Linear Regression contd…

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Machine Learning 10-315
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Linear Regression

$$\widehat{f}_n^L = \arg\min_{f \in \mathcal{F}_L} \frac{1}{n} \sum_{i=1}^{n} (f(X_i) - Y_i)^2 \qquad f(X_i) = X_i \beta$$

⇩

$$\widehat{\beta} = \arg\min_{\beta} \frac{1}{n} \sum_{i=1}^{n} (X_i \beta - Y_i)^2 \qquad \widehat{f}_n^L(X) = X\widehat{\beta}$$

$$= \arg\min_{\beta} \frac{1}{n} (\mathbf{A}\beta - \mathbf{Y})^T (\mathbf{A}\beta - \mathbf{Y})$$

$$\mathbf{A} = \begin{bmatrix} X_1 \\ \vdots \\ X_n \end{bmatrix} = \begin{bmatrix} X_1^{(1)} & \dots & X_1^{(p)} \\ \vdots & \ddots & \vdots \\ X_n^{(1)} & \dots & X_n^{(p)} \end{bmatrix} \quad \mathbf{Y} = \begin{bmatrix} \mathbf{Y}_1 \\ \vdots \\ \mathbf{Y}_n \end{bmatrix}$$

Linear regression solution satisfies Normal Equations

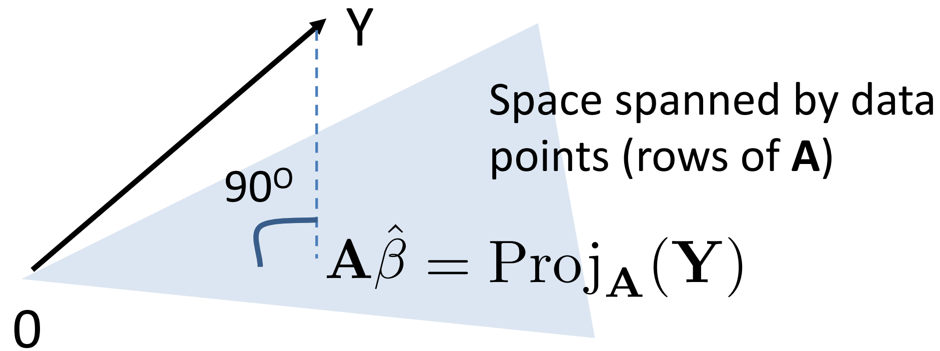
$$(\mathbf{A}^T\mathbf{A})\widehat{\beta} = \mathbf{A}^T\mathbf{Y}$$

p x p   p x1   p x1

If $(\mathbf{A}^T\mathbf{A})$ is invertible,

$$\widehat{\beta} = (\mathbf{A}^T\mathbf{A})^{-1}\mathbf{A}^T\mathbf{Y} \qquad \widehat{f}_n^L(X) = X\widehat{\beta}$$

Predicted labels for training points $\mathbf{A}\hat{\beta} = \mathrm{Proj}_{\mathbf{A}}(\mathbf{Y})$



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Later: When is $(\mathbf{A}^T\mathbf{A})$ invertible ?

Recall: Full rank matrices are invertible. What is rank of $(\mathbf{A}^T\mathbf{A})$?

Now: What if $(\mathbf{A}^T\mathbf{A})$ is invertible but expensive (p very large)?

Gradient Descent

Even when $(\mathbf{A}^T\mathbf{A})$ is invertible, might be computationally expensive if **A** is huge.

$$\widehat{\beta} = \arg\min_{\beta} \frac{1}{n}(\mathbf{A}\beta - \mathbf{Y})^T(\mathbf{A}\beta - \mathbf{Y}) = \arg\min_{\beta} J(\beta)$$

Since J(β) is convex, move along negative of gradient

Initialize: β^0

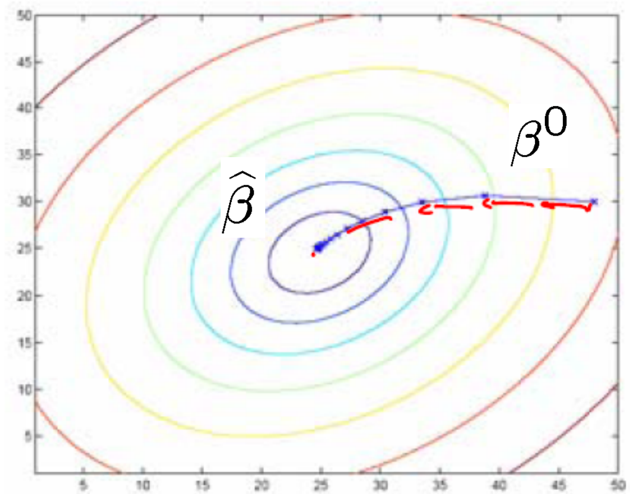
step size

Update:

