Fast Regularization Paths via Coordinate Descent

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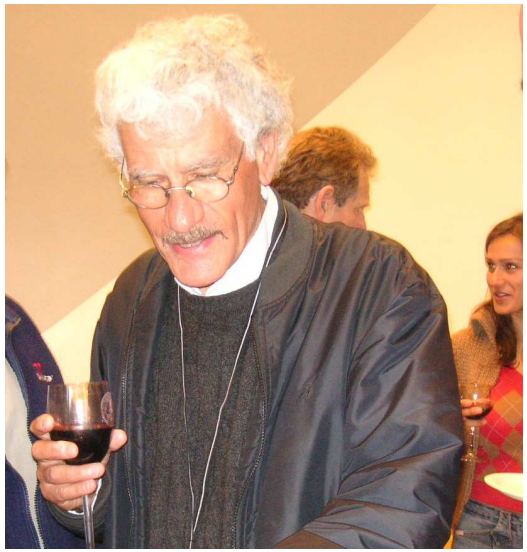
joint work with Jerry Friedman and Rob Tibshirani.



Linear Models in Data Mining

As datasets grow *wide*—i.e. many more features than samples—the linear model has regained favor in the dataminers toolbox.

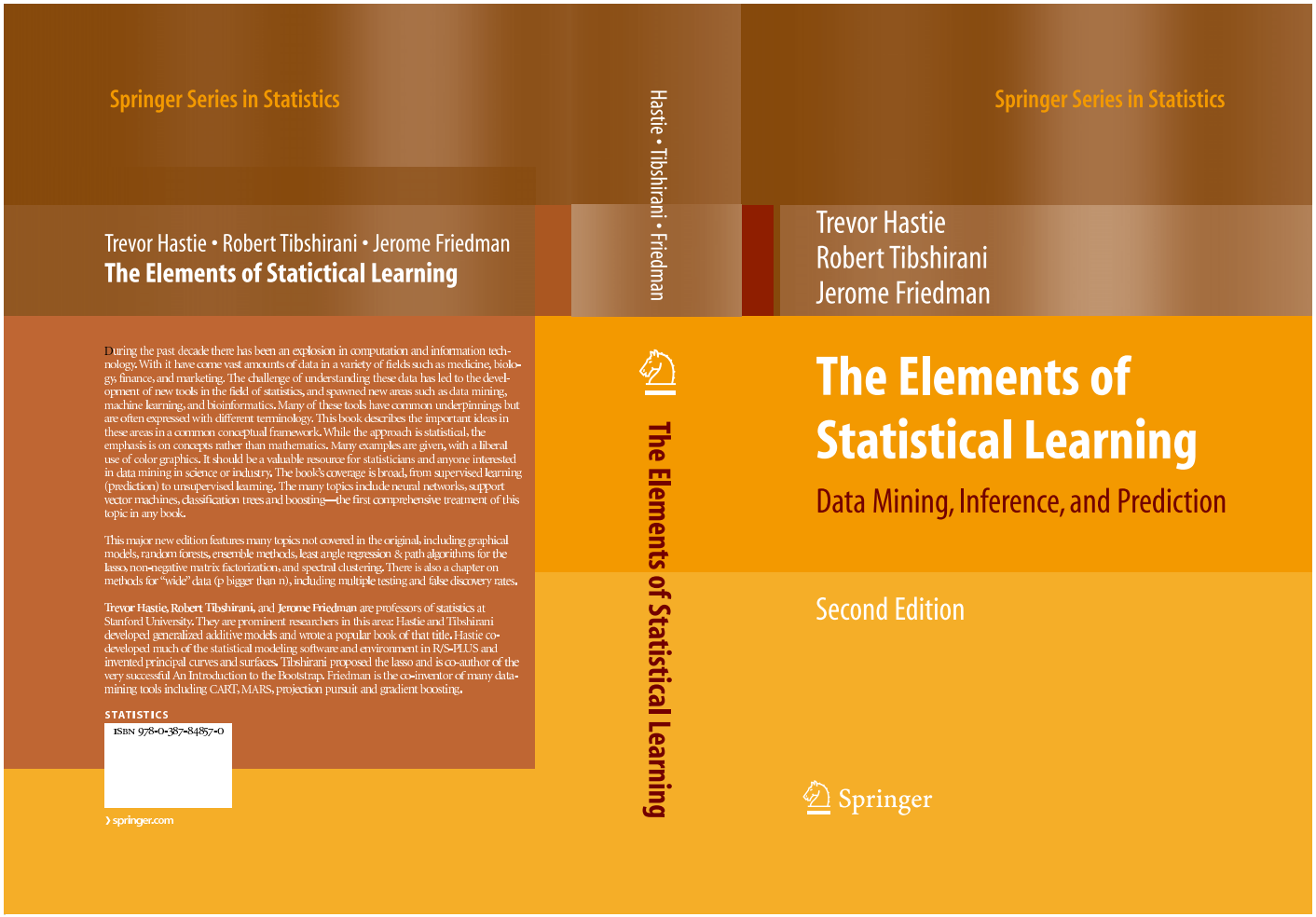
Document classification: bag-of-words can leads to $p = 20K$ features and $N = 5K$ document samples.

