
- Using proper data model (e.g., Bernoulli-SDR for binary data) matters
- SDR ``gets'' the structure (0% error), SVM does not (20% error)

…and on Real-Life Data from fMRI Experiments

Real-valued data, Classification Task

Predict the type of word (tools or buildings) the subject is seeing

84 samples (words presented to a subject), 14043 dimensions (voxels)

Latent dimensionality L = 5, 10, 15, 20, 25

method\ L	5	10	15	20	25
Gaussian-SDR	0.21	0.26	0.23	**0.20**	0.23
Logistic-UDR	0.44	0.42	**0.29**	0.30	0.26
SVM-UDR	**0.49**	0.52	0.56	0.57	0.55
SVDM	0.32	0.25	**0.21**	0.23	0.23
SVM	0.21				

- Gaussian-SDR achieves overall best performance
- SDR matches SVM's performance using only 5 dimensions, while SVDM needs 15
- **SDR greatly outperforms unsupervised DR followed by learning a classifier**

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Summary and Open Issues

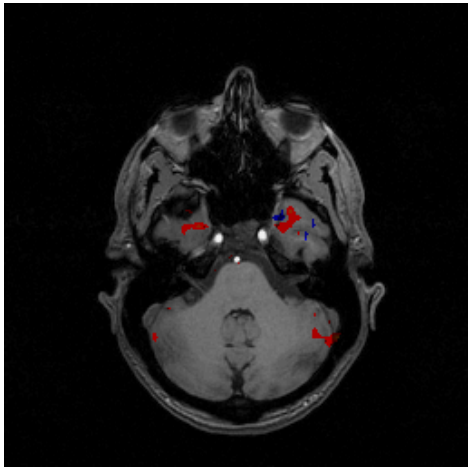
- Common problem: small-sample, high-dimensional inference
- Feasible if the input is structured – e.g. sparse in some basis
- Efficient recovery of sparse input via l_1- relaxation
- Sparse modeling with l_1-regularization: interpretability + prediction
- Beyond l_1-regularization: adding more structure
- Beyond Lasso: M-estimators, dictionary learning, variable construction
- Open issues, still:
  - choice of regularization parameter?
  - choice of proper dictionary?
  - Is interpretability $\Leftrightarrow$ sparsity? (NO!)

Interpretability: Much More than Sparsity?

Data

x - fMRI voxels,

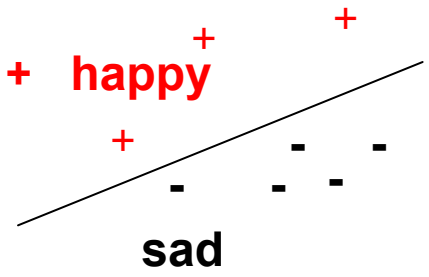
y - mental state



Interpretable Predictive Patterns

Predictive Model

y = f(**x**)



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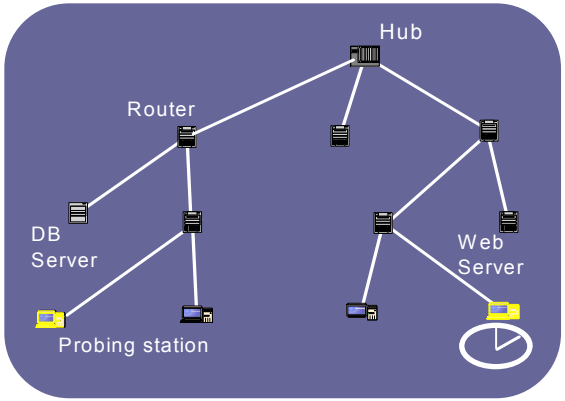
Appendix A

Why Exponential Family Loss?

- Network Management – Problem Diagnosis:
  - binary failures - Bernoulli
  - non-negative delays – exponential



- Collaborative prediction:
  - discrete rankings - multinomial

- DNA microarray data analysis:
  - Real-valued expression level – Gaussian

- fMRI data analysis
  - Real-valued voxel intensities, binary, nominal and continuous responses

Variety of data types: real-valued, binary, nominal, non-negative, etc.