$$\beta^{t+1} = \beta^t - \frac{\alpha}{2}\frac{\partial J(\beta)}{\partial \beta}\bigg|_t$$

$$= \beta^t - \alpha\, \mathbf{A}^T\underbrace{(\mathbf{A}\beta^t - Y)}$$

0 if $\widehat{\beta} = \beta^t$



Stop: when some criterion met e.g. fixed # iterations, or $\frac{\partial J(\beta)}{\partial \beta}\Big|_{\beta^t} < \varepsilon$.

Linear regression solution satisfies Normal Equations

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p x p   p x1   p x1

When is $(\mathbf{A}^T\mathbf{A})$ invertible ?
Recall: Full rank matrices are invertible. What is rank of $(\mathbf{A}^T\mathbf{A})$?

Null space argument

Linear regression solution satisfies Normal Equations

$$(\mathbf{A}^T\mathbf{A})\widehat{\beta} = \mathbf{A}^T\mathbf{Y}$$

p x p   p x1   p x1

When is $(\mathbf{A}^T\mathbf{A})$ invertible ?
Recall: Full rank matrices are invertible. What is rank of $(\mathbf{A}^T\mathbf{A})$?

Rank$(\mathbf{A}^T\mathbf{A})$ = number of non-zero eigenvalues of $(\mathbf{A}^T\mathbf{A})$= number of non-zero singular values of **A** <= min(n,p) since **A** is n x p

So, rank$(\mathbf{A}^T\mathbf{A})$, r <= min(n,p)   not invertible if r < p (e.g. n < p i.e. high-dimensional setting)

Linear regression solution satisfies Normal Equations

$$(\mathbf{A}^T\mathbf{A})\widehat{\beta} = \mathbf{A}^T\mathbf{Y}$$

p x p   p x1   p x1

When is $(\mathbf{A}^T\mathbf{A})$ invertible ?
Recall: Full rank matrices are invertible. What is rank of $(\mathbf{A}^T\mathbf{A})$?

If $\mathbf{A} = \mathbf{U}\mathbf{S}\mathbf{V}^\top$, then normal equations $(\mathbf{S}\mathbf{V}^\top)\hat{\beta} = (\mathbf{U}^\top\mathbf{Y})$

S - r x r   r x p   p x 1   r x 1

r equations in p unknowns. Under-determined if r < p, hence no unique solution.

Regularized Linear Regression

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Regularized Least Squares

What if $(\mathbf{A}^T\mathbf{A})$ is not invertible ?

r equations , p unknowns – underdetermined system of linear equations
many feasible solutions

Need to constrain solution further

e.g. bias solution to "small" values of β (small changes in input don't translate to large changes in output)

$$\widehat{\beta}_{\text{MAP}} = \arg\min_{\beta} \sum_{i=1}^{n} (Y_i - X_i\beta)^2 + \lambda\|\beta\|_2^2$$

Ridge Regression
(l2 penalty)

$$= \arg\min_{\beta} \quad (\mathbf{A}\beta - \mathbf{Y})^T(\mathbf{A}\beta - \mathbf{Y}) + \lambda\|\beta\|_2^2$$

$$\lambda \geq 0$$

$$\hat{\beta}_{\text{MAP}} = (\mathbf{A}^\top\mathbf{A} + \lambda\mathbf{I})^{-1}\mathbf{A}^\top\mathbf{Y}$$

Regularized Least Squares

$$\widehat{\beta}_{\text{MAP}} = \arg\min_{\beta} \sum_{i=1}^{n} (Y_i - X_i\beta)^2 + \lambda\|\beta\|_2^2$$

$$= \arg\min_{\beta} \frac{1}{n}(\mathbf{A}\beta - \mathbf{Y})^T(\mathbf{A}\beta - \mathbf{Y}) + \lambda\|\beta\|_2^2$$

Ridge Regression
(l2 penalty)

