Least Angle Regression, Forward Stagewise and the Lasso

Brad Efron, Trevor Hastie, Iain Johnstone and Robert Tibshirani
Stanford University

Annals of Statistics, 2004 (with discussion)

`http://www-stat.stanford.edu/∼tibs`

Background

- Today's talk is about linear regression
- But the motivation comes from the area of flexible function fitting: "Boosting"— Freund & Schapire (1995)

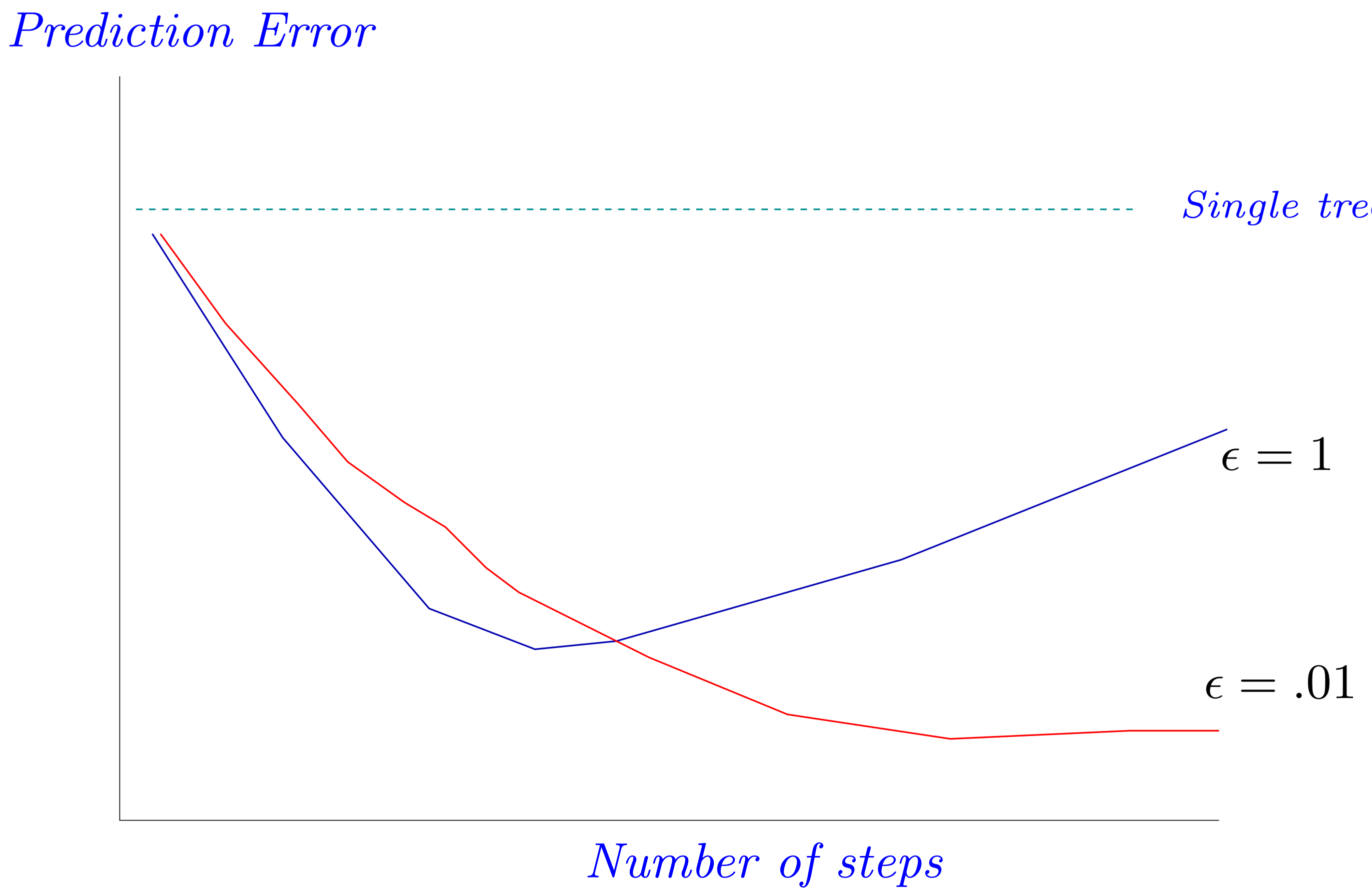
Least Squares Boosting

Friedman, Hastie & Tibshirani — see *Elements of Statistical Learning (chapter 10)*

Supervised learning: Response y, predictors $x = (x_1, x_2 \dots x_p)$.

1. Start with function $F(x) = 0$ and residual $r = y$
2. Fit a CART regression tree to r giving $f(x)$
3. Set $F(x) \leftarrow F(x) + \epsilon f(x)$, $r \leftarrow r - \epsilon f(x)$ and repeat step 2 many times

Least Squares Boosting



Linear Regression

Here is a version of least squares boosting for multiple linear regression: (assume predictors are standardized)

(Incremental) Forward Stagewise

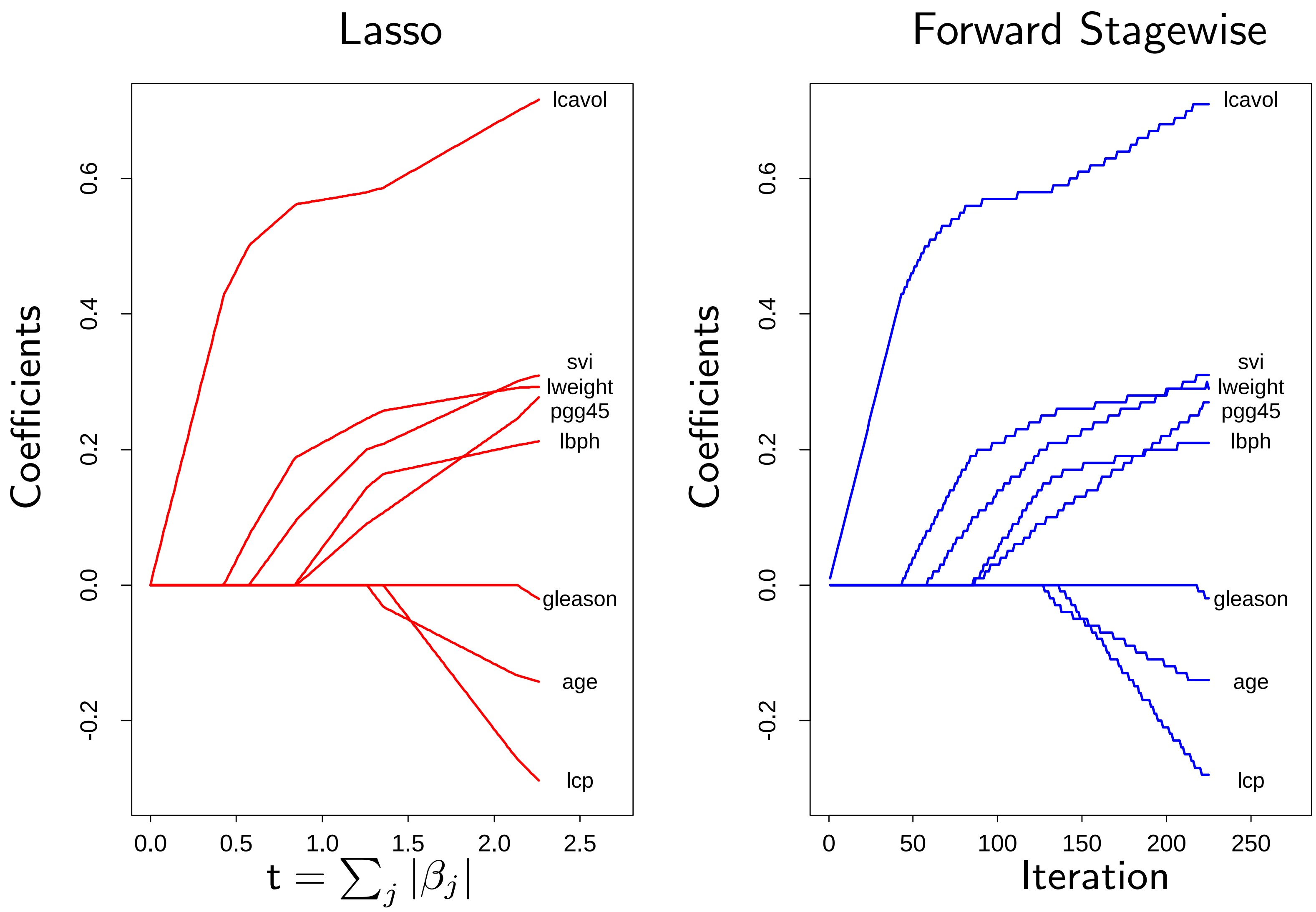
Find co-var with highest
correlation.
Then add a bit of sigma

1. Start with $r = y$, $\beta_1, \beta_2, \ldots \beta_p = 0$.
2. Find the predictor x_j most correlated with r
3. Update $\beta_j \leftarrow \beta_j + \delta_j$, where $\delta_j = \epsilon \cdot \text{sign}\langle r, x_j \rangle$ if they have diff. signs, give -1. otherwise 1
4. Set $r \leftarrow r - \delta_j \cdot x_j$ and repeat steps 2 and 3 many times

$\delta_j = \langle r, x_j \rangle$ gives usual forward stagewise; different from forward stepwise

Analogous to least squares boosting, with *trees=predictors*

Prostate Cancer Data



Linear regression via the Lasso (Tibshirani, 1995)