Noise model: exponential-family

Bregman Divergences

Definition. *Given a strictly convex function $\phi : S \to \mathbb{R}$ defined on a convex set $S \subseteq \mathbb{R}$, and differentiable on the interior of S, $int(S)$, the Bregman divergence $d_\phi : S \times int(S) \to [0, \infty)$ is*

$$d_\phi(\mathbf{x}, \mathbf{y}) = \phi(\mathbf{x}) - h_y(\mathbf{x}),$$

where $h_y(x) = \phi(\mathbf{y}) + < (\mathbf{x} - \mathbf{y}), \nabla\phi(\mathbf{y}) >$ is the value of the first-order Taylor expansion of ϕ around $\mathbf{y}$ evaluated at point $\mathbf{x}$.

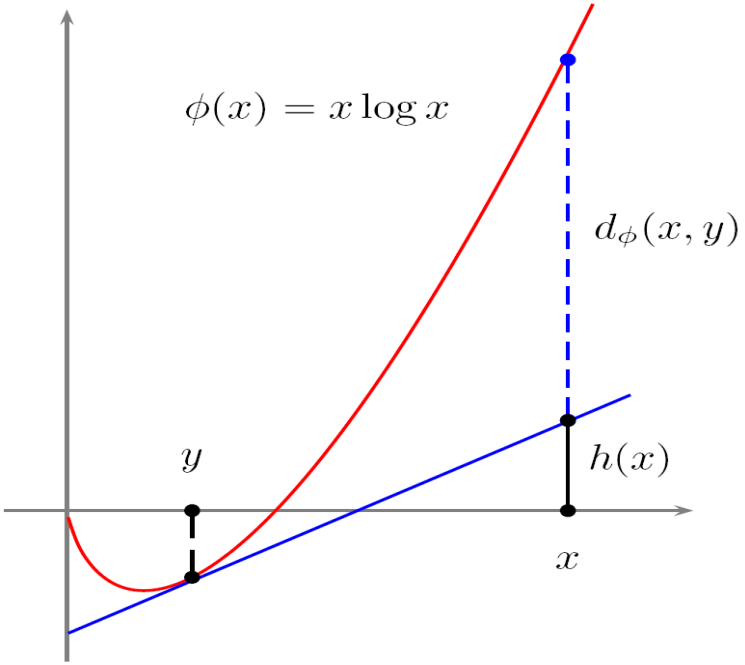


Fig. 1. Relative entropy (KL-divergence)

Bijection Theorem

Theorem [Banerjee et al., 2005]. There is a bijection between the exponential-family densities $p_{\psi,\theta}(\cdot)$ and Bregman divergences $d_\phi(\cdot, \mu)$:

$$p_{\psi,\theta}(\mathbf{y}) = exp(-d_\phi(\mathbf{y}, \mu(\theta)))f_\phi(\mathbf{y}),$$

- $\mu(\theta) = E_{p_{\psi,\theta}}(Y)$
- $\mu = \nabla\psi(\theta)$, $\theta = \nabla\phi(\mu)$
- ϕ - (strictly convex and differentiable) Legendre conjugate of ψ
- $f_\phi(\mathbf{y})$ - a uniquely determined function

Legendre duality:

$$\psi(\theta) \Leftrightarrow \phi(\mu)$$

Exponential-family distribution

Bregman divergence

Image courtesy of Arindam Banerjee

Appendix A

Lemma 1 *Let y denote a random variable following an exponential-family distribution $p_\theta(y)$, with the natural parameter θ, and the corresponding mean parameters $\mu(\theta)$. Let $d_\phi(y, \mu(\theta))$ denote the Bregman divergence associated with this distribution. If If*