$\lambda \geq 0$

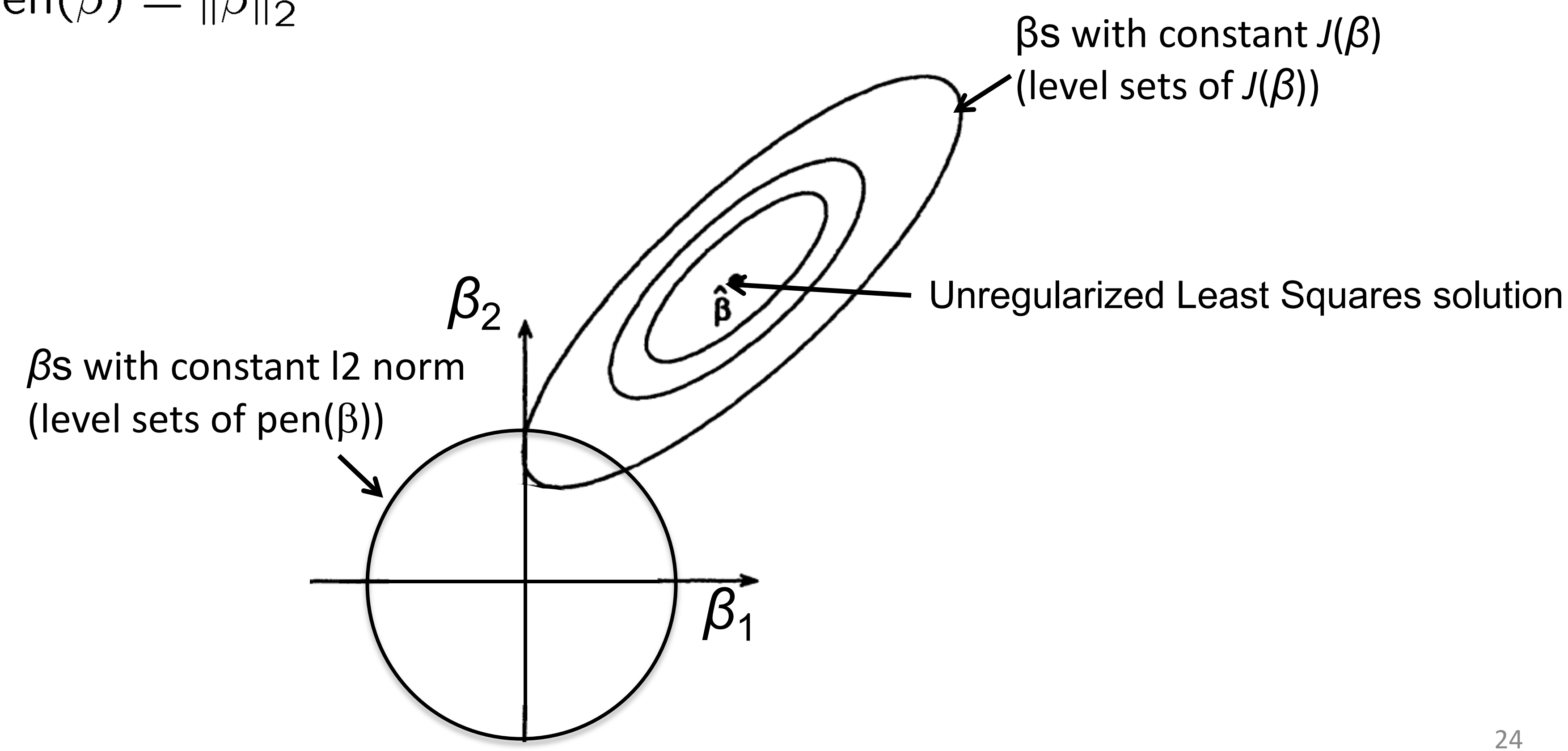
Is $(\mathbf{A}^\top\mathbf{A} + \lambda\mathbf{I})$ invertible ?