Image deblurring, classification: $p = 65K$ pixels are features, $N = 100$ samples.

Genomics, microarray studies: $p = 40K$ genes are measured for each of $N = 100$ subjects.

Genome-wide association studies: $p = 500K$ SNPs measured for $N = 2000$ case-control subjects.

In all of these we use linear models — e.g. linear regression, logistic regression. Since $p \gg N$, we have to regularize.



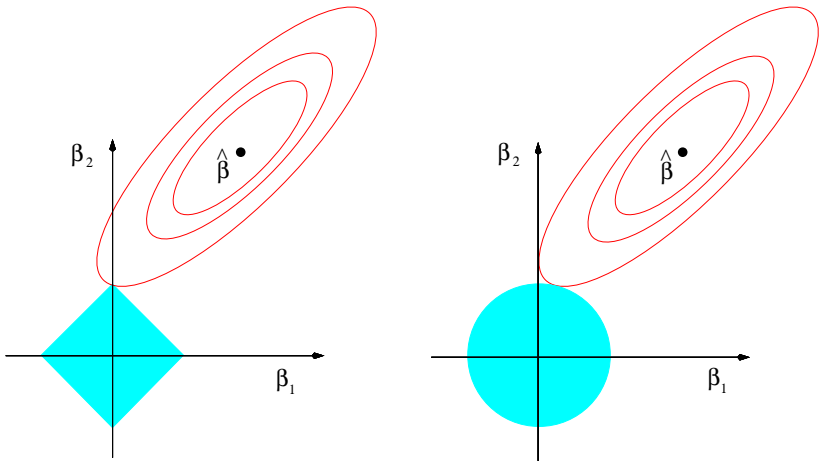
Due December 2008. Additional chapters on wide data, random forests, graphical models and ensemble methods + new material on path algorithms, kernel methods and more.

Linear regression via the Lasso (Tibshirani, 1995)

- Given observations $\{y_i,\ x_{i1}, \ldots, x_{ip}\}_{i=1}^N$

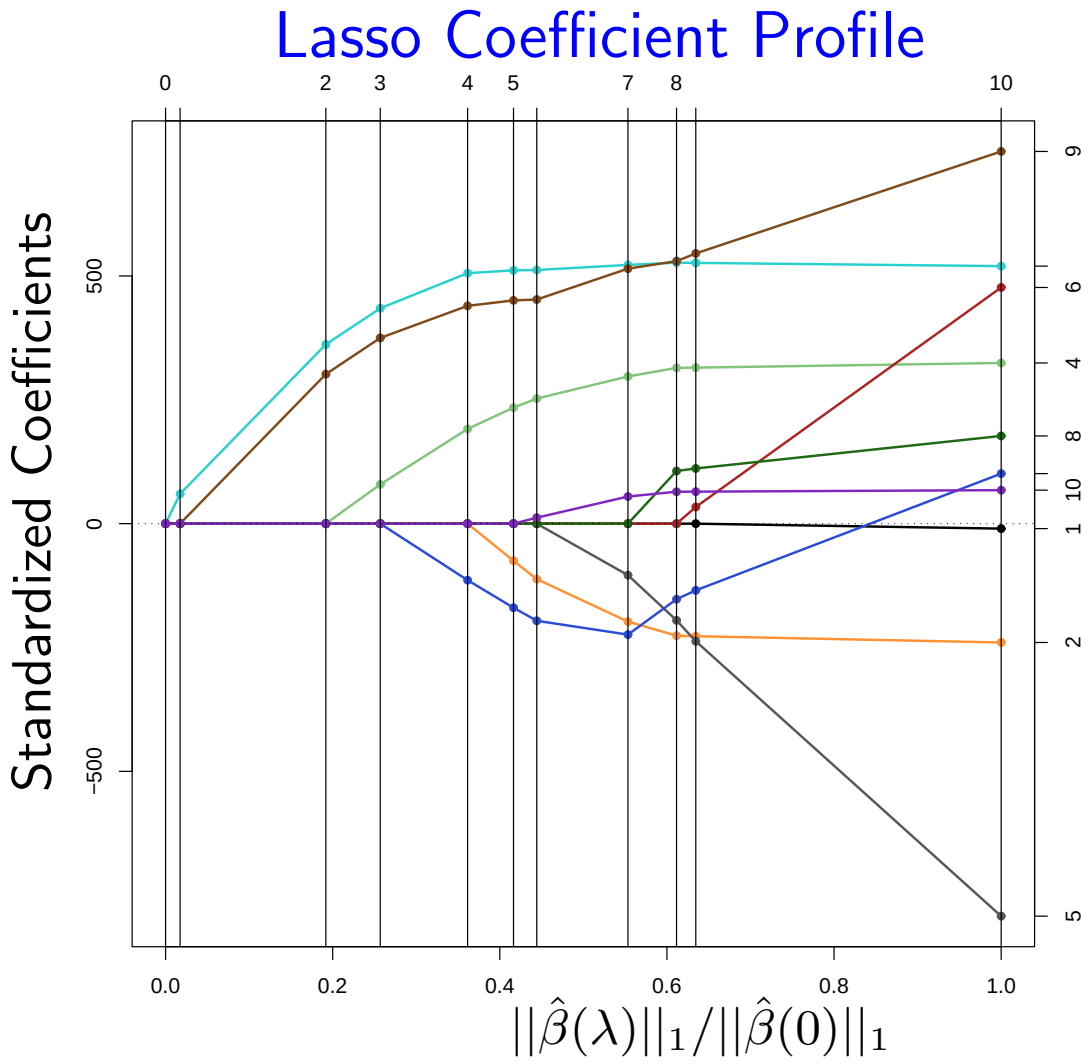
$$\min_\beta \sum_{i=1}^N (y_i - \beta_0 - \sum_{j=1}^p x_{ij}\beta_j)^2 \text{ subject to } \sum_{j=1}^p |\beta_j| \le t$$

