Regularization, Ridge Regression

Machine Learning – CSEP546

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The regression problem

- **Instances:** $\langle \mathbf{x}_j, t_j \rangle$
- **Learn:** Mapping from x to t(**x**)
- **Hypothesis space:**
  - Given, basis functions
  - Find coeffs **w**={$w_1,\ldots,w_k$}

$$H = \{h_1, \ldots, h_K\}$$

$$\underbrace{t(\mathbf{x})}_{\text{data}} \approx \widehat{f}(\mathbf{x}) = \sum_i w_i h_i(\mathbf{x})$$

  - Why is this called linear regression???
    - model is linear in the parameters

- Precisely, minimize the residual squared error:

$$\mathbf{w}^* = \arg\min_{\mathbf{w}} \sum_{j=1}^{N} \left(t(\mathbf{x}_j) - \sum_i w_i h_i(\mathbf{x}_j) \right)^2$$

The regression problem in matrix notation

$$\mathbf{w}^* = \arg\min_{\mathbf{w}} \sum_{j=1}^{N} \left(t(\mathbf{x}_j) - \sum_{i=1}^{K} w_i h_i(\mathbf{x}_j) \right)^2$$

$$\mathbf{w}^* = \arg\min_{\mathbf{w}} \underbrace{(\mathbf{Hw} - \mathbf{t})^T (\mathbf{Hw} - \mathbf{t})}_{\text{residual error}}$$

$$\mathbf{H} = \begin{bmatrix} h_1 \dots h_K \\ \vdots \end{bmatrix} \quad \mathbf{w} = \begin{bmatrix} w_1 \\ \vdots \end{bmatrix} \quad \mathbf{t} = \begin{bmatrix} t \\ \vdots \end{bmatrix}$$

N data points; K basis functions; K basis func; N data points

weights; observations

Regression solution = simple matrix operations

$$\mathbf{w}^* = \arg\min_{\mathbf{w}} \underbrace{(\mathbf{Hw} - \mathbf{t})^T (\mathbf{Hw} - \mathbf{t})}_{\text{residual error}}$$

loss function

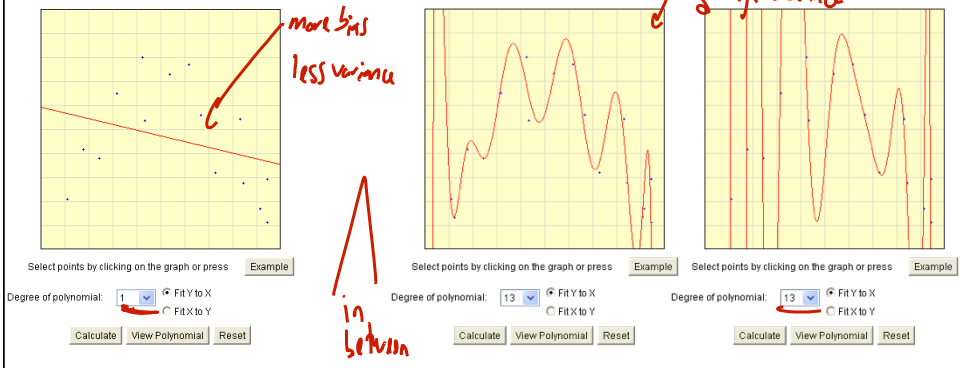
$$\text{solution: } \mathbf{w}^* = \underbrace{(\mathbf{H}^T\mathbf{H})^{-1}}_{\mathbf{A}^{-1}} \underbrace{\mathbf{H}^T\mathbf{t}}_{\mathbf{b}} = \mathbf{A}^{-1}\mathbf{b}$$

$$\text{where } \mathbf{A} = \mathbf{H}^T\mathbf{H} = \begin{bmatrix} \\ \\ \\ \end{bmatrix} \quad \mathbf{b} = \mathbf{H}^T\mathbf{t} = \begin{bmatrix} \\ \\ \\ \end{bmatrix}$$

k×k matrix for k basis functions; k×1 vector

Bias-Variance Tradeoff

- Choice of hypothesis class introduces learning bias
  - More complex class → less bias
  - More complex class → more variance