Understanding regularized Least Squares

$$\min_\beta (\mathbf{A}\beta - \mathbf{Y})^T(\mathbf{A}\beta - \mathbf{Y}) + \lambda \text{pen}(\beta) = \min_\beta J(\beta) + \lambda \text{pen}(\beta)$$

Ridge Regression:

$$\text{pen}(\beta) = \|\beta\|_2^2$$



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$$\widehat{\beta}_{\text{MAP}} = \arg\min_{\beta} \sum_{i=1}^{n} (Y_i - X_i\beta)^2 + \lambda\|\beta\|_1$$

$\lambda \geq 0$

Lasso
(l1 penalty)

Many β can be zero – many inputs are irrelevant to prediction in high-dimensional settings (typically intercept term not penalized)

Regularized Least Squares

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Ridge Regression
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Lasso
(l1 penalty)

$\lambda \geq 0$

No closed form solution, but can optimize using sub-gradient descent (packages available)

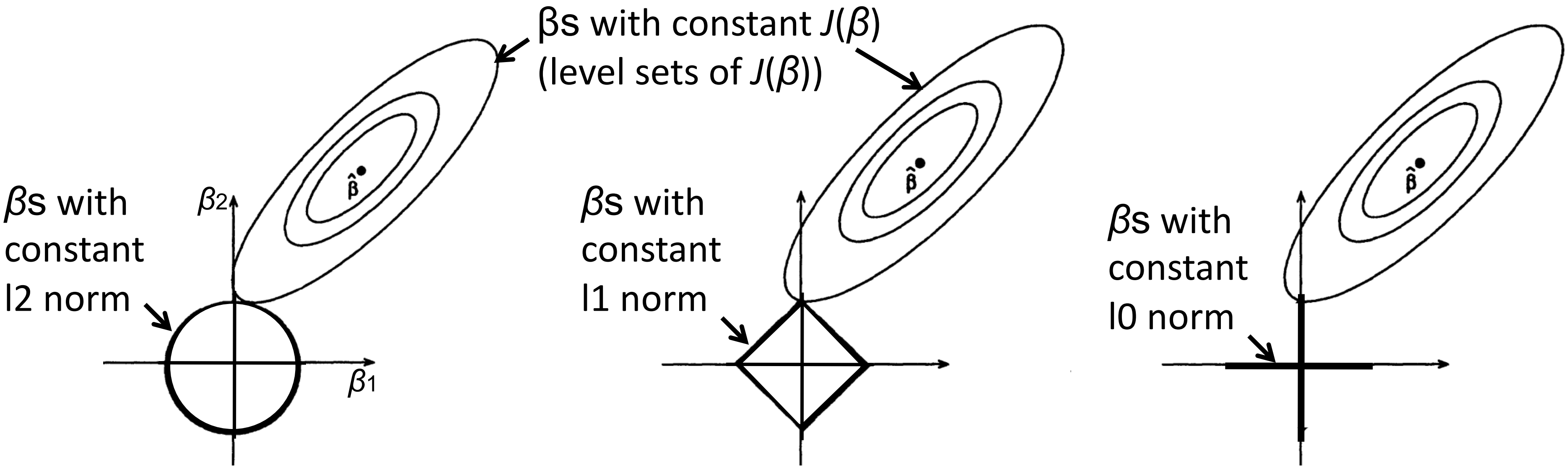
Ridge Regression vs Lasso

$$\min_{\beta}(\mathbf{A}\beta - \mathbf{Y})^T(\mathbf{A}\beta - \mathbf{Y}) + \lambda \text{pen}(\beta) = \min_{\beta} J(\beta) + \lambda \text{pen}(\beta)$$

Ridge Regression:
$\text{pen}(\beta) = \|\beta\|_2^2$

Lasso:
$\text{pen}(\beta) = \|\beta\|_1$

Ideally l0 penalty, but optimization becomes non-convex



Lasso (l1 penalty) results in sparse solutions – vector with more zero coordinates
Good for high-dimensional problems – don't have to store all coordinates, interpretable solution!