- Similar to *ridge regression*, which has constraint $\sum_j \beta_j^2 \le t$
- Lasso does variable selection and shrinkage, while ridge only shrinks.



Brief History of ℓ_1 Regularization

- Wavelet *Soft Thresholding* (Donoho and Johnstone 1994) in orthonormal setting.
- Tibshirani introduces *Lasso* for regression in 1995.
- Same idea used in *Basis Pursuit* (Chen, Donoho and Saunders 1996).
- Extended to many linear-model settings e.g. Survival models (Tibshirani, 1997)
- Gives rise to a new field *Compressed Sensing* (Donoho 2004, Candes and Tao 2005)—near exact recovery of sparse signals in very high dimensions. In many cases ℓ_1 a good surrogate for ℓ_0.



Lasso: $\hat{\beta}(\lambda) = \text{argmin}_\beta \sum_{i=1}^{N}(y_i - \beta_0 - x_i^T\beta)^2 + \lambda||\beta||_1$

History of Path Algorithms

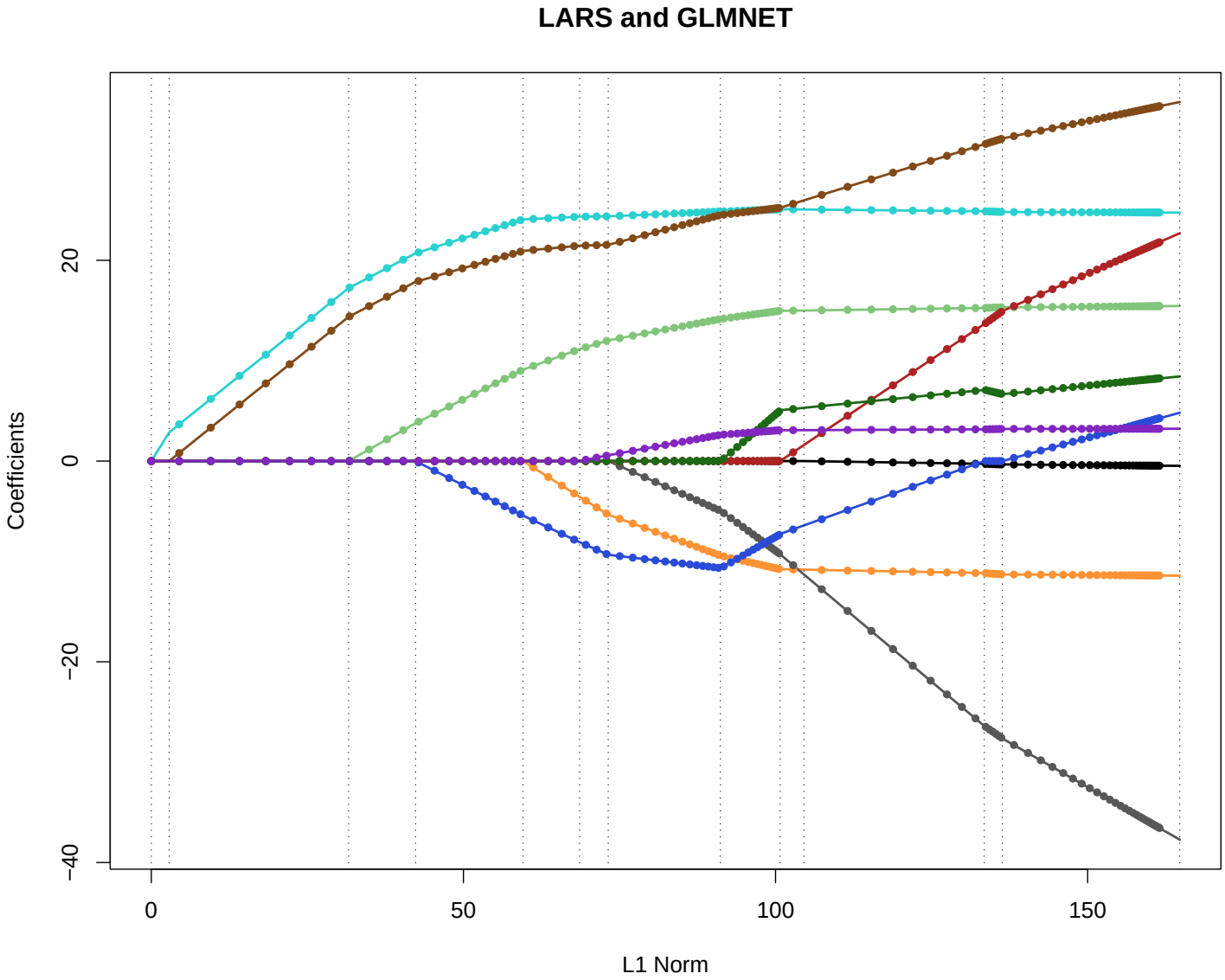
Efficient path algorithms for $\hat{\beta}(\lambda)$ allow for easy and exact cross-validation and model selection.