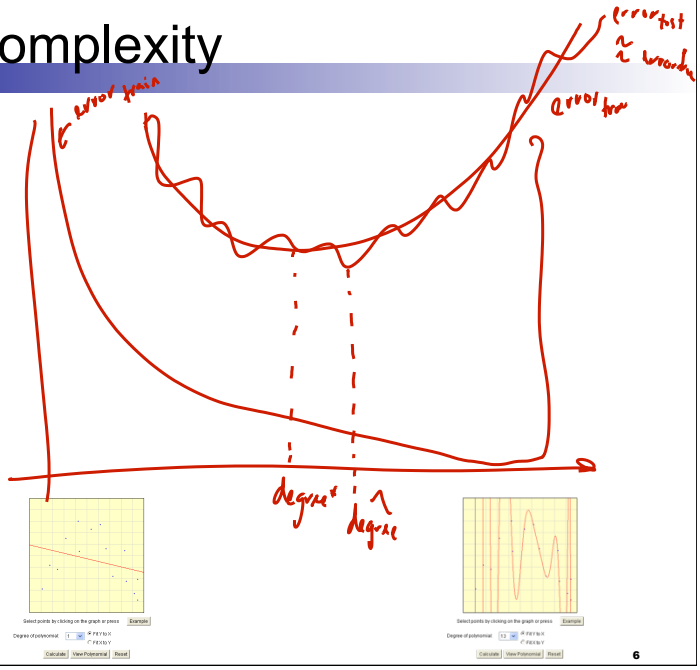


Test set error as a function of model complexity

$$error_{train}(\mathbf{w}) = \frac{1}{N_{train}} \sum_{j=1}^{N_{train}} \left(t(\mathbf{x}_j) - \sum_i w_i h_i(\mathbf{x}_j) \right)^2$$

$$error_{true}(\mathbf{w}) = \int_{\mathbf{x}} \left(t(\mathbf{x}) - \sum_i w_i h_i(\mathbf{x}) \right)^2 p(\mathbf{x}) d\mathbf{x}$$

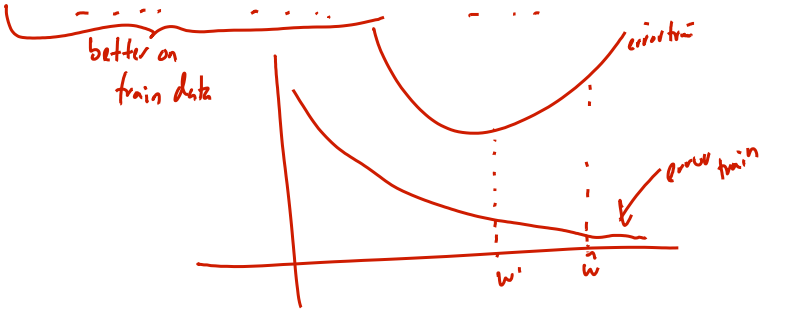
$$error_{test}(\mathbf{w}) = \frac{1}{N_{test}} \sum_{j=1}^{N_{test}} \left(t(\mathbf{x}_j) - \sum_i w_i h_i(\mathbf{x}_j) \right)^2$$



Overfitting

- **Overfitting:** a learning algorithm overfits the training data if it outputs a solution $\hat{\mathbf{w}}$ when there exists another solution $\mathbf{w}'$ such that:

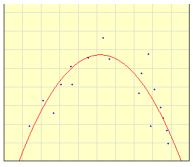
$$[error_{train}(\hat{\mathbf{w}}) < error_{train}(\mathbf{w}')] \wedge [error_{true}(\mathbf{w}') < error_{true}(\hat{\mathbf{w}})]$$



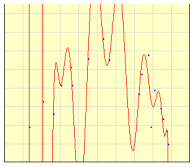
Regularization in Linear Regression

- Overfitting usually leads to very large parameter choices, e.g.:

-2.2 + 3.1 X – 0.30 X^2



-1.1 + 4,700,910.7 X – 8,585,638.4 X^2 + …



- ***Regularized*** or ***penalized*** regression aims to impose a "complexity" penalty by penalizing large weights
  - "Shrinkage" method

Quadratic Penalty (regularization)