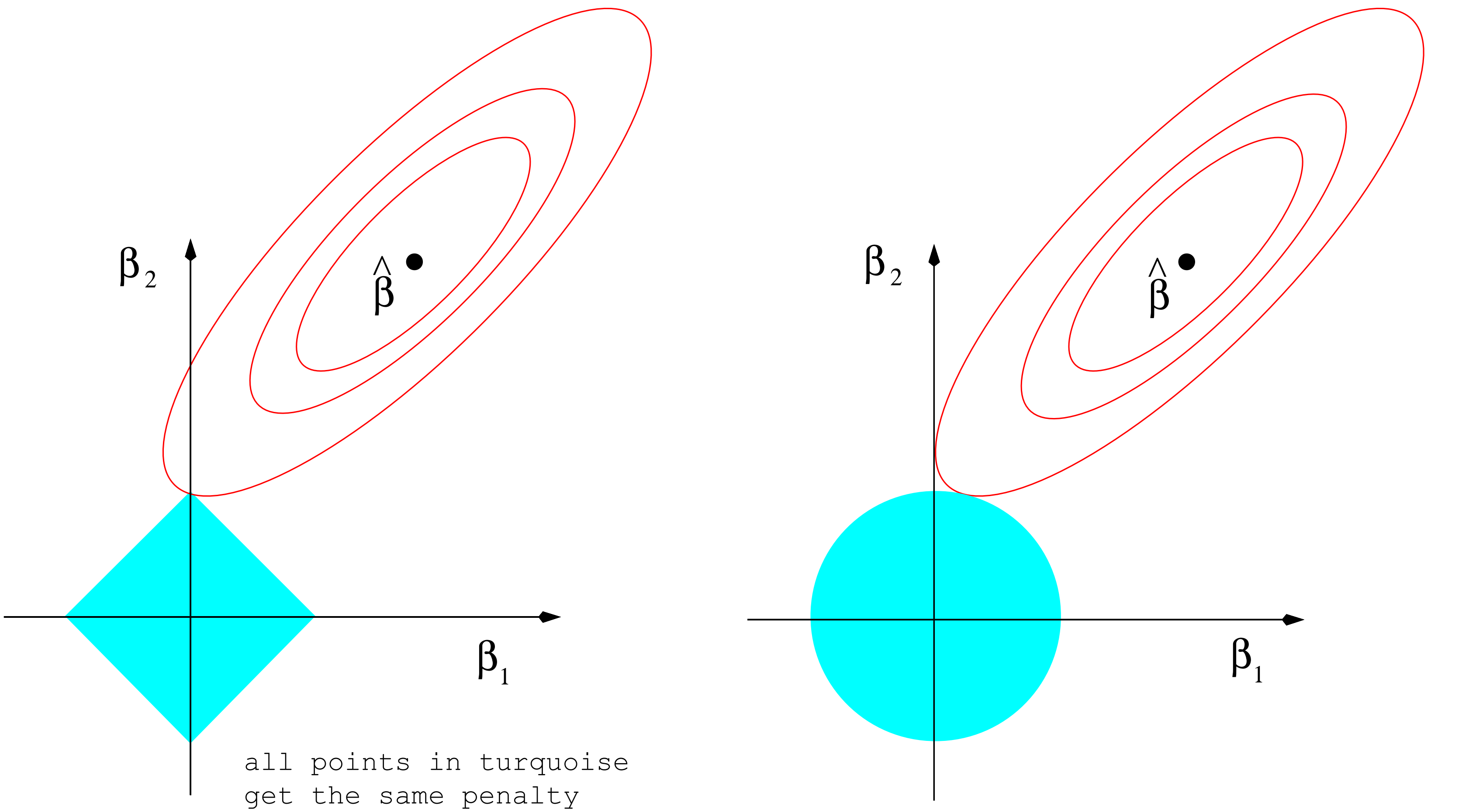
- Assume $\bar{y} = 0$, $\bar{x}_j = 0$, $\text{Var}(x_j) = 1$ for all j.
- Minimize $\sum_i (y_i - \sum_j x_{ij}\beta_j)^2$ subject to $\sum_j |\beta_j| \le s$
- With orthogonal predictors, solutions are soft thresholded version of least squares coefficients:

$$\text{sign}(\hat{\beta}_j)(|\hat{\beta}_j| - \gamma)_+$$

(γ is a function of s)

- For small values of the bound s, Lasso does variable selection. See pictures

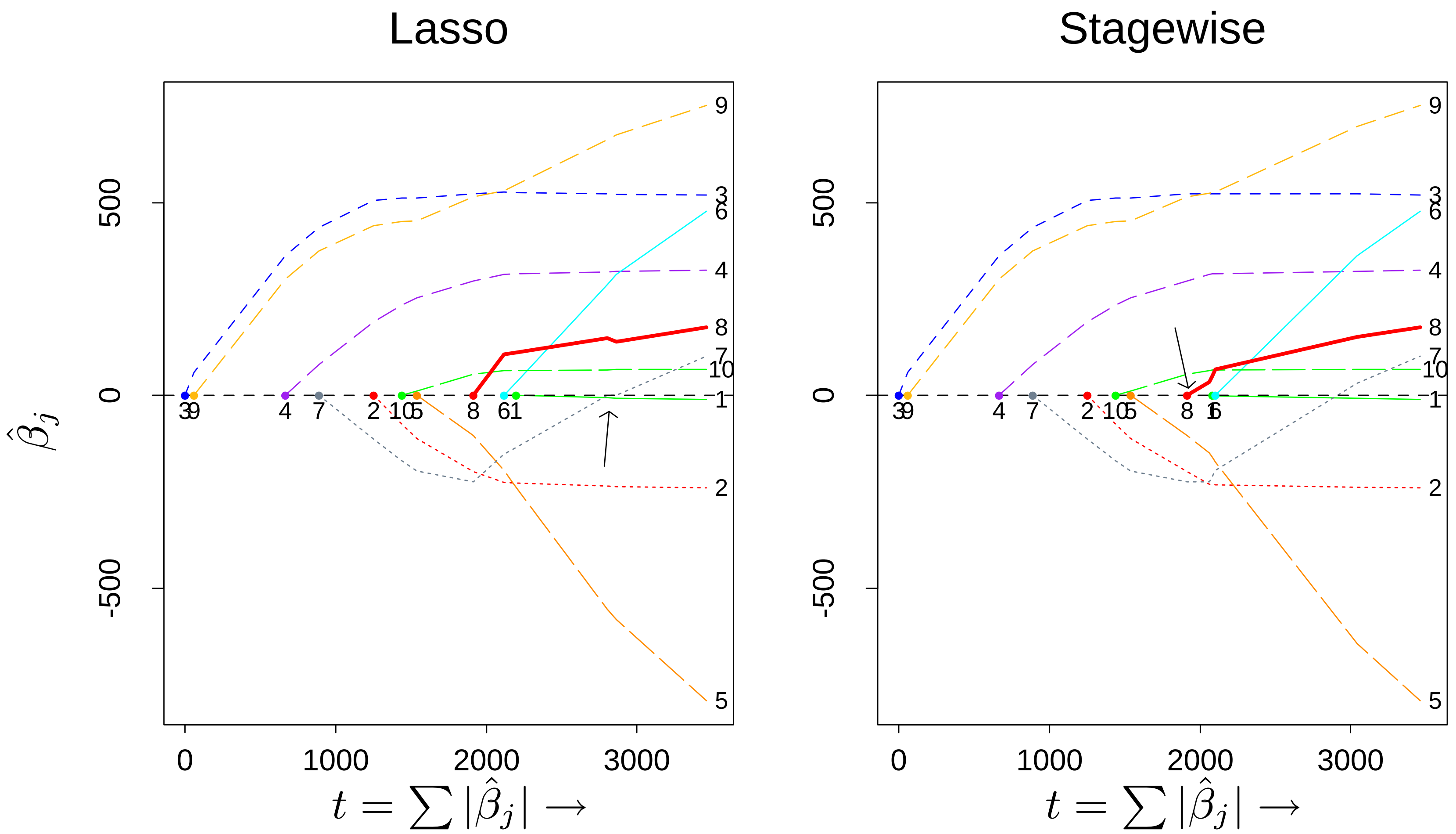
Lasso and Ridge regression



More on Lasso

- Current implementations use quadratic programming to compute solutions
- Can be applied when $p > n$. In that case, number of non-zero coefficients is at most $n - 1$ (by convex duality)
- interesting consequences for applications, eg microarray data

