

# Regularized Linear Regression

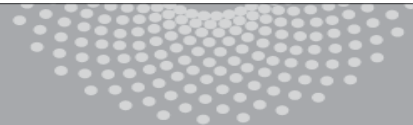
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Machine Learning 10-701

Mar 22, 2023

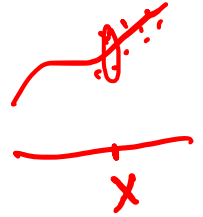


**MACHINE LEARNING** DEPARTMENT



**Carnegie Mellon.**  
School of Computer Science

# Mean square error regression



Optimal predictor:

$$f^* = \arg \min_f \mathbb{E}[(f(X) - Y)^2]$$

$$= E[Y|X]$$

$P(X, Y)$   
known

Empirical Minimizer:

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

Class of predictors

$\{X_i, Y_i\}_{i=1}^n \stackrel{iid}{\sim} P(X, Y)$

- $\mathcal{F}$  - Class of Linear functions ✓
- Class of Polynomial functions
- Class of nonlinear functions

$$f(x) = X\beta = [x^{(1)} \dots x^{(p)}] \begin{bmatrix} \beta_1 \\ \vdots \\ \beta_p \end{bmatrix}$$

# Least Square solution satisfies Normal Equations

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

$p \times p$     $p \times 1$     $p \times 1$

$$Y = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix}_{n \times 1}$$
$$A = \begin{bmatrix} X_1^{(1)} & \dots & X_1^{(p)} \\ \vdots & & \vdots \\ X_n^{(1)} & \dots & X_n^{(p)} \end{bmatrix}_{n \times p}$$

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

1) If dimension  $p$  not too large, analytical solution:

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

2) If dimension  $p$  is large, computing inverse is expensive  $O(p^3)$

Gradient descent since objective is convex ( $\mathbf{A}^T \mathbf{A} \succeq 0$ )

$$\begin{aligned} \beta^{t+1} &= \beta^t - \frac{\alpha}{2} \frac{\partial J(\beta)}{\partial \beta} \Big|_t \\ &= \beta^t - \alpha \mathbf{A}^T (\mathbf{A} \beta^t - Y) \end{aligned}$$

# Linear regression solution satisfies Normal Equations

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

$p \times p$     $p \times 1$     $p \times 1$

$$\mathbf{A} = \begin{bmatrix} X_1^{(1)} & \dots & X_p^{(1)} \\ \vdots & & \vdots \\ X_1^{(n)} & \dots & X_p^{(n)} \end{bmatrix}_{n \times p}$$

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

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

$$\mathbf{A}_{n \times p} = \mathbf{U} \mathbf{S} \mathbf{V}^T$$

$n \times r$     $r \times r$     $r \times p$

$$\text{rank}(\mathbf{A}) = r \leq p \quad r \leq \min(n, p)$$

$$\mathbf{S} = \begin{bmatrix} s_1 & & 0 \\ & \ddots & \\ 0 & & s_r \end{bmatrix}$$

$$\mathbf{A}^T \mathbf{A} = (\mathbf{U} \mathbf{S} \mathbf{V}^T)^T \mathbf{U} \mathbf{S} \mathbf{V}$$

$$= \mathbf{V} \mathbf{S} \mathbf{U}^T \mathbf{U} \mathbf{S} \mathbf{V} = \mathbf{V} \mathbf{S}^2 \mathbf{V}^T$$

$$\Rightarrow \text{eig}(\mathbf{A}^T \mathbf{A}) = s_1^2 \dots s_r^2$$

no. of datapoints  
 $\uparrow$   
 if  $n < p$  → no. of features  
 then  $\mathbf{A}^T \mathbf{A}$  is not invertible

# Linear regression solution satisfies Normal Equations

$$\underbrace{(\mathbf{A}^T \mathbf{A})}_{p \times p} \hat{\beta} = \underbrace{\mathbf{A}^T \mathbf{Y}}_{p \times 1} \leftarrow \begin{array}{l} p \text{ equations in} \\ p \text{ unknowns } (\hat{\beta}) \end{array}$$

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

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

If  $\mathbf{A} = \mathbf{U} \mathbf{S} \mathbf{V}^T$ , then  
S -  $r \times r$

normal equations  $\underbrace{(\mathbf{S} \mathbf{V}^T)}_{r \times p} \hat{\beta} = \underbrace{(\mathbf{U}^T \mathbf{Y})}_{r \times 1} \leftarrow$

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

# Regularized Least Squares

$$Y = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} \quad A = \begin{bmatrix} x_1^{(1)} & \dots & x_1^{(p)} \\ \vdots & & \vdots \\ x_n^{(1)} & \dots & x_n^{(p)} \end{bmatrix}$$

What if  $(A^T A)$  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  $\beta$  (small changes in input don't translate to large changes in output)

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

Ridge Regression  
(l2 penalty)

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

$$\lambda \geq 0$$

$$2 \underline{A^T A} \beta - 2 \underline{A^T Y} + 2 \underline{\lambda} \beta = 0$$