- What we thought we wanted to minimize:
- But weights got too big, penalize large weights:

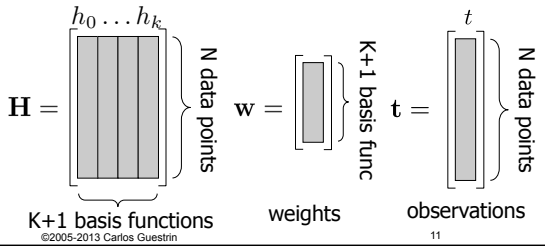
Ridge Regression

- Ameliorating issues with overfitting:
- New objective:

Ridge Regression in Matrix Notation

$$\hat{\mathbf{w}}_{ridge} = \arg\min_{w} \sum_{j=1}^{N} \left(t(x_j) - (w_0 + \sum_{i=1}^{k} w_i h_i(x_j)) \right)^2 + \lambda \sum_{i=1}^{k} w_i^2$$

$$= \arg\min_{\mathbf{w}} \underbrace{(\mathbf{Hw} - \mathbf{t})^T (\mathbf{Hw} - \mathbf{t})}_{\text{residual error}} + \lambda\ \mathbf{w}^T I_{0+k} \mathbf{w}$$



Minimizing the Ridge Regression Objective

$$\mathbf{w}^*_{\text{MLE}} = \underbrace{(\mathbf{H}^{\mathrm{T}}\mathbf{H})^{-1}}_{\mathbf{A}^{-1}} \underbrace{\mathbf{H}^{\mathrm{T}}\mathbf{t}}_{\mathbf{b}} = \mathbf{A}^{-1}\mathbf{b}$$

$$\hat{\mathbf{w}}_{ridge} = \arg\min_{w} \sum_{j=1}^{N} \left(t(x_j) - (w_0 + \sum_{i=1}^{k} w_i h_i(x_j)) \right)^2 + \lambda \sum_{i=1}^{k} w_i^2$$

$$= (H\mathbf{w} - \mathbf{t})^T (H\mathbf{w} - \mathbf{t}) + \lambda\ \mathbf{w}^T I_{0+k} \mathbf{w}$$

Shrinkage Properties

$$\hat{\mathbf{w}}_{ridge} = (H^T H + \lambda\ I_{0+k})^{-1} H^T \mathbf{t}$$

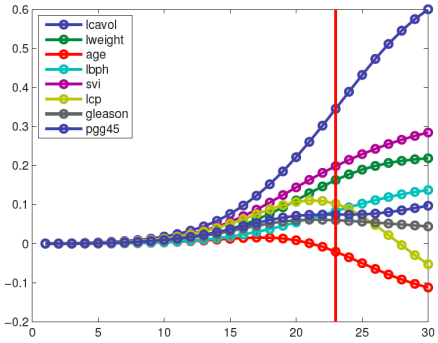
- If orthonormal features/basis: $H^T H = I$

Ridge Regression: Effect of Regularization

$$\hat{\mathbf{w}}_{ridge} = \arg\min_{w} \sum_{j=1}^{N} \left(t(x_j) - (w_0 + \sum_{i=1}^{k} w_i h_i(x_j)) \right)^2 + \lambda \sum_{i=1}^{k} w_i^2$$

- Solution is indexed by the regularization parameter λ
- Larger λ
- Smaller λ
- As λ → 0
- As λ →∞

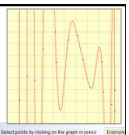
Ridge Coefficient Path



From
Kevin Murphy
textbook

- Typical approach: select λ using cross validation, more on this later in the quarter

Error as a function of regularization parameter for a fixed model complexity



$$error_{train}(\mathbf{w}) = \frac{1}{N_{train}} \sum_{j=1}^{N_{train}} \left(t(\mathbf{x}_j) - \sum_i w_i h_i(\mathbf{x}_j) \right)^2$$

$$error_{true}(\mathbf{w}) = \int_{\mathbf{x}} \left(t(\mathbf{x}) - \sum_i w_i h_i(\mathbf{x}) \right)^2 p(\mathbf{x}) d\mathbf{x}$$