Diabetes Data



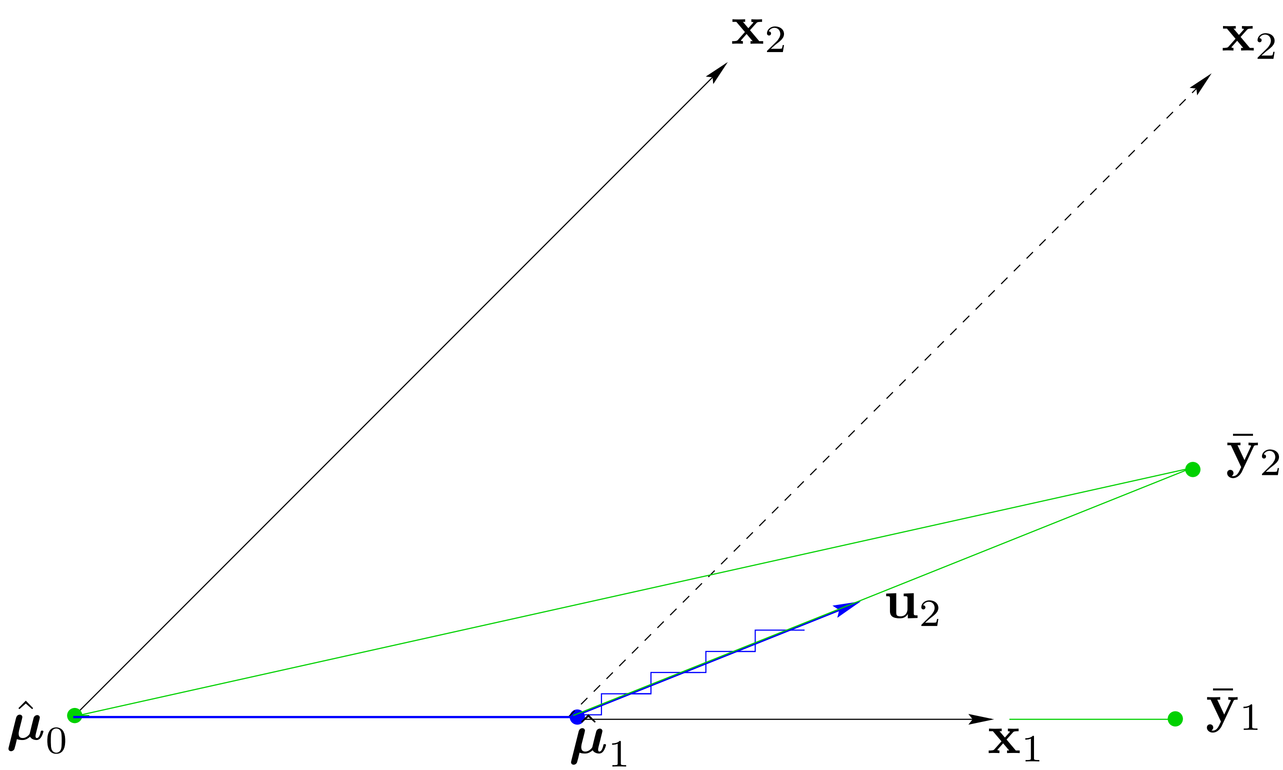
Why are Forward Stagewise and Lasso so similar?

- Are they identical?
- In orthogonal predictor case: *yes*
- In hard to verify case of *monotone* coefficient paths: *yes*
- In general, almost!
- Least angle regression (LAR) provides answers to these questions, and an efficient way to compute the complete Lasso sequence of solutions.

Least Angle Regression — LAR

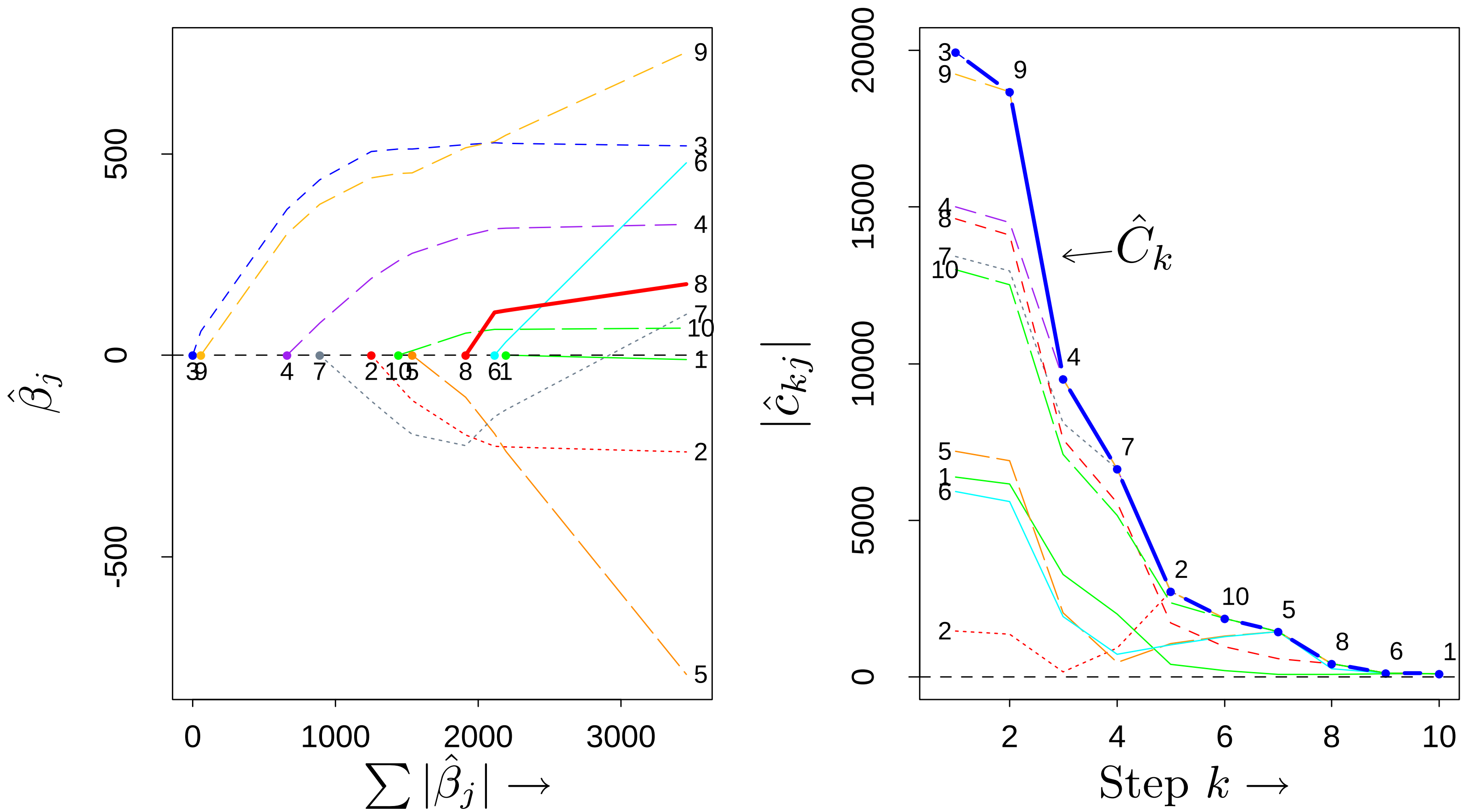
Like a "more democratic" version of forward stepwise regression.

1. Start with $r = y$, $\hat{\beta}_1, \hat{\beta}_2, \ldots \hat{\beta}_p = 0$. Assume x_j standardized.
2. Find predictor x_j most correlated with r.
3. Increase β_j in the direction of sign(corr(r, x_j)) until some other competitor x_k has as much correlation with current residual as does x_j.
4. Move $(\hat{\beta}_j, \hat{\beta}_k)$ in the joint least squares direction for (x_j, x_k) until some other competitor x_ℓ has as much correlation with the current residual
5. Continue in this way until all predictors have been entered. Stop when $\text{corr}(r, x_j) = 0 \; \forall \; j$, i.e. OLS solution.



The LAR direction $\mathbf{u}_2$ at step 2 makes an equal angle with $\mathbf{x}_1$ and $\mathbf{x}_2$.

LARS



$\hat{\beta}_j$
$\sum |\hat{\beta}_j| \rightarrow$
$|\hat{c}_{kj}|$
$\hat{C}_k$
Step $k \rightarrow$

Relationship between the 3 algorithms

- Lasso and forward stagewise can be thought of as restricted versions of LAR
- *For Lasso*: Start with LAR. If a coefficient crosses zero, stop. Drop that predictor, recompute the best direction and continue. This gives the Lasso path

Proof (lengthy): use Karush-Kuhn-Tucker theory of convex optimization. Informally:

$$\begin{aligned} \frac{\partial}{\partial \beta_j}\{||\mathbf{y}-\mathbf{X}\beta||^2 \quad &+ \quad \lambda \sum_j |\beta_j|\} = 0 \\ &\Leftrightarrow \\ \langle \mathbf{x}_j, \mathbf{r} \rangle \quad &= \quad \frac{\lambda}{2}\text{sign}(\hat{\beta}_j) \quad \text{if } \hat{\beta}_j \neq 0 \text{ (active)} \end{aligned}$$