Matlab example

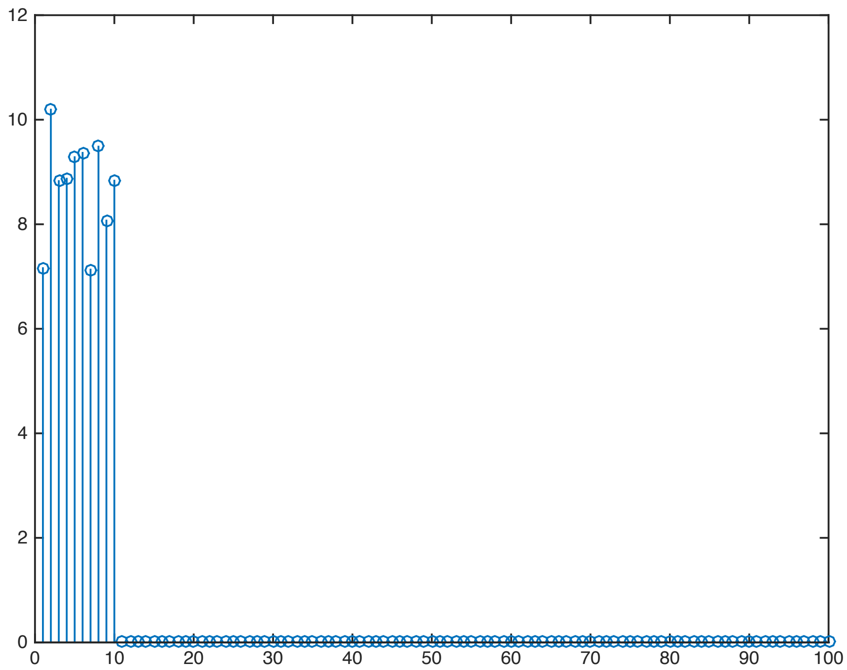
```
clear all
close all

n = 80;     % datapoints
p = 100;   % features
k = 10;      % non-zero features

rng(20);
X = randn(n,p);
weights = zeros(p,1);
weights(1:k) = randn(k,1)+10;
noise = randn(n,1) * 0.5;
Y = X*weights +  noise;

Xtest = randn(n,p);
noise = randn(n,1) * 0.5;
Ytest = Xtest*weights + noise;

lassoWeights = lasso(X,Y,'Lambda',1,
'Alpha', 1.0);
Ylasso = Xtest*lassoWeights;
norm(Ytest-Ylasso)

ridgeWeights = lasso(X,Y,'Lambda',1,
'Alpha', 0.0001);
Yridge = Xtest*ridgeWeights;
norm(Ytest-Yridge)

stem(lassoWeights)
pause
stem(ridgeWeights)
```