λ=∞ ⟶ λ=0

What you need to know…

- Regularization
  - Penalizes for complex models
- Ridge regression
  - L_2 penalized least-squares regression
  - Regularization parameter trades off model complexity with training error

Cross-Validation

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Test set error as a function of model complexity

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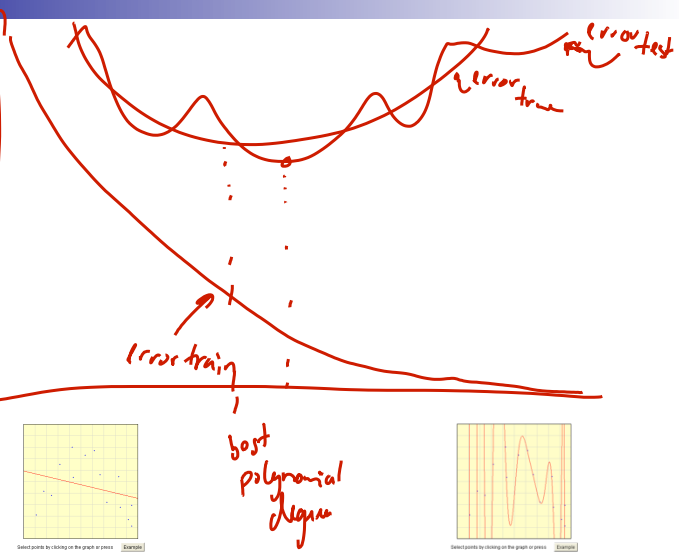


How… How… How???????

- How do we pick the regularization constant λ…
  - And all other constants in ML, 'cause one thing ML doesn't lack is constants to tune… ☹
- We could use the test data, but…

(LOO) Leave-one-out cross validation

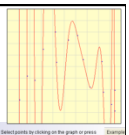
- Consider a **validation set with 1 example**:
  - *D* – training data
  - *D*\j – training data with *j*th data point moved to validation set
- **Learn classifier $h_{D\setminus j}$ with *D*\j dataset**
- **Estimate true error** as squared error on predicting t($\mathbf{x}_j$):
  - Unbiased estimate of $error_{true}(h_{D\setminus j})$!
  - Seems really bad estimator, but wait!
- **LOO cross validation**: Average over all data points *j*:
  - **For each data point you leave out, learn a new classifier $h_{D\setminus j}$**
  - **Estimate error** as:

$$error_{LOO} = \frac{1}{N}\sum_{j=1}^{N}\left(t(\mathbf{x}_j) - h_{\mathcal{D}\setminus j}(\mathbf{x}_j)\right)^2$$

LOO cross validation is (almost) unbiased estimate of true error of h_D!

- When computing **LOOCV error, we only use *N-1* data points**
  - So it's not estimate of true error of learning with *N* data points!
  - Usually pessimistic, though – learning with less data typically gives worse answer
- **LOO is almost unbiased**!
- **Great news!**
  - **Use LOO error for model selection!!!**
  - **E.g., picking λ**

Using LOO to Pick λ



$$error_{train}(\mathbf{w}) = \frac{1}{N_{train}} \sum_{j=1}^{N_{train}} \left(t(\mathbf{x}_j) - \sum_i w_i h_i(\mathbf{x}_j) \right)^2$$

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$$error_{LOO} = \frac{1}{N} \sum_{j=1}^{N} \left(t(\mathbf{x}_j) - h_{\mathcal{D}\setminus j}(\mathbf{x}_j) \right)^2$$

λ=∞ λ=0

Using LOO error for model selection

$$error_{train}(\mathbf{w}) = \frac{1}{N_{train}} \sum_{j=1}^{N_{train}} \left(t(\mathbf{x}_j) - \sum_i w_i h_i(\mathbf{x}_j) \right)^2$$

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$$error_{LOO} = \frac{1}{N} \sum_{j=1}^{N} \left(t(\mathbf{x}_j) - h_{\mathcal{D}\setminus j}(\mathbf{x}_j) \right)^2$$

Computational cost of LOO

- Suppose you have 100,000 data points
- You implemented a great version of your learning algorithm
  - Learns in only 1 second
- Computing LOO will take about 1 day!!!
  - If you have to do for each choice of basis functions, it will take fooooooreeeve'!!!
- Solution 1: Preferred, but not usually possible
  - Find a cool trick to compute LOO (e.g., see homework)