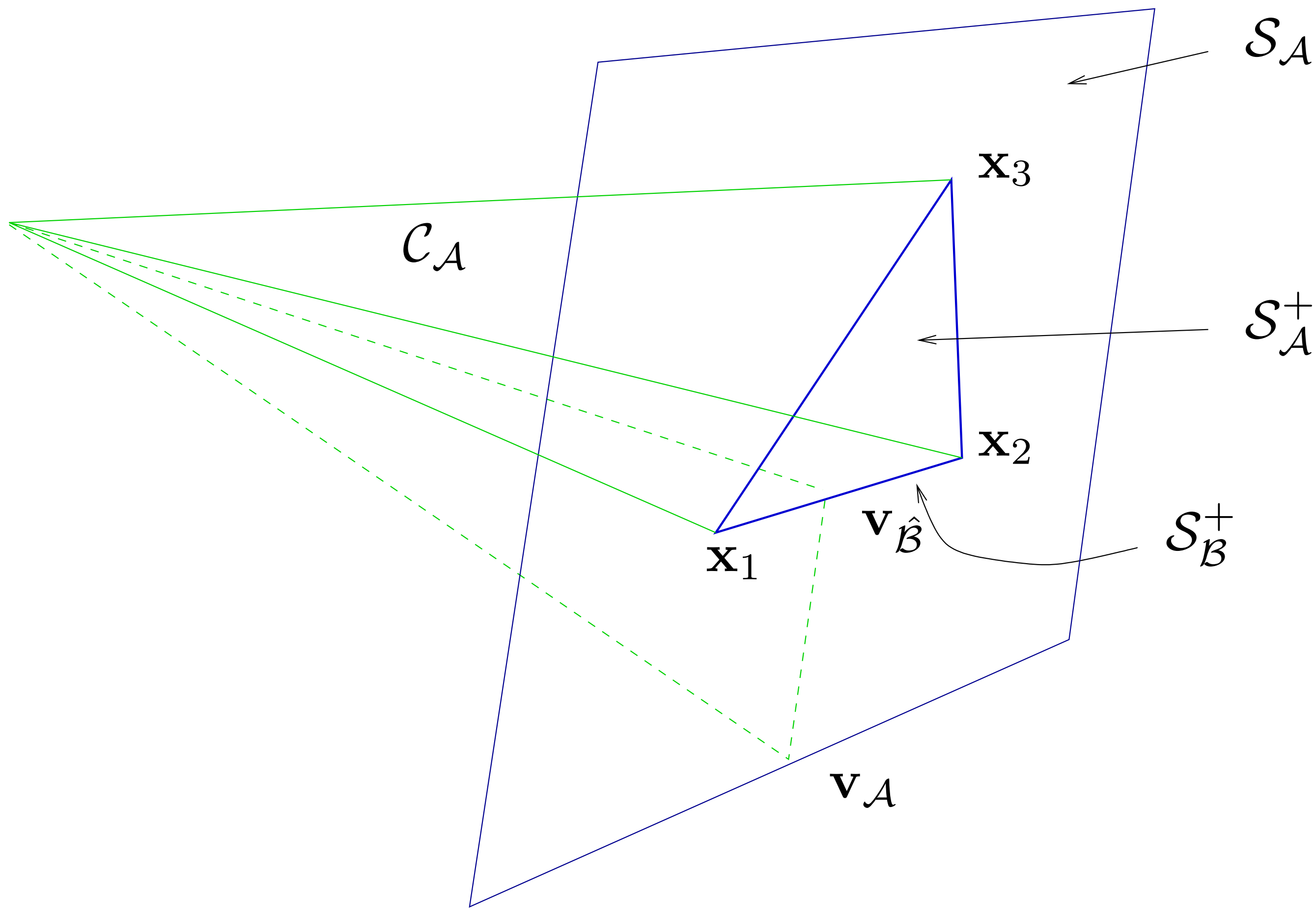
- *For forward stagewise:* Start with LAR. Compute best (equal angular) direction at each stage. If direction for any predictor j doesn't agree in sign with $\mathrm{corr}(r, x_j)$, project direction into the "positive cone" and use the projected direction instead.
- in other words, forward stagewise always moves each predictor in the direction of $\mathrm{corr}(r, x_j)$.
- The incremental forward stagewise procedure approximates these steps, one predictor at a time. As step size $\epsilon \to 0$, can show that it coincides with this modified version of LAR

More on forward stagewise

- Let A be the active set of predictors at some stage. Suppose the procedure takes $M = \sum M_j$ steps of size ϵ in these predictors, M_j in predictor j ($M_j = 0$ for $j \notin A$).
- Then $\hat{\beta}$ is changed to $\hat{\beta} + (s_1 M_1/M, s_2 M_2/M, \cdots s_p M_p/M)$ where $s_j = \mathrm{sign}(\mathrm{corr}(r, x_j))$
- $\theta = (M_1/M, \cdots M_p/M)$ satisfies

$$\theta = \mathrm{argmin} \sum_i (r_i - \sum_{j \in A} x_{ij} s_j \theta_j)^2,$$

subject to $\theta_j \geq 0$ for all j. This is a *non-negative least squares estimate*.



The forward stagewise direction lies in the positive cone spanned by the (signed) predictors with equal correlation with the current residual.

Summary

- LARS—uses least squares directions in the active set of variables.
- Lasso—uses least square directions; if a variable crosses zero, it is removed from the active set.
- Forward stagewise—uses non-negative least squares directions in the active set.

Benefits

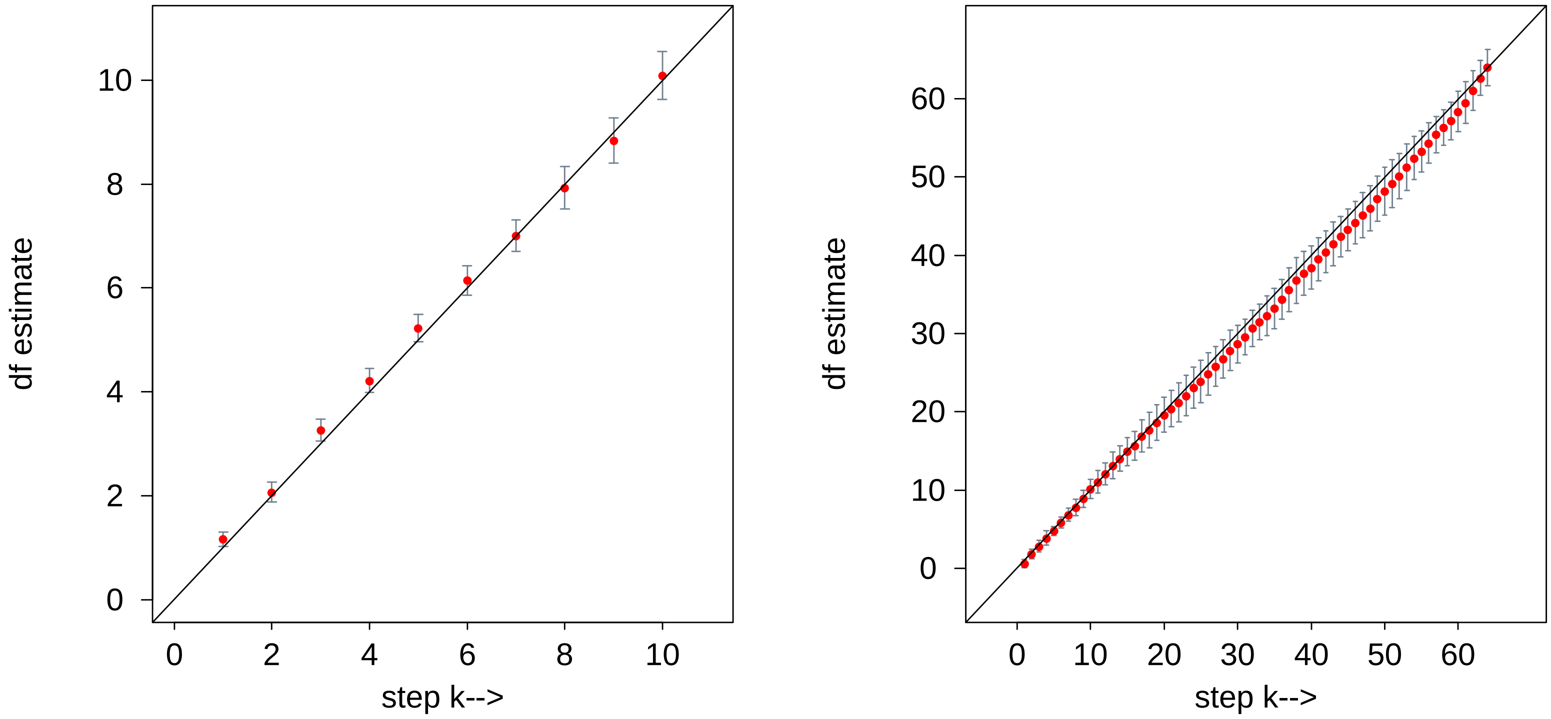
- Possible explanation of the benefit of "slow learning" in boosting: it is approximately fitting via an L_1 (lasso) penalty
- new algorithm computes entire Lasso path in same order of computation as one full least squares fit. Splus/R Software on Hastie's website:

  `www-stat.stanford.edu/~hastie/Papers#LARS`
- Degrees of freedom formula for LAR:

  After k steps, degrees of freedom of fit $= k$ (with some regularity conditions)
- For Lasso, the procedure often takes $> p$ steps, since predictors can drop out. Corresponding formula (conjecture):

  Degrees of freedom for last model in sequence with k predictors is equal to k.

Degrees of freedom



Degree of Freedom result

$$\mathrm{df}(\hat{\mu}) \equiv \sum_{i=1}^{n} \mathrm{cov}(\hat{\mu}_i, y_i)/\sigma^2 = k$$

Proof is based on is an application of Stein's unbiased risk estimate (SURE). Suppose that $g : \mathbb{R}^n \to \mathbb{R}^n$ is almost differentiable and set $\nabla \cdot g = \sum_{i=1}^{n} \partial g_i / \partial x_i$. If $\mathbf{y} \sim N_n(\mu, \sigma^2 \mathbf{I})$, then Stein's formula states that

$$\sum_{i=1}^{n} \mathrm{cov}(g_i, y_i)/\sigma^2 = E[\nabla \cdot g(\mathbf{y})].$$

LHS is degrees of freedom. Set $g(\cdot)$ equal to the LAR estimate. In orthogonal case, $\partial g_i / \partial x_i$ is 1 if predictor is in model, 0 otherwise. Hence RHS equals number of predictors in model $(= k)$.

Non-orthogonal case is much harder.