Matlab example

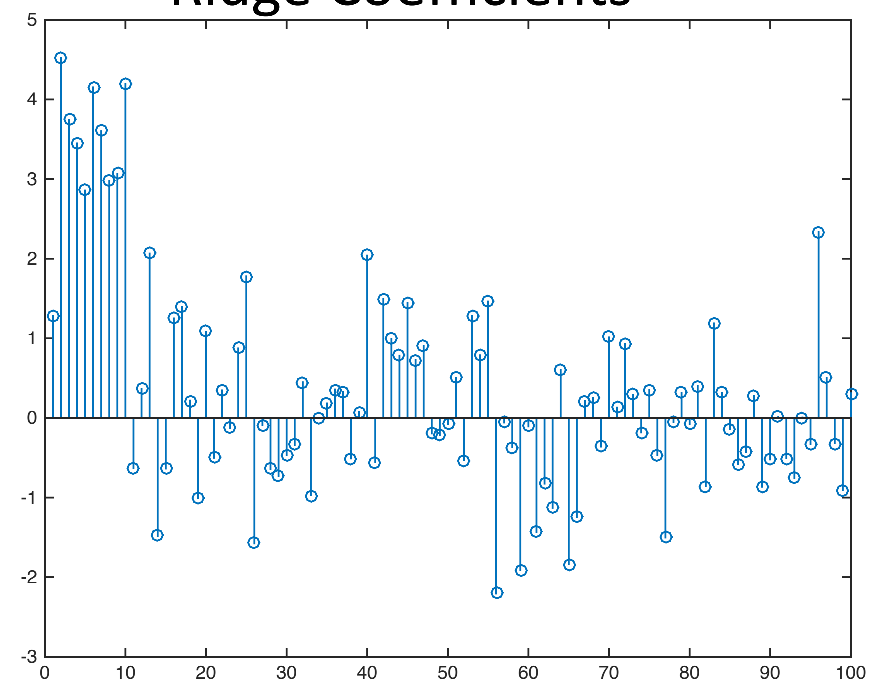
Test MSE = 33.7997

Test MSE = 185.9948

Lasso Coefficients

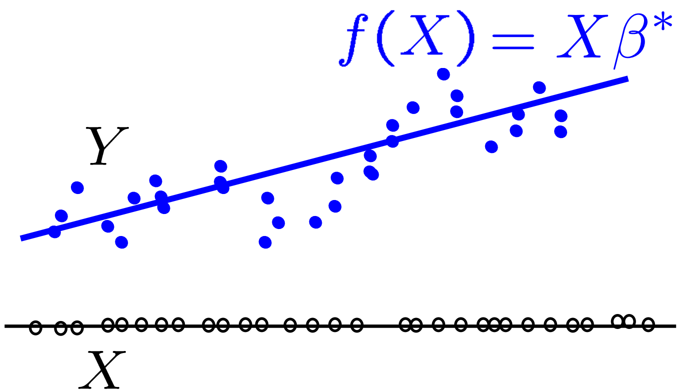


Ridge Coefficients



Least Squares and M(C)LE

Intuition: Signal plus (zero-mean) Noise model



$$Y = f^*(X) + \epsilon = X\beta^* + \epsilon$$

$$\epsilon \sim \mathcal{N}(0, \sigma^2 \mathbf{I}) \quad Y \sim \mathcal{N}(X\beta^*, \sigma^2 \mathbf{I})$$

$$\widehat{\beta}_{\text{MLE}} = \arg\max_{\beta} \underbrace{\log p(\{Y_i\}_{i=1}^n | \beta, \sigma^2, \{X_i\}_{i=1}^n)}_{\text{Conditional log likelihood}}$$

- Breakout

$$= \arg\min_{\beta} \sum_{i=1}^{n} (X_i\beta - Y_i)^2 = \widehat{\beta}$$

Groups 1-10: Jamboard_1_10
Groups 11-20: Jamboard_11_20

Least Square Estimate is same as Maximum Conditional Likelihood Estimate under a Gaussian model !

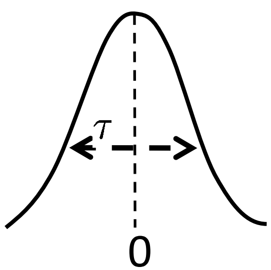
Regularized Least Squares and M(C)AP

What if $(\mathbf{A}^T\mathbf{A})$ is not invertible ?

$$\widehat{\beta}_{\text{MAP}} = \arg\max_{\beta} \underbrace{\log p(\{Y_i\}_{i=1}^n | \beta, \sigma^2, \{X_i\}_{i=}^n}_{\text{Conditional log likelihood}} + \underbrace{\log p(\beta)}_{\text{log prior}}$$

I) Gaussian Prior

$$\beta \sim \mathcal{N}(0, \tau^2\mathbf{I}) \qquad p(\beta) \propto e^{-\beta^T\beta/2\tau^2}$$



$$\widehat{\beta}_{\text{MAP}} = \arg\min_{\beta} \sum_{i=1}^{n} (Y_i - X_i\beta)^2 + \lambda \|\beta\|_2^2$$

$\lambda \rightarrow$ constant(σ^2, τ^2)

Ridge Regression

$$\widehat{\beta}_{\text{MAP}} = (\boldsymbol{A}^\top \boldsymbol{A} + \lambda \boldsymbol{I})^{-1} \boldsymbol{A}^\top \boldsymbol{Y}$$

Regularized Least Squares and M(C)AP

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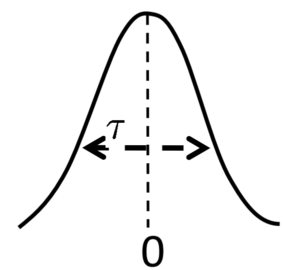

$$\widehat{\beta}_{\text{MAP}} = \arg\min_{\beta} \sum_{i=1}^{n} (Y_i - X_i\beta)^2 + \lambda\|\beta\|_2^2$$

Ridge Regression

$\lambda \downarrow$ constant(σ^2, τ^2)

Prior belief that β is Gaussian with zero-mean biases solution to “small” β

Regularized Least Squares and M(C)AP

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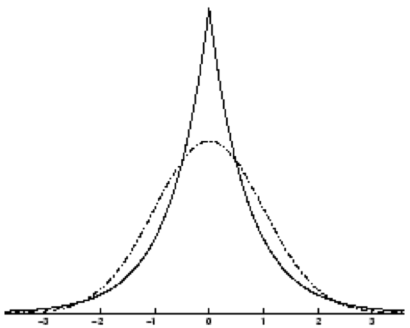
II) Laplace Prior