- In 2001 the LARS algorithm (Efron et al) provides a way to compute the entire lasso coefficient path efficiently at the cost of a full least-squares fit.
- 2001 – present: path algorithms pop up for a wide variety of related problems: Grouped lasso (Yuan & Lin 2006), support-vector machine (Hastie, Rosset, Tibshirani & Zhu 2004), elastic net (Zou & Hastie 2004), quantile regression (Li & Zhu, 2007), logistic regression and glms (Park & Hastie, 2007), Dantzig selector (James & Radchenko 2008), ...
- Many of these do not enjoy the piecewise-linearity of LARS, and seize up on very large problems.

Coordinate Descent

- Solve the lasso problem by coordinate descent: optimize each parameter separately, holding all the others fixed. Updates are trivial. Cycle around till coefficients stabilize.
- Do this on a grid of λ values, from λ_{max} down to λ_{min} (uniform on log scale), using warms starts.
- Can do this with a variety of loss functions and additive penalties.

Coordinate descent achieves dramatic speedups over all competitors, by factors of 10, 100 and more.


LARS and GLMNET
Coefficients
20
0
−20
−40
0
50
100
150
L1 Norm

Speed Trials

Competitors:

`lars` As implemented in R package, for squared-error loss.

`glmnet` Fortran based R package using coordinate descent — topic of this talk. Does squared error and logistic (2- and K-class).

`l1logreg` Lasso-logistic regression package by Koh, Kim and Boyd, using state-of-art interior point methods for convex optimization.

`BBR/BMR` Bayesian binomial/multinomial regression package by Genkin, Lewis and Madigan. Also uses coordinate descent to compute posterior mode with Laplace prior—the lasso fit.

Based on simulations (next 3 slides) and real data (4th slide).

Linear Regression — Dense Features

	Average Correlation between Features					
	0	0.1	0.2	0.5	0.9	0.95
	$N = 5000,\ p = 100$					
glmnet	0.05	0.05	0.05	0.05	0.05	0.05
lars	0.29	0.29	0.29	0.30	0.29	0.29
	$N = 100,\ p = 50000$					
glmnet	2.66	2.46	2.84	3.53	3.39	2.43
lars	58.68	64.00	64.79	58.20	66.39	79.79

Timings (secs) for `glmnet` and `lars` algorithms for linear regression with lasso penalty. Total time for 100 λ values, averaged over 3 runs.

Logistic Regression — Dense Features

	Average Correlation between Features					
	0	0.1	0.2	0.5	0.9	0.95
	$N = 5000,\ p = 100$					
glmnet	7.89	8.48	9.01	13.39	26.68	26.36
l1logreg	239.88	232.00	229.62	229.49	223.19	223.09
	$N = 100,\ p = 5000$					
glmnet	5.24	4.43	5.12	7.05	7.87	6.05
l1logreg	165.02	161.90	163.25	166.50	151.91	135.28

Timings (seconds) for logistic models with lasso penalty. Total time for tenfold cross-validation over a grid of 100 λ values.

Logistic Regression — Sparse Features

	0	0.1	0.2	0.5	0.9	0.95
	$N = 10,000,\ p = 100$					
glmnet	3.21	3.02	2.95	3.25	4.58	5.08
BBR	11.80	11.64	11.58	13.30	12.46	11.83
l1lognet	45.87	46.63	44.33	43.99	45.60	43.16
	$N = 100,\ p = 10,000$					
glmnet	10.18	10.35	9.93	10.04	9.02	8.91
BBR	45.72	47.50	47.46	48.49	56.29	60.21
l1lognet	130.27	124.88	124.18	129.84	137.21	159.54

Timings (seconds) for logistic model with lasso penalty and sparse features (95% zeros in X). Total time for ten-fold cross-validation over a grid of 100 λ values.