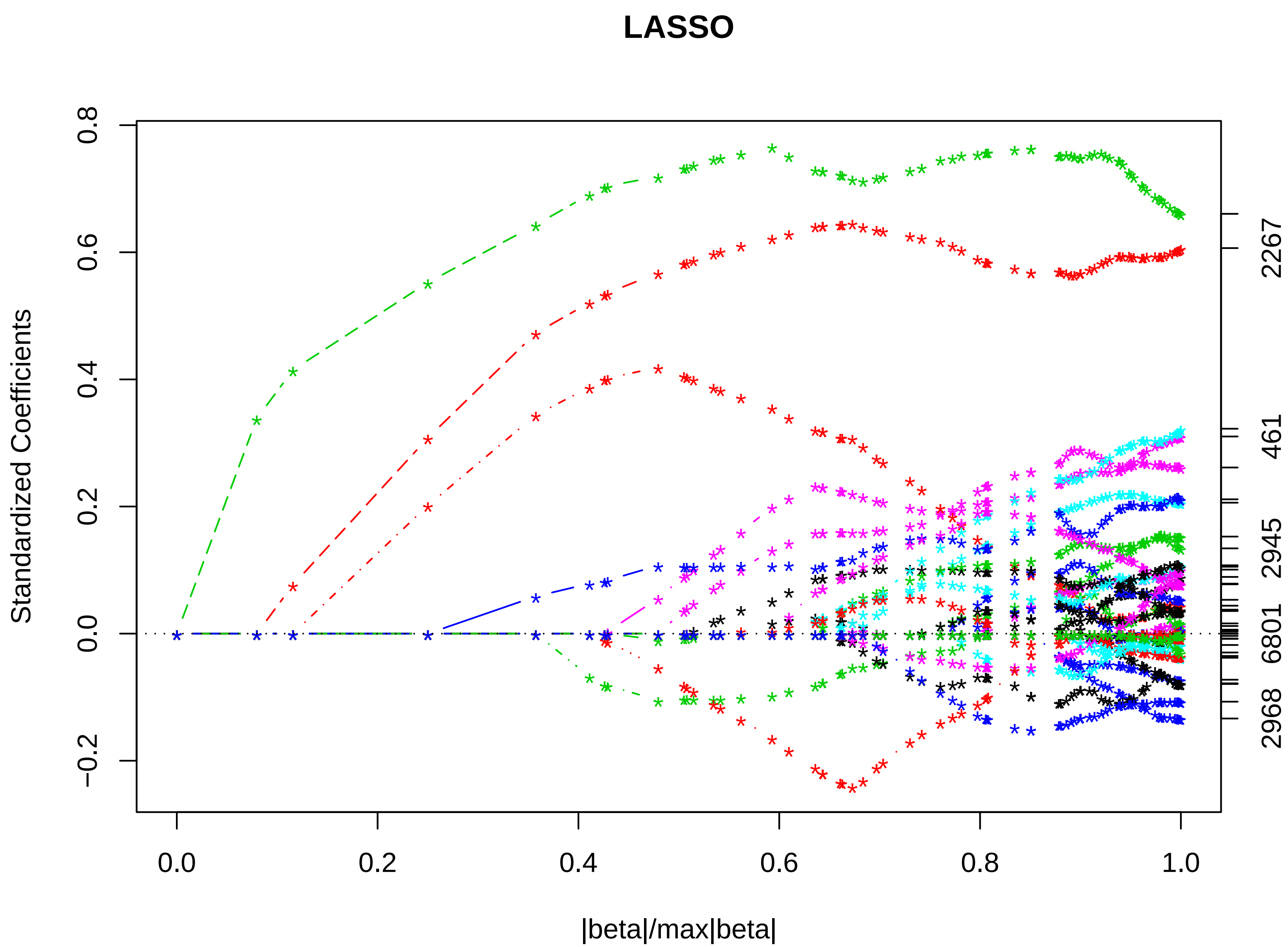
Software for R and Splus

`lars()` function fits all three models: `lasso`, `lar` or `forward.stagewise`. Methods for prediction, plotting, and cross-validation. Detailed documentation provided. Visit `www-stat.stanford.edu/~hastie/Papers/#LARS`

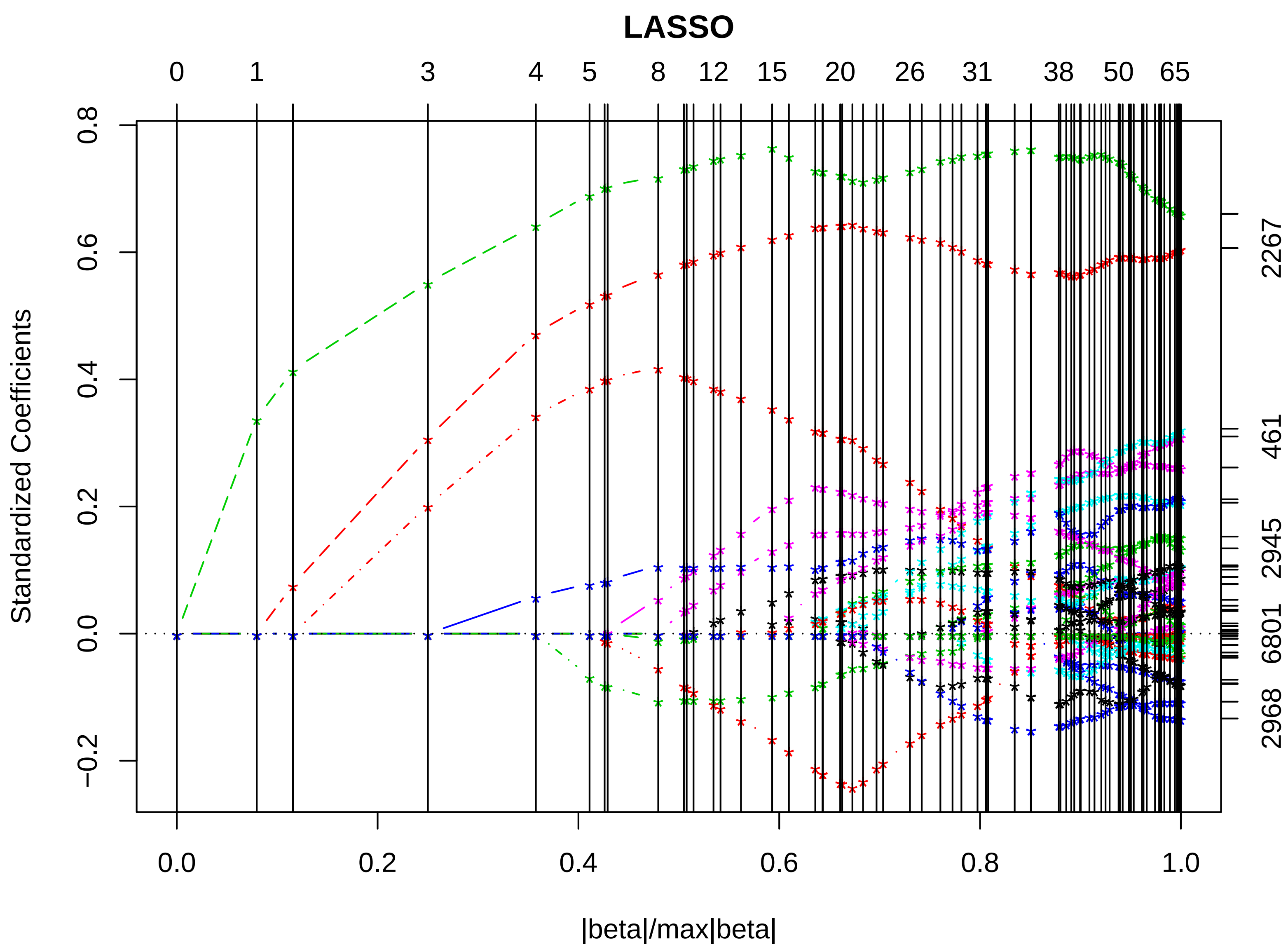
Main computations involve least squares fitting using the *active set* of variables. Computations managed by updating the Choleski R matrix (and frequent downdating for lasso and forward stagewise).