# Ridge Regression

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

Ridge Regression  
(l2 penalty)

$$= \arg \min_{\beta} (\mathbf{A}\beta - \mathbf{Y})^T (\mathbf{A}\beta - \mathbf{Y}) + \lambda \|\beta\|_2^2 \quad \lambda \geq 0$$

$$= 2\mathbf{A}^T \mathbf{A} \beta - 2\mathbf{A}^T \mathbf{Y} + \underbrace{2\lambda \beta}_{2\lambda \mathbf{I} \beta}$$

$$= 2(\mathbf{A}^T \mathbf{A} + \lambda \mathbf{I}) \beta - 2\mathbf{A}^T \mathbf{Y} = 0$$

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

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

always  $\lambda > 0$  ✓

$$\Sigma = \begin{bmatrix} \lambda_1 & 0 \\ 0 & \dots \lambda_p \end{bmatrix}$$

$$\mathbf{M} + \lambda \mathbf{I}$$

$$V \Sigma V^T + \lambda V V^T$$

$$V(\Sigma + \lambda \mathbf{I})V^T$$

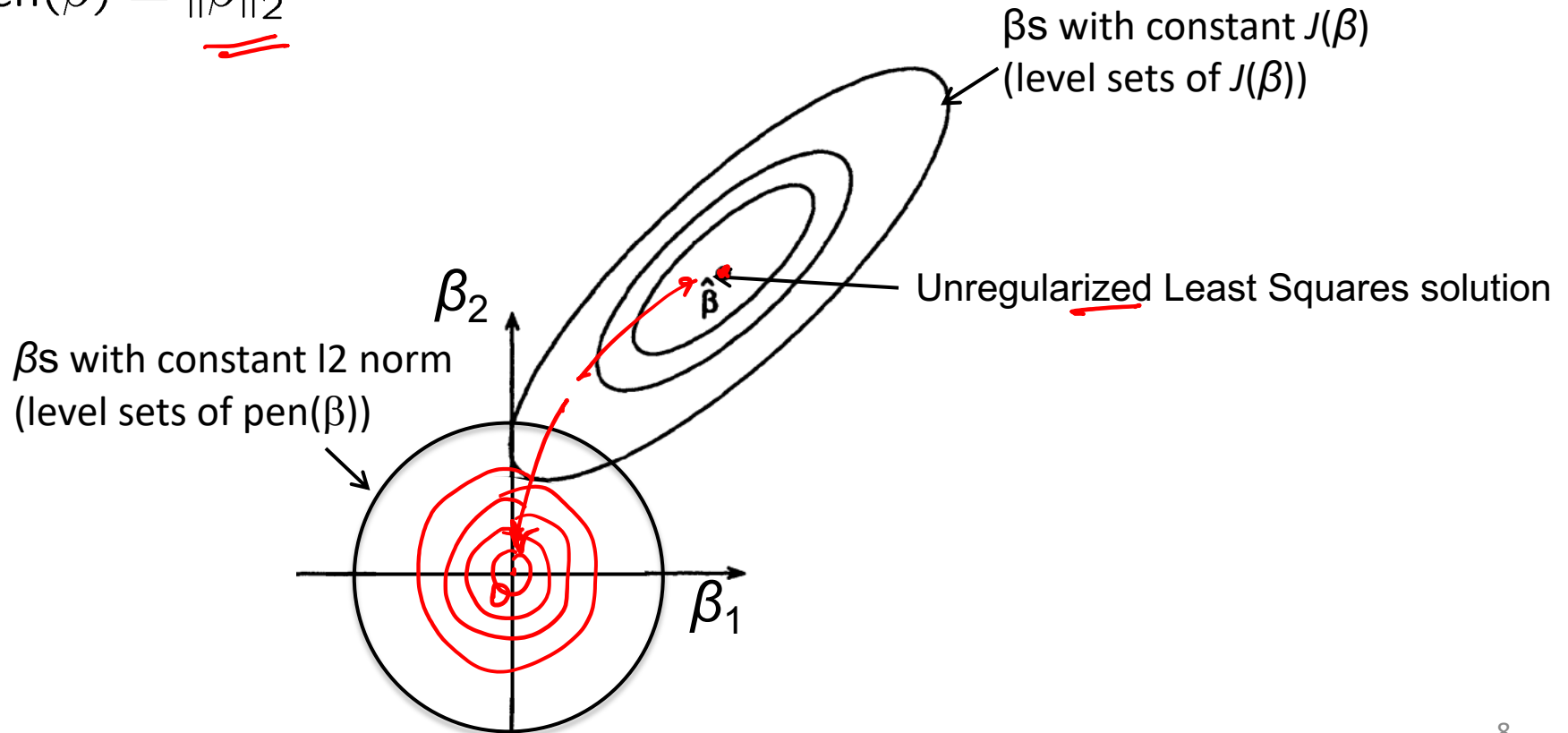
$$\text{eig}(\mathbf{M} + \lambda \mathbf{I}) = \text{eig}(\mathbf{M}) + \lambda \geq \lambda > 0$$

# Understanding regularized Least Squares

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

Ridge Regression:

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





# 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  $\beta$  (small changes in input don’t translate to large changes in output)