Logistic Regression — Real Datasets

Name	Type	N	p	**glmnet**	**l1logreg**	**BBR BMR**
			Dense			
Cancer	14 class	144	16,063	2.5 mins	NA	2.1 hrs
Leukemia	2 class	72	3571	2.50	55.0	450
			Sparse			
Internet ad	2 class	2359	1430	5.0	20.9	34.7
Newsgroup	2 class	11,314	777,811	2 mins	3.5 hrs	

Timings in seconds (unless stated otherwise). For Cancer, Leukemia and Internet-Ad, times are for ten-fold cross-validation over 100 λ values; for Newsgroup we performed a single run with 100 values of λ, with $\lambda_{min} = 0.05\lambda_{max}$.

A brief history of coordinate descent for the lasso

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2006 Friedman is external examiner at PhD oral of Anita van der Kooij (Leiden) who uses coordinate descent for elastic net. Friedman, Hastie + Tibshirani revisit this problem. Others have too — Krishnapuram and Hartemink (2005), Genkin, Lewis and Madigan (2007), Wu and Lange (2008), Meier, van de Geer and Buehlmann (2008).

Coordinate descent for the lasso

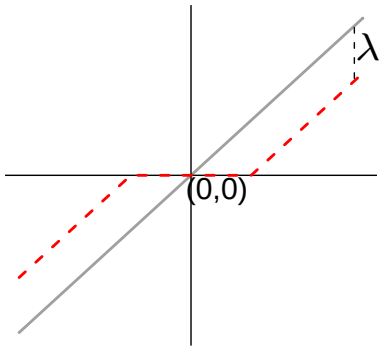
$$\min_\beta \frac{1}{2N}\sum_{i=1}^N (y_i - \sum_{j=1}^p x_{ij}\beta_j)^2 + \lambda \sum_{j=1}^p |\beta_j|$$

Suppose the p predictors and response are standardized to have mean zero and variance 1. Initialize all the $\beta_j = 0$.

Cycle over $j = 1, 2, \ldots, p, 1, 2, \ldots$ till convergence:

- Compute the partial residuals $r_{ij} = y_i - \sum_{k \neq j} x_{ik}\beta_k$.
- Compute the simple least squares coefficient of these residuals on jth predictor: $\beta_j^* = \frac{1}{N}\sum_{i=1}^N x_{ij} r_{ij}$
- Update β_j by *soft-thresholding*:

$$\begin{aligned} \beta_j &\leftarrow S(\beta_j^*, \lambda) \\ &= \text{sign}(\beta_j^*)(|\beta_j^*| - \lambda)_+ \end{aligned}$$



Why is coordinate descent so fast?

Naive Updates: $\beta_j^* = \frac{1}{N}\sum_{i=1}^N x_{ij}r_{ij} = \frac{1}{N}\sum_{i=1}^N x_{ij}r_i + \beta_j$, where r_i is current model residual; $O(N)$. Many coefficients are zero, and stay zero. If a coefficient changes, residuals are updated in $O(N)$ computations.

Covariance Updates: $\sum_{i=1}^N x_{ij}r_i = \langle x_j, y\rangle - \sum_{k:|\beta_k|>0}\langle x_j, x_k\rangle\beta_k$ Cross-covariance terms are computed once for active variables and stored (helps a lot when $N \gg p$).

Sparse Updates: If data is sparse (many zeros), inner products can be computed efficiently.

Active Set Convergence: After a cycle through p variables, we can restrict further iterations to the *active set* till convergence + one more cycle through p to check if active set has changed. Helps when $p \gg N$.

Warm Starts: We fits a sequence of models from $\lambda_{\max}$ down to $\lambda_{\min} = \epsilon\lambda_{max}$ (on log scale). λ_{max} is smallest value of λ for which all coefficients are zero. Solutions don't change much from one λ to the next. Convergence is often faster for entire sequence than for single solution at small value of λ.

FFT: Friedman + Fortran + Tricks — no sloppy flops!

Binary Logistic Models

Newton Updates: For binary logistic regression we have an outer Newton loop at each λ. This amounts to fitting a lasso with weighted squared error-loss. Uses weighted soft thresholding.

Multinomial: We use a symmetric formulation for multi- class logistic:

$$\Pr(G = \ell|x) = \frac{e^{\beta_{0\ell}+x^T\beta_\ell}}{\sum_{k=1}^K e^{\beta_{0k}+x^T\beta_k}}.$$

This creates an additional loop, as we cycle through classes, and compute the quadratic approximation to the multinomial log-likelihood, holding all but one classes parameters fixed.