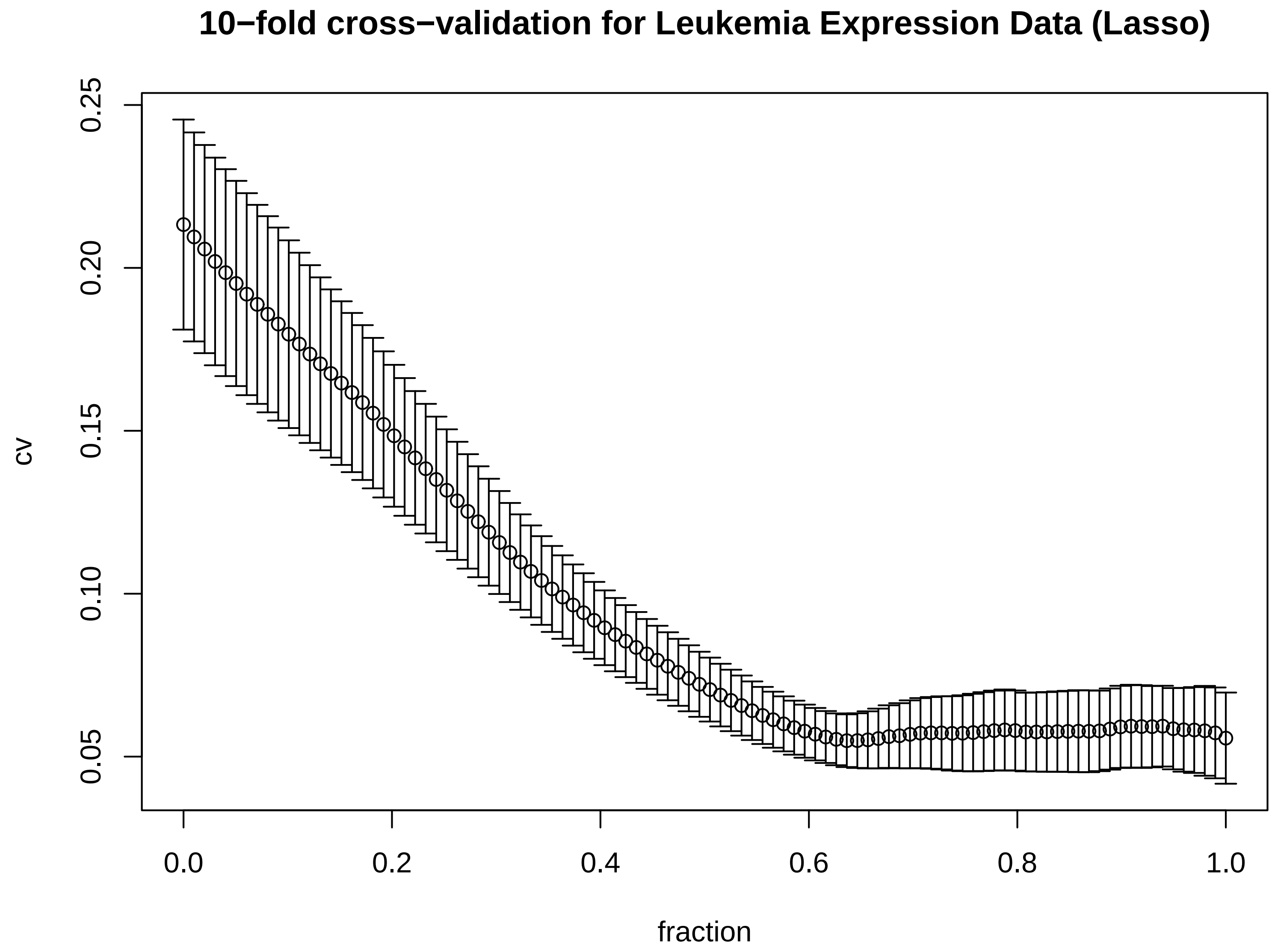
MicroArray Example

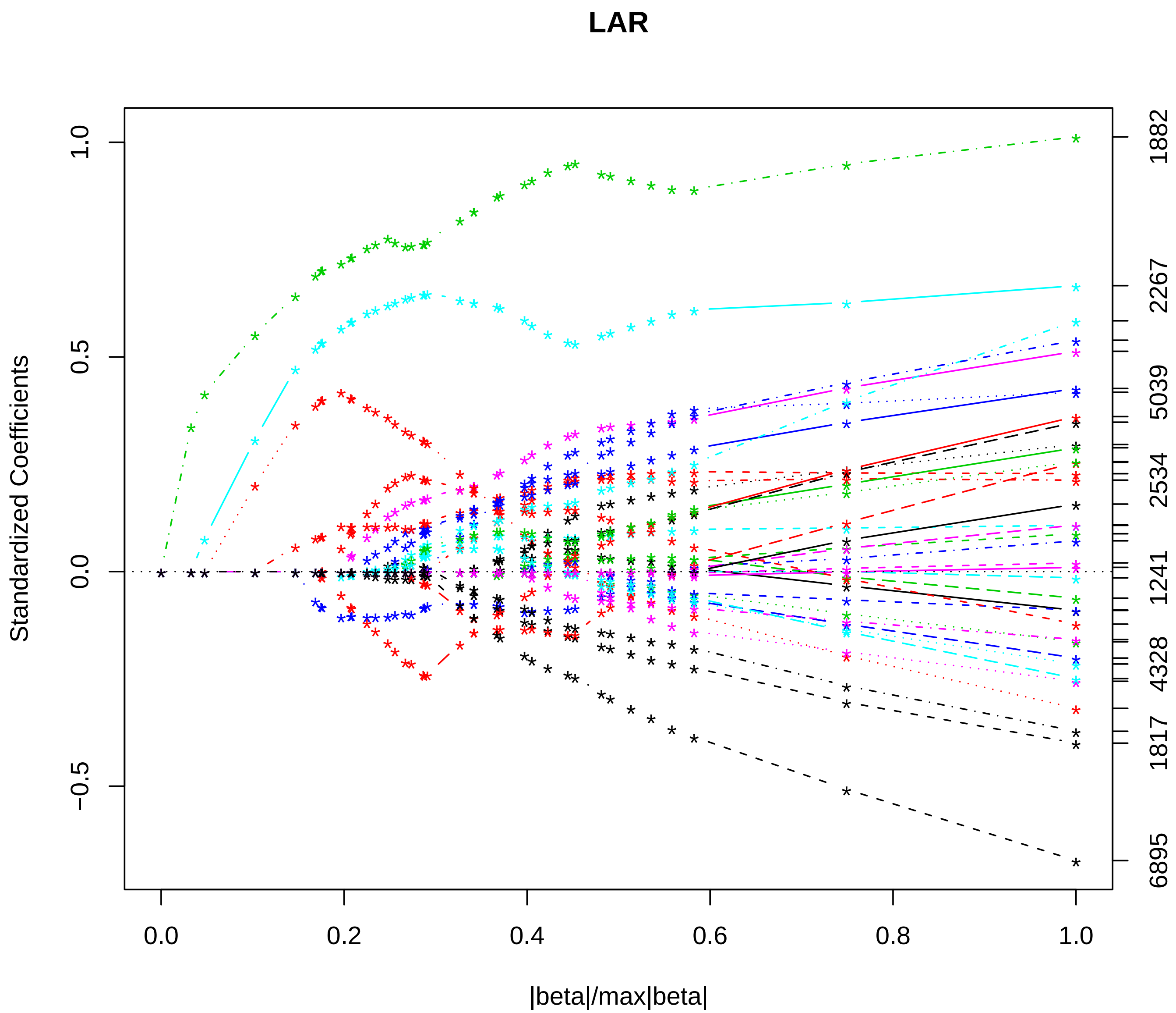
- Expression data for 38 Leukemia patients ("Golub" data).
- X matrix with 38 samples and 7129 variables (genes)
- Response Y is dichotomous ALL (27) vs AML (11)
- LARS (lasso) took 4 seconds in R version 1.7 on a 1.8Ghz Dell workstation running Linux.
- In 70 steps, 52 variables ever non zero, at most 37 at a time.