$\beta_i \overset{iid}{\sim} \text{Laplace}(0, t)$ $\qquad p(\beta_i) \propto e^{-|\beta_i|/t}$



$$\widehat{\beta}_{\text{MAP}} = \arg\min_{\beta} \sum_{i=1}^{n} (Y_i - X_i\beta)^2 + \lambda \|\beta\|_1$$

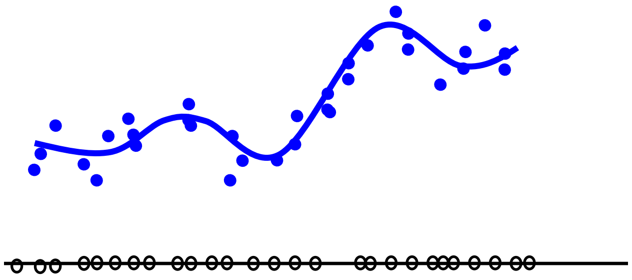
Lasso

$\lambda \downarrow$ constant(σ^2, t)

Prior belief that β is Laplace with zero-mean biases solution to "sparse" β

Beyond Linear Regression

Polynomial regression
Regression with nonlinear features



Kernelized Ridge Regression (Later)

Local Kernel Regression (Later)

Polynomial Regression

degree m

Univariate (1-dim) case: $f(X) = \beta_0 + \beta_1 X + \beta_2 X^2 + \cdots + \beta_m X^m = \mathbf{X}\beta$

where $\mathbf{X} = [1 \;\; X \;\; X^2 \ldots X^m], \beta = [\beta_1 \ldots \beta_m]^T$

$$\widehat{\beta} = (\mathbf{A}^T\mathbf{A})^{-1}\mathbf{A}^T\mathbf{Y} \text{ or } (\mathbf{A}^T\mathbf{A} + \lambda\mathbf{I})^{-1}\mathbf{A}^T\mathbf{Y} \qquad \widehat{f}_n(X) = \mathbf{X}\widehat{\beta}$$

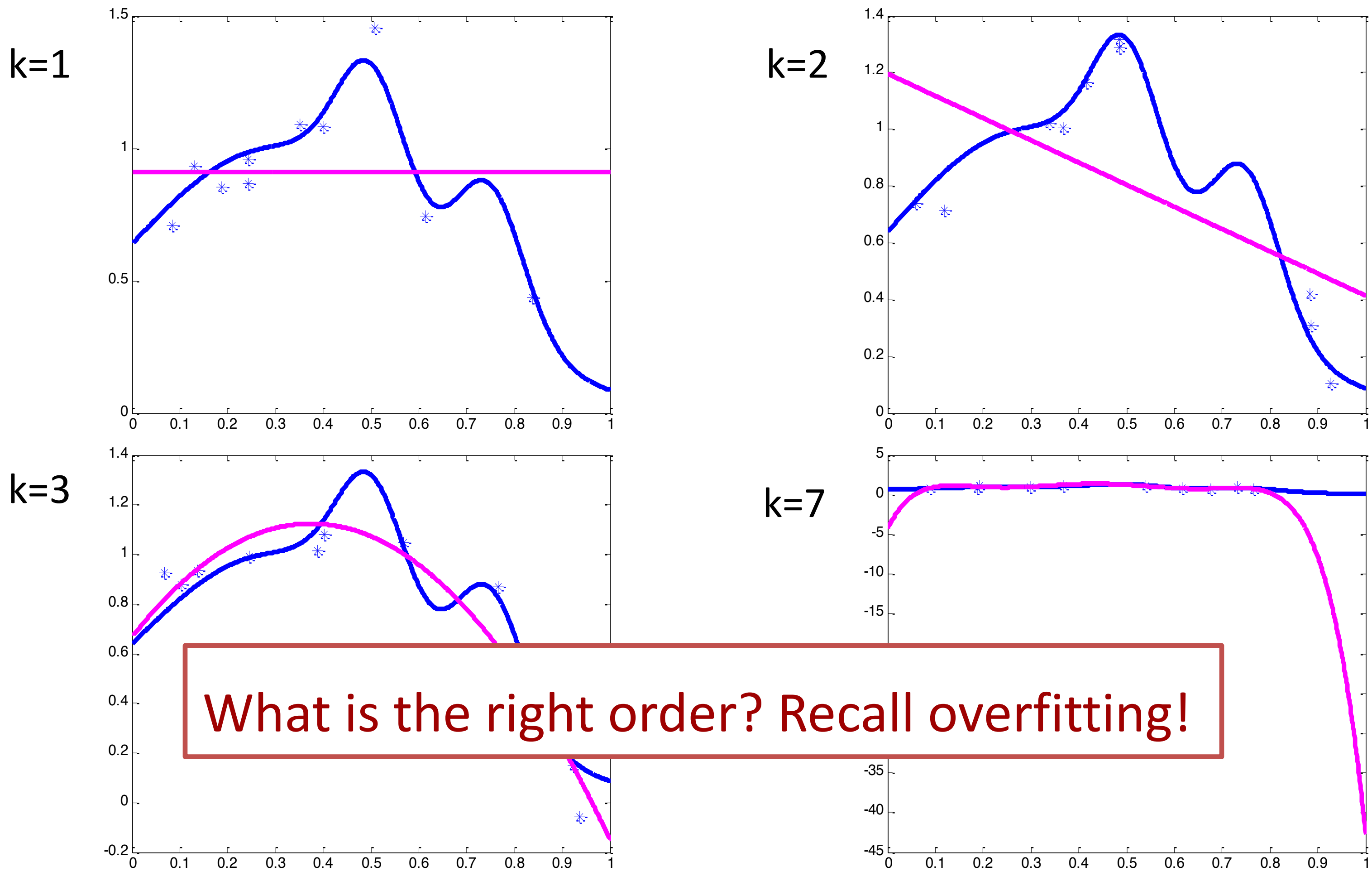
where $\mathbf{A} = \begin{bmatrix} 1 & X_1 & X_1^2 & \ldots & X_1^m \\ \vdots & & & \ddots & \vdots \\ 1 & X_n & X_n^2 & \ldots & X_n^m \end{bmatrix}$