Details Many important but tedious details with logistic models. e.g. if $p \gg N$, cannot let λ run down to zero.

Elastic-net Penalty

Proposed in Zou and Hastie (2005) for $p \gg N$ situations, where predictors are correlated in groups.

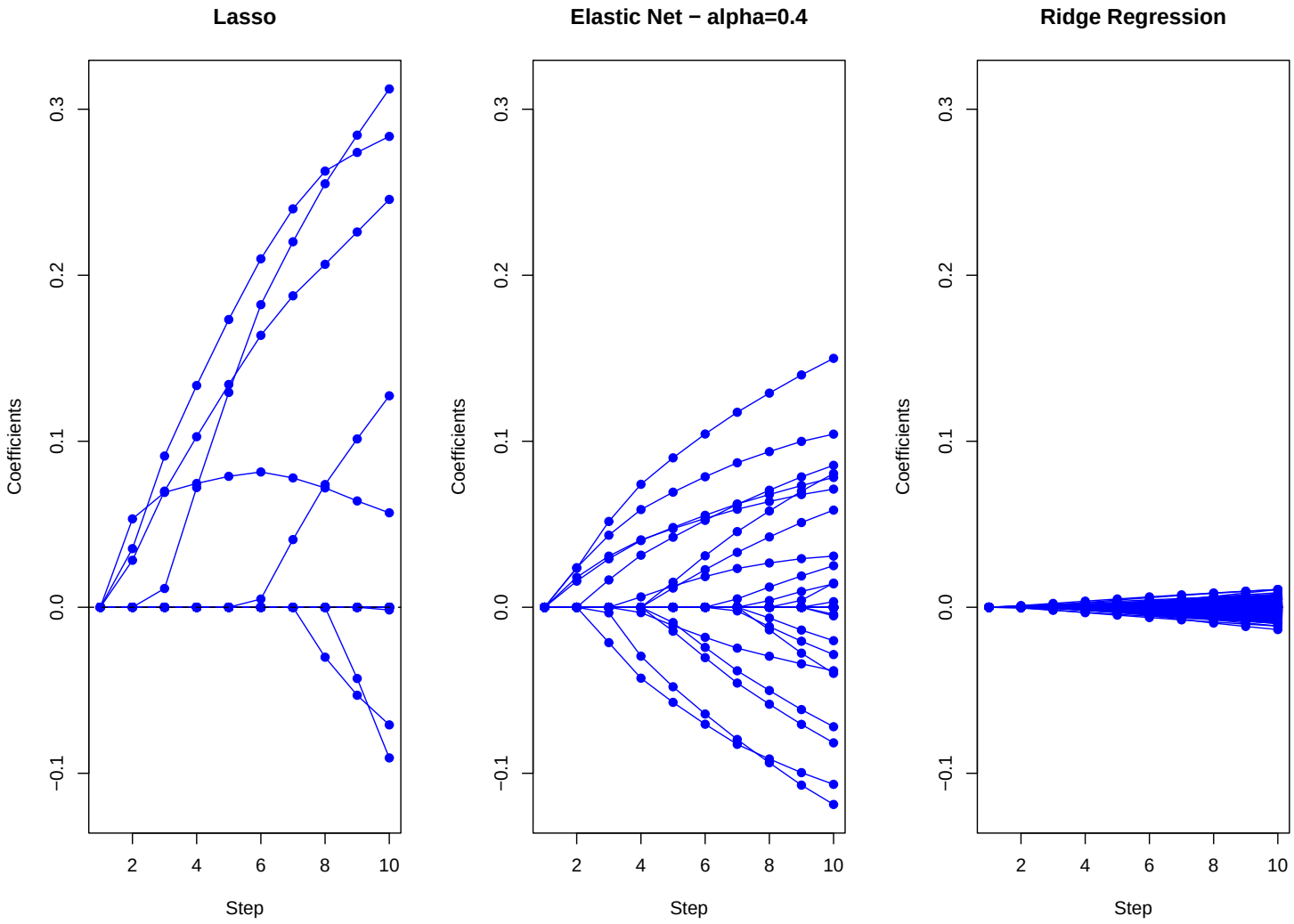
$$P_\alpha(\beta) = \sum_{j=1}^{p} \left[\tfrac{1}{2}(1-\alpha)\beta_j^2 + \alpha|\beta_j|\right].$$

α creates a compromise between the *lasso* and *ridge*.

Coordinate update is now

$$\beta_j \leftarrow \frac{S(\beta_j^*,\ \lambda\alpha)}{1+\lambda(1-\alpha)}$$

where $\beta_j^* = \frac{1}{N}\sum_{i=1}^{N} x_{ij} r_{ij}$ as before.



Leukemia Data, Logistic, N=72, p=3571, first 10 steps shown

Multiclass classification

Microarray classification: 16,063 genes, 144 training samples 54 test samples, 14 cancer classes. Multinomial regression model.