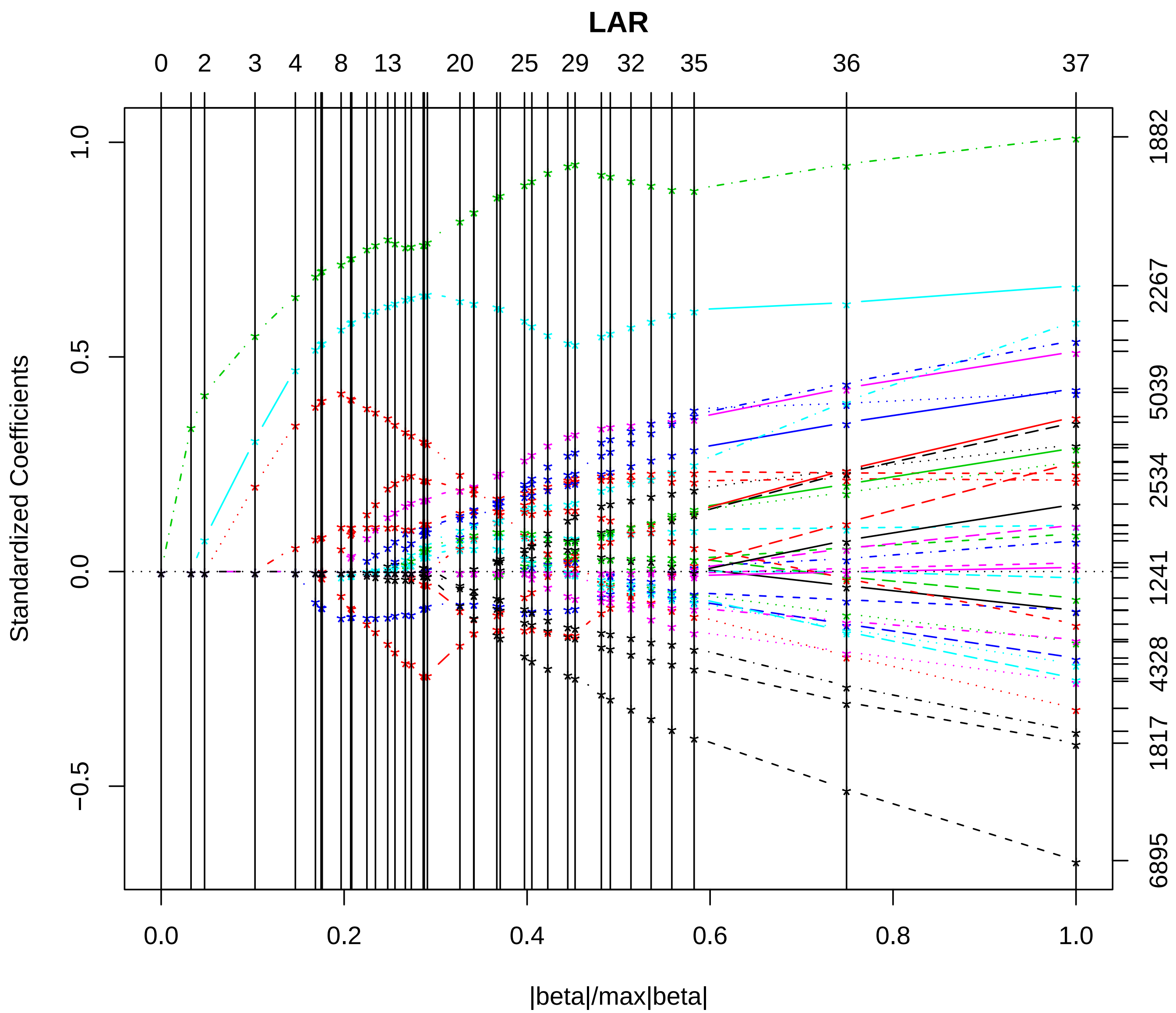


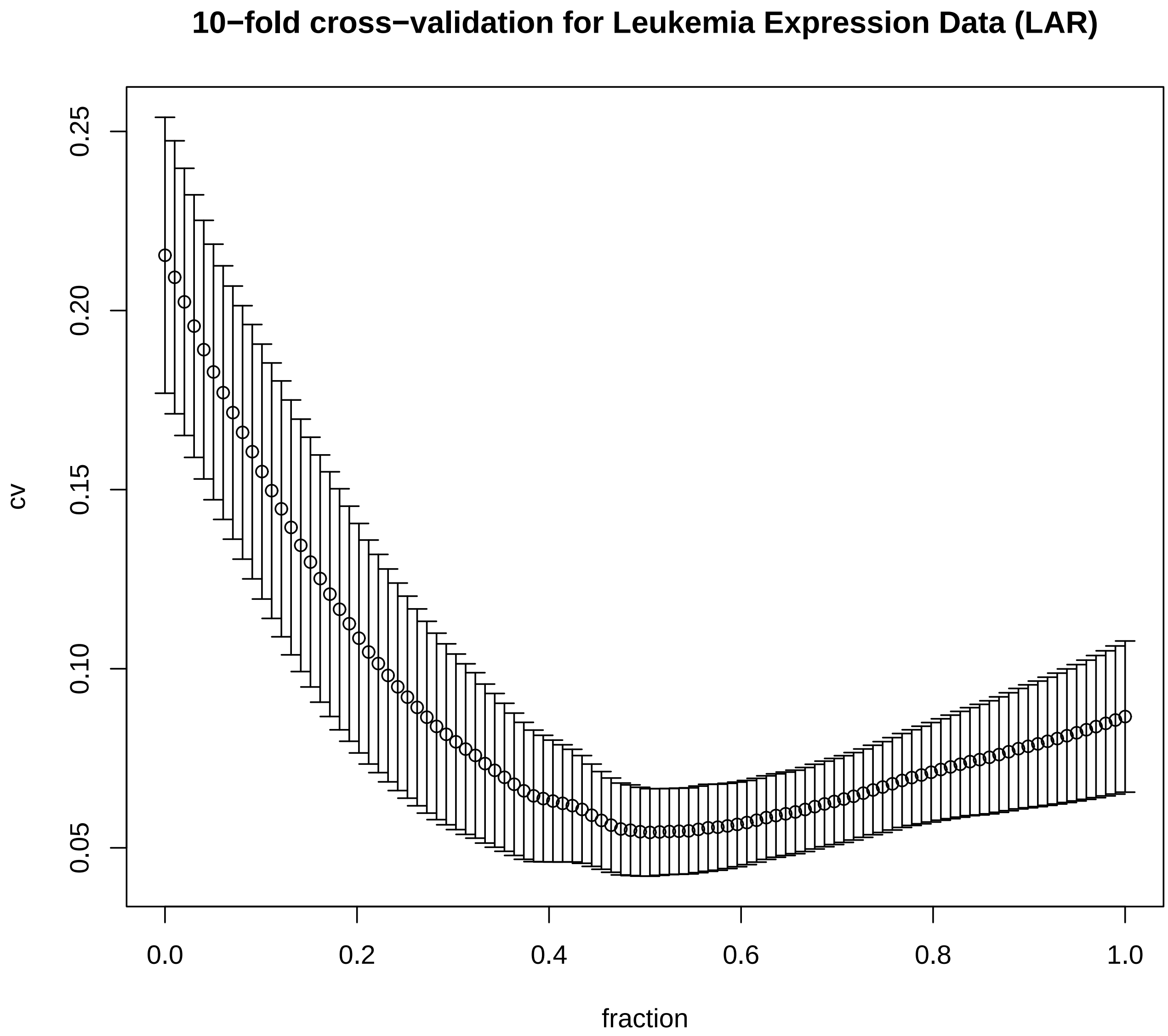
LASSO
Standardized Coefficients
|beta|/max|beta|
0.0
0.2
0.4
0.6
0.8
1.0
−0.2
0.0
0.2
0.4
0.6
0.8
2267
461
2945
6801
2968

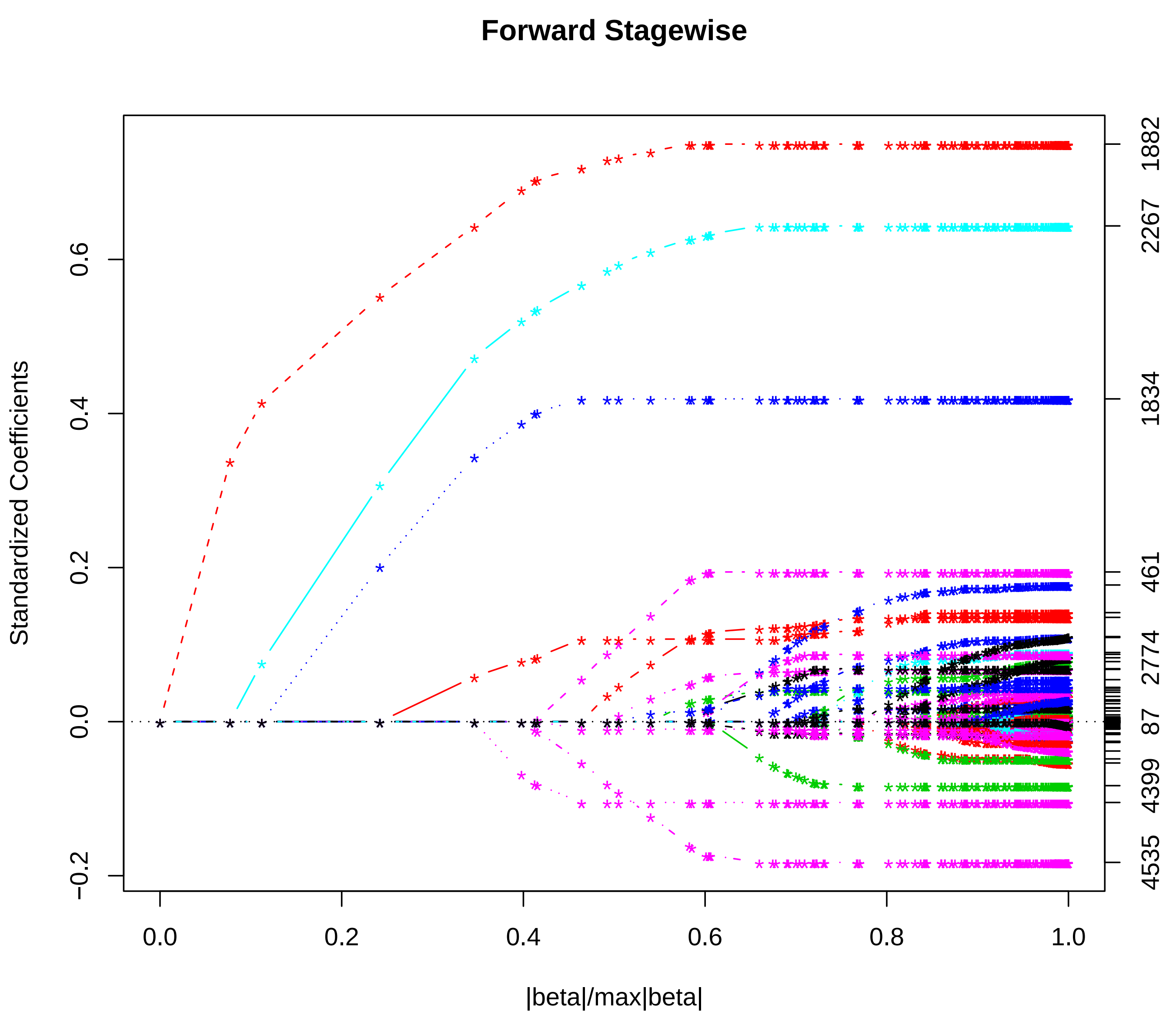

LASSO
0
1
3
4
5
8
12
15
20
26
31
38
50
65
Standardized Coefficients
0.8
0.6
0.4
0.2
0.0
−0.2
0.0
0.2
0.4
0.6
0.8
1.0
|beta|/max|beta|
2267
461
2945
6801
2968