Solution 2 to complexity of computing LOO: (More typical) **Use *k*-fold cross validation**

- Randomly **divide training data into *k* equal parts**
  - $D_1,\ldots,D_k$
- For each *i*
  - **Learn classifier $h_{D\setminus Di}$ using data point not in D_i**
  - **Estimate error of $h_{D\setminus Di}$ on validation set D_i:**

$$error_{\mathcal{D}_i} = \frac{k}{N} \sum_{\mathbf{x}_j \in \mathcal{D}_i} \left(t(\mathbf{x}_j) - h_{\mathcal{D}\setminus\mathcal{D}_i}(\mathbf{x}_j)\right)^2$$

- ***k*-fold cross validation error is average** over data splits:

$$error_{k-fold} = \frac{1}{k} \sum_{i=1}^{k} error_{\mathcal{D}_i}$$

- *k*-fold cross validation properties:
  - **Much faster to compute** than LOO
  - **More (pessimistically) biased** – using much less data, only *m(k-1)/k*
  - Usually, **k = 10** ☺

ML Pipeline

What you need to know…

- Never ever ever ever ever ever ever ever ever ever ever ever ever ever ever ever ever ever ever ever ever ever ever ever ever ever ever ever ever ever train on the test data
- Use cross-validation to choose magic parameters such as λ
- Leave-one-out is the best you can do, but sometimes too slow
  - In that case, use k-fold cross-validation

Variable Selection LASSO: Sparse Regression

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Sparsity

- Vector **w** is sparse, if many entries are zero:
- Very useful for many tasks, e.g.,
  - **Efficiency**: If size(**w**) = 100B, each prediction is expensive:
    - If part of an online system, too slow
    - If **w** is sparse, prediction computation only depends on number of non-zeros
  - **Interpretability**: What are the relevant dimension to make a prediction?
    - E.g., what are the parts of the brain associated with particular words?
- But computationally intractable to perform "all subsets" regression

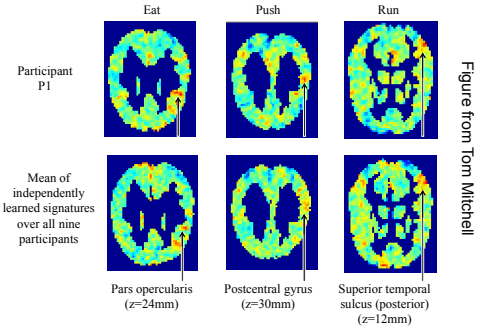


Figure from Tom Mitchell

Simple greedy model selection algorithm

- Pick a dictionary of features
  - e.g., polynomials for linear regression
- Greedy heuristic:
  - Start from empty (or simple) set of features $F_0 = \varnothing$
  - Run learning algorithm for current set of features F_t
    - Obtain h_t
  - Select **next best feature X_i^***
    - e.g., X_j that results in lowest training error learner when learning with $F_t + \{X_j\}$
  - $F_{t+1} \leftarrow F_t + \{X_i^*\}$
  - Recurse

Greedy model selection

- Applicable in many settings:
  - Linear regression: Selecting basis functions
  - Naïve Bayes: Selecting (independent) features $P(X_i|Y)$
  - Logistic regression: Selecting features (basis functions)
  - Decision trees: Selecting leaves to expand
- Only a heuristic!
  - But, sometimes you can prove something cool about it
    - e.g., [Krause & Guestrin '05]: Near-optimal in some settings that include Naïve Bayes
- There are many more elaborate methods out there

When do we stop???

- Greedy heuristic:
  - …
  - Select **next best feature X_i^***
    - e.g., X_j that results in lowest training error learner when learning with $F_t + \{X_j\}$
  - $F_{t+1} \leftarrow F_t + \{X_i^*\}$
  - Recurse

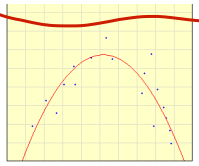
When do you stop???