Methods	CV errors out of 144	Test errors out of 54	# of genes used
1. Nearest shrunken centroids	35 (5)	17	6520
2. L_2-penalized discriminant analysis	25 (4.1)	12	16063
3. Support vector classifier	26 (4.2)	14	16063
4. Lasso regression (one vs all)	30.7 (1.8)	12.5	1429
5. K-nearest neighbors	41 (4.6)	26	16063
6. L_2-penalized multinomial	26 (4.2)	15	16063
7. Lasso-penalized multinomial	17 (2.8)	13	269
8. Elastic-net penalized multinomial	22 (3.7)	11.8	384

6–8 fit using `glmnet`

Summary

Many problems have the form

$$\min_{\{\beta_j\}_1^p} \left[R(y, \beta) + \lambda \sum_{j=1}^{p} P_j(\beta_j) \right].$$

- If R and P_j are convex, and R is differentiable, then coordinate descent converges to the solution (Tseng, 1988).
- Often each coordinate step is trivial. E.g. for lasso, it amounts to soft-thresholding, with many steps leaving $\hat{\beta}_j = 0$.
- Decreasing λ slowly means not much cycling is needed.
- Coordinate moves can exploit sparsity.

Other Applications

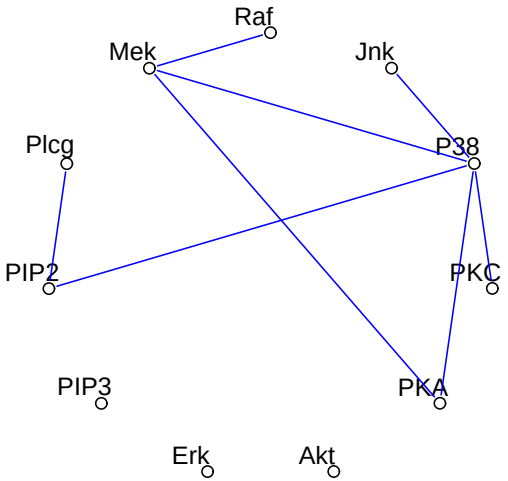
Undirected Graphical Models — learning dependence structure via the lasso. Model the inverse covariance $\mathbf{\Theta}$ in the Gaussian family with L_1 penalties applied to elements.

$$\max_{\mathbf{\Theta}} \log\det \mathbf{\Theta} - \mathrm{Tr}(\mathbf{S\Theta}) - \lambda||\mathbf{\Theta}||_1$$

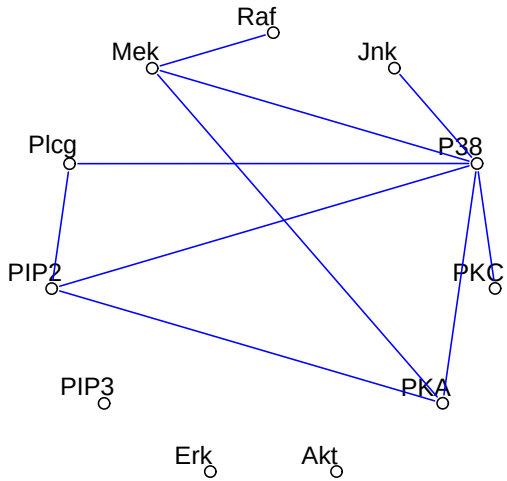
Modified block-wise lasso algorithm, which we solve by coordinate descent (FHT 2007). Algorithm is very fast, and solve moderately sparse graphs with 1000 nodes in under a minute.

Example: flow cytometry - $p = 11$ proteins measured in $N = 7466$ cells (Sachs et al 2003) (next page)

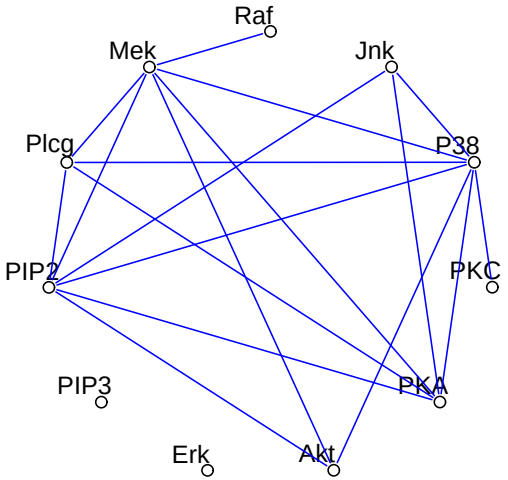
$\lambda = 36$



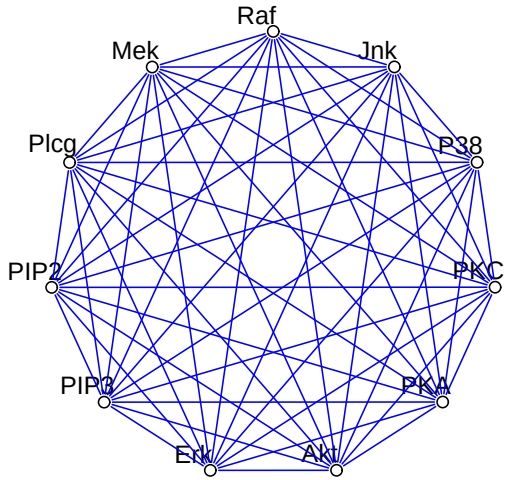
$\lambda = 27$



$\lambda = 7$



$\lambda = 0$



Grouped lasso (Yuan and Lin, 2007, Meier, Van de Geer, Buehlmann, 2008) — each term $P_j(\beta_j)$ applies to *sets* of parameters:

$$\sum_{j=1}^{J} ||\beta_j||_2.$$

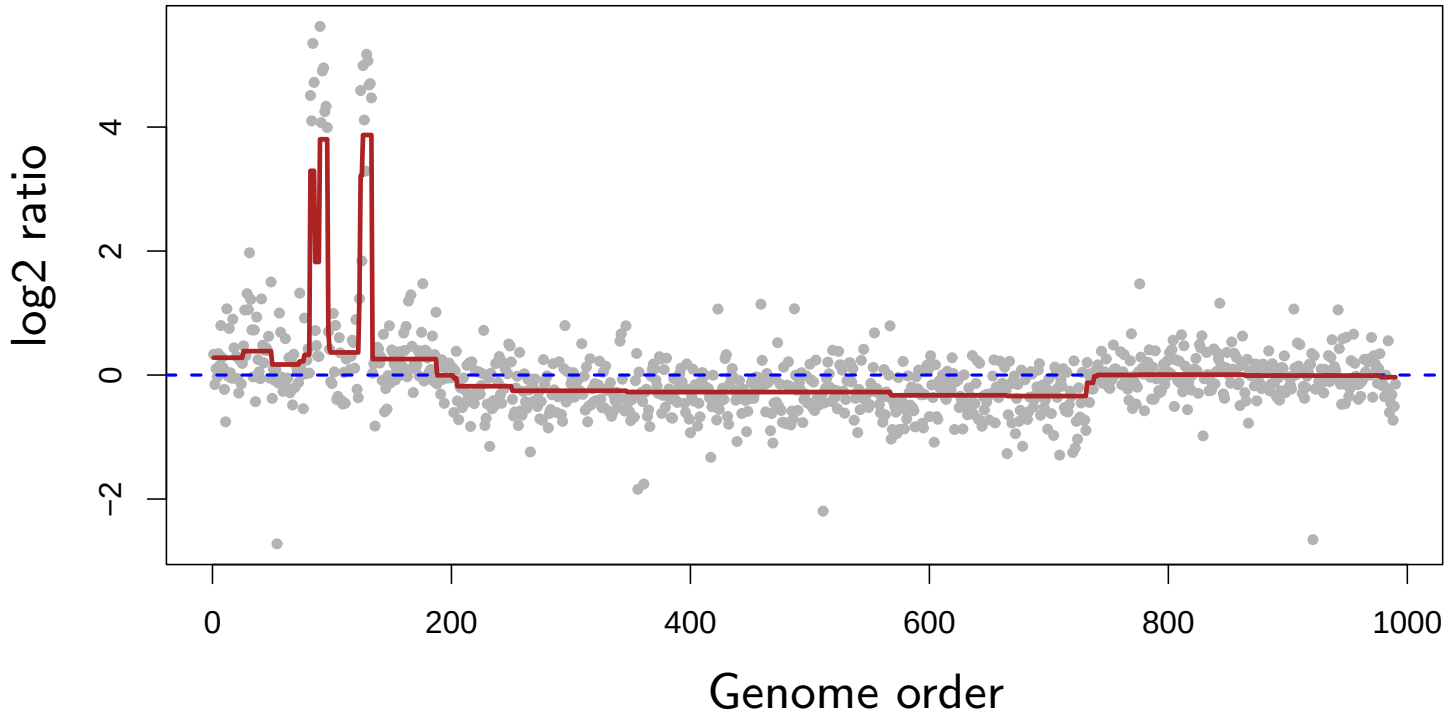
Example: each block represents the levels for a categorical predictor.

Leads to a block-updating form of coordinate descent.

CGH modeling and the fused lasso. Here the penalty has the form

$$\sum_{j=1}^{p} |\beta_j| + \alpha \sum_{j=1}^{p-1} |\beta_{j+1} - \beta_j|.$$

This is not additive, so a modified coordinate descent algorithm is required (FHT + Hoeffling 2007).



Summary

- ℓ_1 regularization (and variants) has become a powerful tool with the advent of wide data.
- In compressed sensing, often exact sparse signal recovery is possible with ℓ_1 methods.
- Coordinate descent is fastest known algorithm for solving these problems—along a path of values for the tuning parameter.