$d_\phi(y, \mu^0(\theta^0)) \leq \epsilon$ *(small noise),*

$d_\phi(y, \mu^*(\theta^*)) \leq \epsilon$ *(constraint in GLM problem), and*

$\phi''(y)$ *exists and is bounded on* $[y_{min}, y_{max}]$*, where* $y_{min} = \min\{y, \mu^0, \mu^*\}$ *and* $y_{max} = \max\{y, \mu^0, \mu^*\}$,

then

$$|\theta^* - \theta^0| \leq \frac{2\sqrt{2\epsilon}}{\sqrt{\min_{\hat{y} \in [y_{min}; y_{max}]} \phi''(\hat{y})}} \max_{\hat{\mu} \in [\mu^*; \mu^0]} |\phi''(\hat{\mu})|.$$

However, in some specific cases when condition on $\phi(y)$ is not satisfied (e.g., logistic loss $\phi''(y) = \frac{1}{y(1-y)}$ and some others), similar result can still be shown, i.e. $|\theta^* - \theta^0| < \beta(\epsilon)$, where $\beta(\epsilon)$ is continuous monotone increasing function, and $\delta(0) = 0$, i.e. $\delta(\epsilon)$ is small when ϵ is small (Rish and Grabarnik, 2009).

Appendix B

Theorem 1.
If

- x^0 is s-sparse
- A obeys RIP with same constants as in [CR&T, 2006]
- observation noise in y_i follows exponential-family distributions $p_{\theta_i}(y_i)$, with the natural parameter $\theta_i = (A_{i,:}x^0)$
- the noise is sufficiently small, i.e. $\forall i,\ d_{\phi_i}(y_i, \mu(A_{i,:}x^0)) \leq \epsilon$, and
- ϕ_i satisfies certain conditions (specified below)

Then the solution to the sparse GLM regression problem

$$min||x||_1 \ \ subject\ to \ \sum_i d(y_i, \mu(A_i x)) \leq \epsilon$$

is a good approximation of x^0, i.e. $||x^* - x^0||_{l_2} \leq C_S \cdot \delta(\epsilon)$,

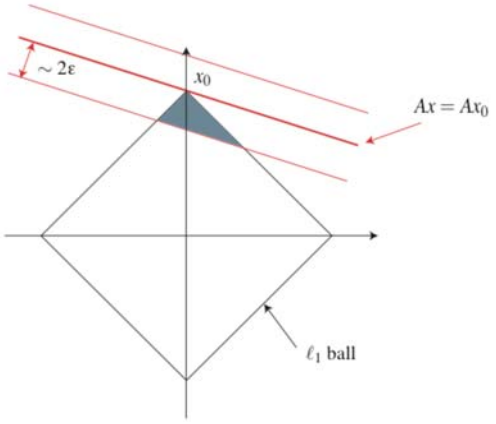
$\delta(\epsilon)$ - continuous monotone increasing function, and $\delta(0) = 0$
(i.e. $\delta(\epsilon)$ is small when ϵ is small).

Proof Idea

- Follows the proof of Theorem 1 in [CR&T]
- Only have to prove condition 1 ("tube constraint"):

$$||\theta^* - \theta^0||_{l_2} = ||Ax^* - Ax^0||_{l_2} \leq \delta(\epsilon)$$

given that $\forall i,\ d(y_i, \mu(A_{i,:}x^0)) \leq \epsilon$
and $\forall i,\ d(y_i, \mu(A_{i,:}x^*)) \leq \epsilon$



For Gaussian noise (Euclidean distance),
this follows easily from triangle inequality
(given $||y - Ax^0||_{l_2} \leq \epsilon$ and $||y - Ax^*||_{l_2} \leq \epsilon$),
which does not hold for Bregman divergences, in general.

- Condition 2 ("cone constraint") remains intact: it does not depend on the particular form of the constraint in the l_1-minimization problem, and only makes use of the sparsity of x^0 and l_1-optimality of x^*.

Appendix B

Beyond LASSO