- When training error is low enough?
- When test set error is low enough?
-

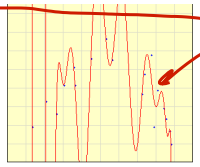
Regularization in Linear Regression

- Overfitting usually leads to very large parameter choices, e.g.:

$-2.2 + 3.1\,X - 0.30\,X^2$



$-1.1 + 4{,}700{,}910.7\,X - 8{,}585{,}638.4\,X^2 + \ldots$



penalty for large weights

overfitting

- ***Regularized*** or ***penalized*** regression aims to impose a "complexity" penalty by penalizing large weights
  - "Shrinkage" method

L_2 regularization → penalizes towards smoother functions

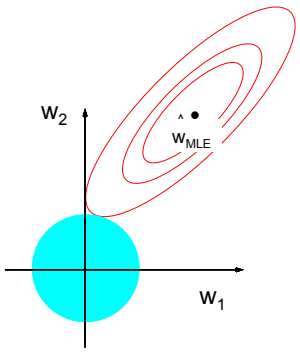
Variable Selection by Regularization

- Ridge regression: Penalizes large weights
- What if we want to perform "feature selection"?
  - E.g., Which regions of the brain are important for word prediction?
  - Can't simply choose features with largest coefficients in ridge solution
- Try new penalty: Penalize non-zero weights
  - Regularization penalty:
  - Leads to sparse solutions
  - Just like ridge regression, solution is indexed by a continuous param λ
  - This simple approach has changed statistics, machine learning & electrical engineering

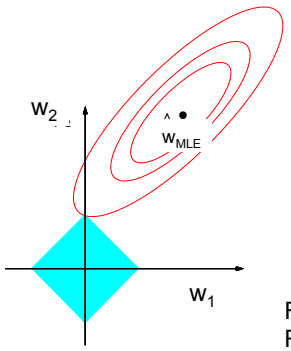
LASSO Regression

- **LASSO:** least absolute shrinkage and selection operator
- New objective:

Geometric Intuition for Sparsity



Ridge Regression



Lasso

From Rob Tibshirani slides

Optimizing the LASSO Objective

- LASSO solution:

$$\hat{\mathbf{w}}_{LASSO} = \arg\min_{w} \sum_{j=1}^{N} \left(t(x_j) - (w_0 + \sum_{i=1}^{k} w_i h_i(x_j)) \right)^2 + \lambda \sum_{i=1}^{k} |w_i|$$

Coordinate Descent

- Given a function F
  - Want to find minimum
- Often, hard to find minimum for all coordinates, but easy for one coordinate
- Coordinate descent:
- How do we pick next coordinate?
- Super useful approach for *many* problems
  - Converges to optimum in some cases, such as LASSO

How do we find the minimum over each coordinate?

- Key step in coordinate descent:
  - Find minimum over each coordinate

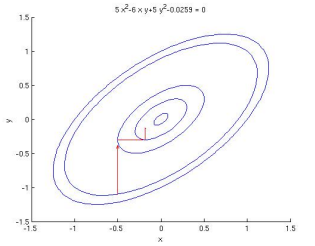


Illustration from Wikipedia

- Standard approach:

Optimizing LASSO Objective One Coordinate at a Time

$$\sum_{j=1}^{N}\left(t(x_j)-(w_0+\sum_{i=1}^{k}w_i h_i(x_j))\right)^2+\lambda\sum_{i=1}^{k}|w_i|$$

- Taking the derivative:
  - Residual sum of squares (RSS):

$$\frac{\partial}{\partial w_\ell}RSS(\mathbf{w})=-2\sum_{j=1}^{N}h_\ell(x_j)\left(t(x_j)-(w_0+\sum_{i=1}^{k}w_i h_i(x_j))\right)$$

  - Penalty term:

Coordinate Descent for LASSO (aka Shooting Algorithm)

- Repeat until convergence
  - Pick a coordinate *l* at (random or sequentially)
    - Set:

$$\hat{w}_\ell=\begin{cases}(c_\ell+\lambda)/a_\ell & c_\ell<-\lambda\\ 0 & c_\ell\in[-\lambda,\lambda]\\ (c_\ell-\lambda)/a_\ell & c_\ell>\lambda\end{cases}$$