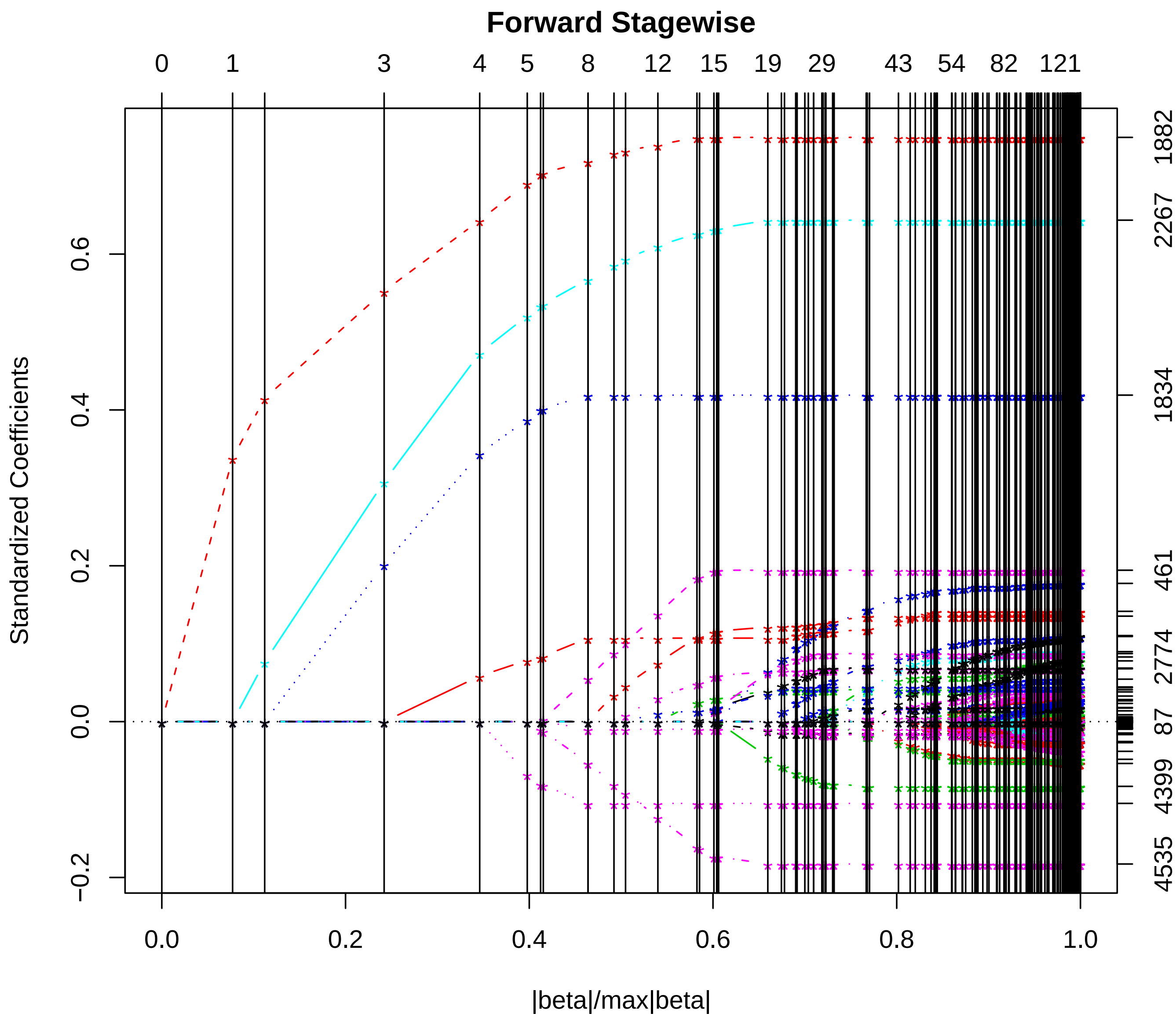

10−fold cross−validation for Leukemia Expression Data (Lasso)
cv
0.05
0.10
0.15
0.20
0.25
0.0
0.2
0.4
0.6
0.8
1.0
fraction

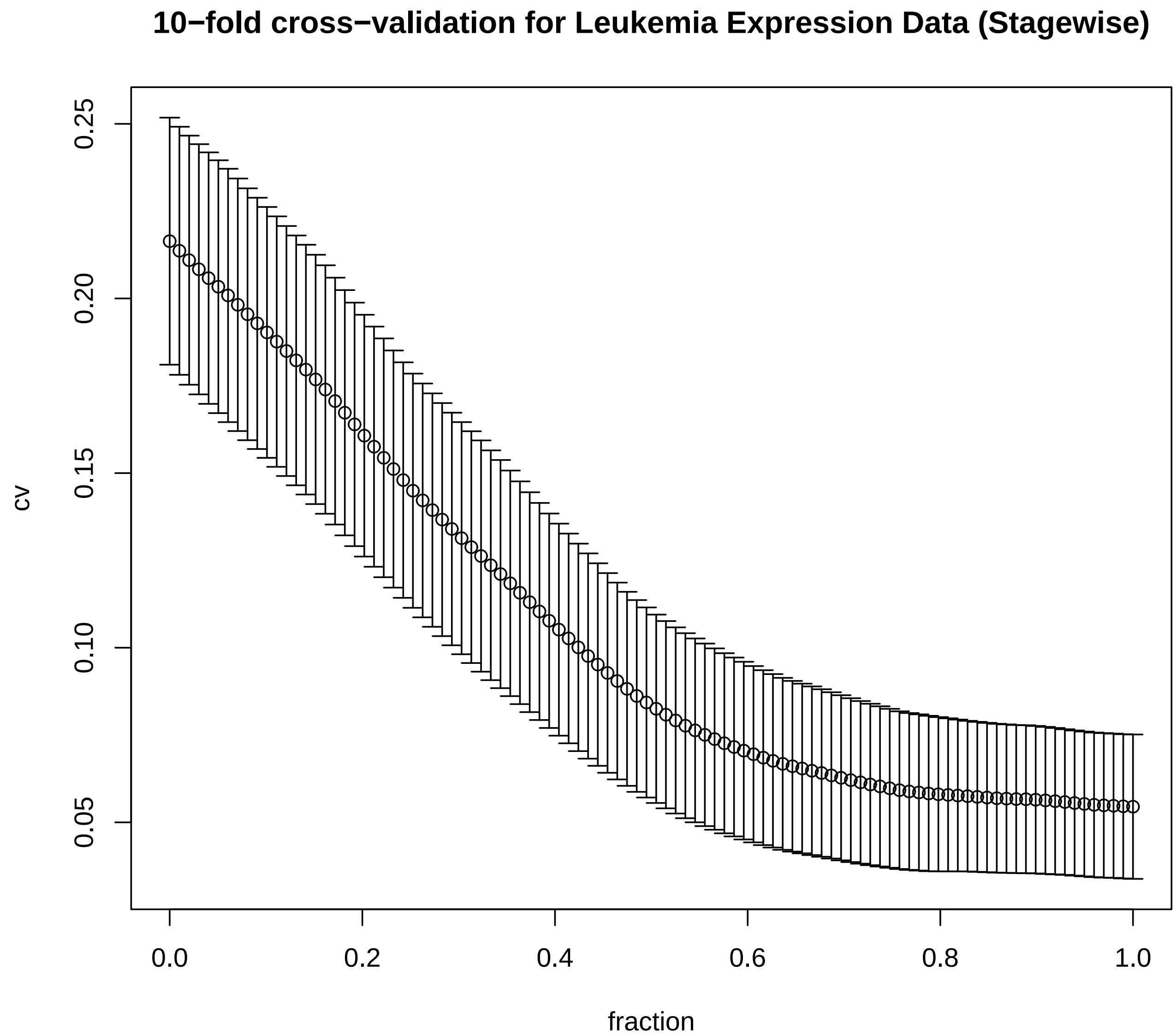

LAR
Standardized Coefficients
|beta|/max|beta|
0.0
0.2
0.4
0.6
0.8
1.0
−0.5
0.0
0.5
1.0
1882
2267
5039
2534
1241
4328
1817
6895


LAR
0
2
3
4
8
13
20
25
29
32
35
36
37
Standardized Coefficients
1.0
0.5
0.0
−0.5
0.0
0.2
0.4
0.6
0.8
1.0
|beta|/max|beta|
1882
2267
5039
2534
1241
4328
1817
6895


10−fold cross−validation for Leukemia Expression Data (LAR)
cv
0.05
0.10
0.15
0.20
0.25
0.0
0.2
0.4
0.6
0.8
1.0
fraction


Forward Stagewise
Standardized Coefficients
|beta|/max|beta|
0.0
0.2
0.4
0.6
0.8
1.0
−0.2
1882
2267
1834
461
2774
87
4399
4535


Forward Stagewise
0 1 3 4 5 8 12 15 19 29 43 54 82 121
Standardized Coefficients
−0.2 0.0 0.2 0.4 0.6
0.0 0.2 0.4 0.6 0.8 1.0
|beta|/max|beta|
1882
2267
1834
461
2774
87
4399
4535


10−fold cross−validation for Leukemia Expression Data (Stagewise)
cv
0.05
0.10
0.15
0.20
0.25
0.0
0.2
0.4
0.6
0.8
1.0
fraction

A new result

(Hastie, Taylor, Tibshirani, Walther)

Criterion for forward stagewise

Minimize $\sum_i \left(y_i - \sum_j x_{ij}\beta_j(t)\right)^2$

Subject to $\sum_j \int_0^t |\beta_j'(s)|ds \leq t$ (Bounded L_1 arc-length)

Future directions

- use ideas to make better versions of boosting (Friedman and Popescu)
- Application to support vector machines (Zhu, Rosset, Hastie, Tibshirani)
- "fused lasso":

$$\hat{\beta} = \text{argmin} \sum_i (y_i - \sum_j x_{ij}\beta_j)^2$$

$$\text{subject to} \sum_{j=1}^{p} |\beta_j| \le s_1$$

$$\text{and} \quad \sum_{j=2}^{p} |\beta_j - \beta_{j-1}| \le s_2$$

Has applications to microarrays and protein mass spec