Multivariate (p-dim) case:

$$\begin{aligned} f(X) &= \beta_0 + \beta_1 X^{(1)} + \beta_2 X^{(2)} + \cdots + \beta_p X^{(p)} \\ &+ \sum_{i=1}^{p}\sum_{j=1}^{p}\beta_{ij}X^{(i)}X^{(j)} + \sum_{i=1}^{p}\sum_{j=1}^{p}\sum_{k=1}^{p}X^{(i)}X^{(j)}X^{(k)} \\ &+ \ldots \text{terms up to degree m} \end{aligned}$$

Polynomial Regression

Polynomial of order k, equivalently of degree up to k-1



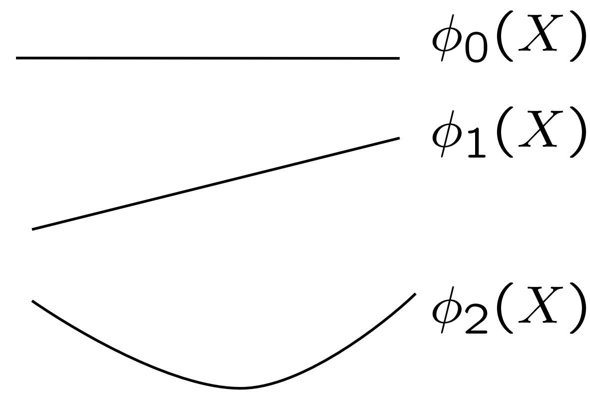
What is the right order? Recall overfitting!

Regression with nonlinear features

$$f(X) = \sum_{j=0}^{m} \beta_j X^j = \sum_{j=0}^{m} \beta_j \phi_j(X)$$

Weight of each feature

Nonlinear features



In general, use any nonlinear features

e.g. e^X, log X, 1/X, sin(X), …

$$\widehat{\beta} = (\mathbf{A}^T\mathbf{A})^{-1}\mathbf{A}^T\mathbf{Y}$$

or

$$(\mathbf{A}^T\mathbf{A} + \lambda\mathbf{I})^{-1}\mathbf{A}^T\mathbf{Y}$$

$$\mathbf{A} = \begin{bmatrix} \phi_0(X_1) & \phi_1(X_1) & \dots & \phi_m(X_1) \\ \vdots & & \ddots & \vdots \\ \phi_0(X_n) & \phi_1(X_n) & \dots & \phi_m(X_n) \end{bmatrix}$$

$$\widehat{f}_n(X) = \mathbf{X}\widehat{\beta}$$

$$\mathbf{X} = [\phi_0(X)\ \phi_1(X)\ \dots\ \phi_m(X)]$$