    - Where:

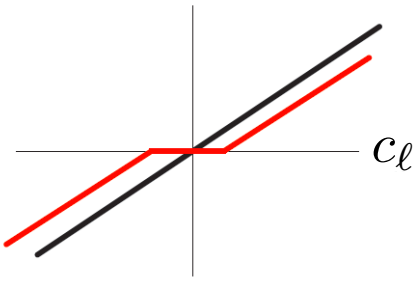
$$a_\ell=2\sum_{j=1}^{N}(h_\ell(\mathbf{x}_j))^2$$

$$c_\ell=2\sum_{j=1}^{N}h_\ell(\mathbf{x}_j)\left(t(\mathbf{x}_j)-(w_0+\sum_{i\neq\ell}w_i h_i(\mathbf{x}_j))\right)$$

  - For convergence rates, see Shalev-Shwartz and Tewari 2009
- Other common technique = LARS
  - Least angle regression and shrinkage, Efron et al. 2004

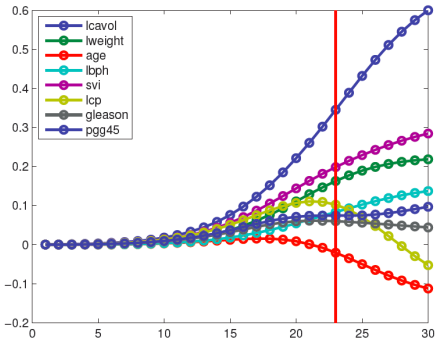
Soft Thresholding

$$\hat{w}_\ell = \begin{cases} (c_\ell + \lambda)/a_\ell & c_\ell < -\lambda \\ 0 & c_\ell \in [-\lambda, \lambda] \\ (c_\ell - \lambda)/a_\ell & c_\ell > \lambda \end{cases}$$



From
Kevin Murphy
textbook

Recall: *Ridge Coefficient Path*



From
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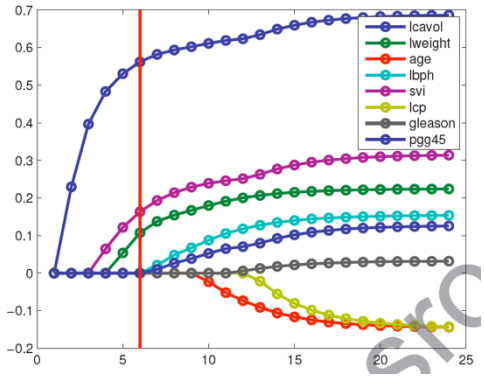
textbook

- Typical approach: select λ using cross validation

Now: *LASSO Coefficient Path*



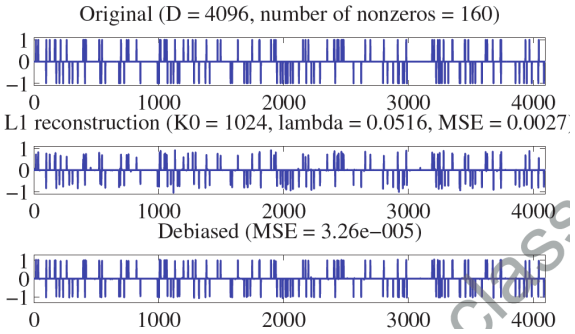
From Kevin Murphy textbook

LASSO Example

Term	Least Squares	Ridge	Lasso
Intercept	2.465	2.452	2.468
lcavol	0.680	0.420	0.533
lweight	0.263	0.238	0.169
age	−0.141	−0.046	
lbph	0.210	0.162	0.002
svi	0.305	0.227	0.094
lcp	−0.288	0.000	
gleason	−0.021	0.040	
pgg45	0.267	0.133	

From Rob Tibshirani slides

Debiasing



From Kevin Murphy textbook

What you need to know

- Variable Selection: find a sparse solution to learning problem
- L_1 regularization is one way to do variable selection
  - Applies beyond regressions
  - Hundreds of other approaches out there
- LASSO objective non-differentiable, but convex ➔ Use subgradient
- No closed-form solution for minimization ➔ Use coordinate descent
- Shooting algorithm is very simple approach for solving LASSO