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

Ridge Regression  
(l2 penalty)

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

Lasso  
(l1 penalty)

$$\lambda \geq 0$$

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

# 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  $\beta$  (small changes in input don’t translate to large changes in output)

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

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

Ridge Regression  
(l2 penalty)

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

Lasso  
(l1 penalty)  $\lambda \geq 0$

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

# Ridge Regression vs Lasso

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

*Handwritten:*  
 $\|\beta\|_0 = \sum_i \mathbb{1}_{\beta_i \neq 0}$

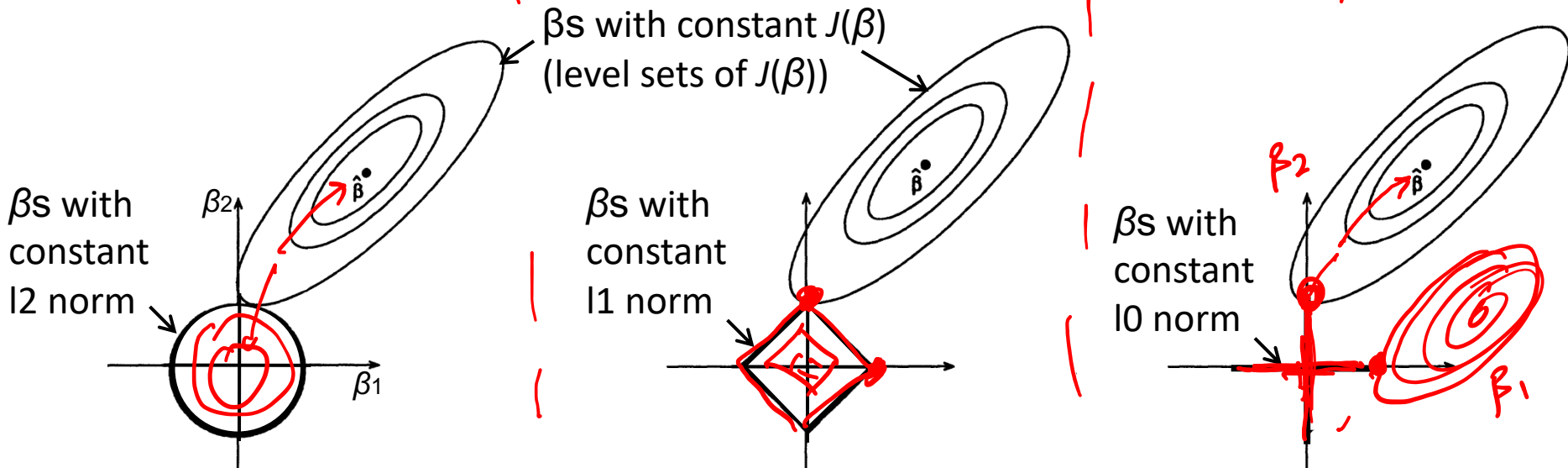
Ridge Regression:

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

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
```

$n < p$

```
→ 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)
```

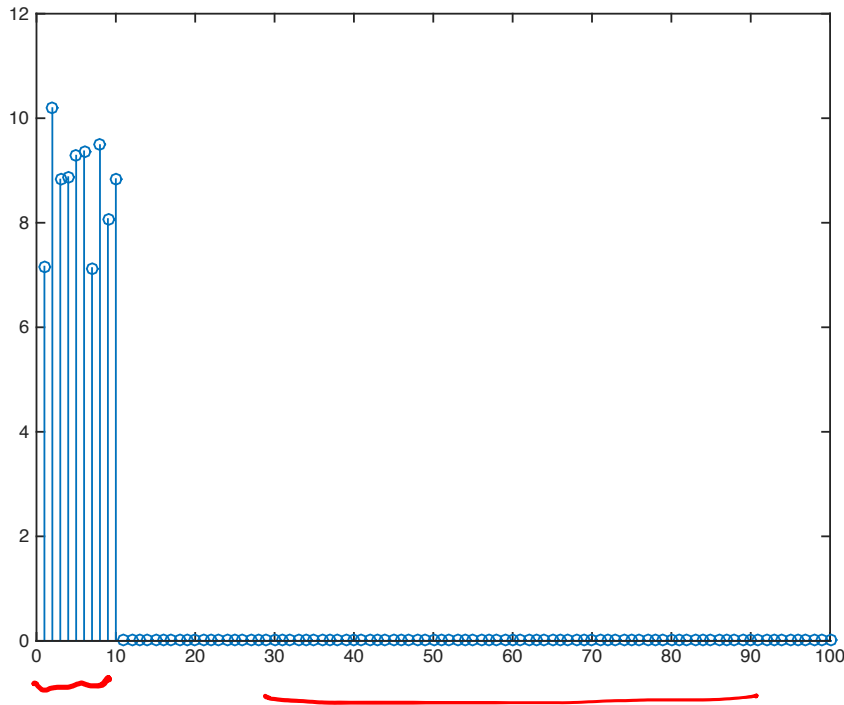
```
pause
```

```
stem(ridgeWeights)
```

# Matlab example

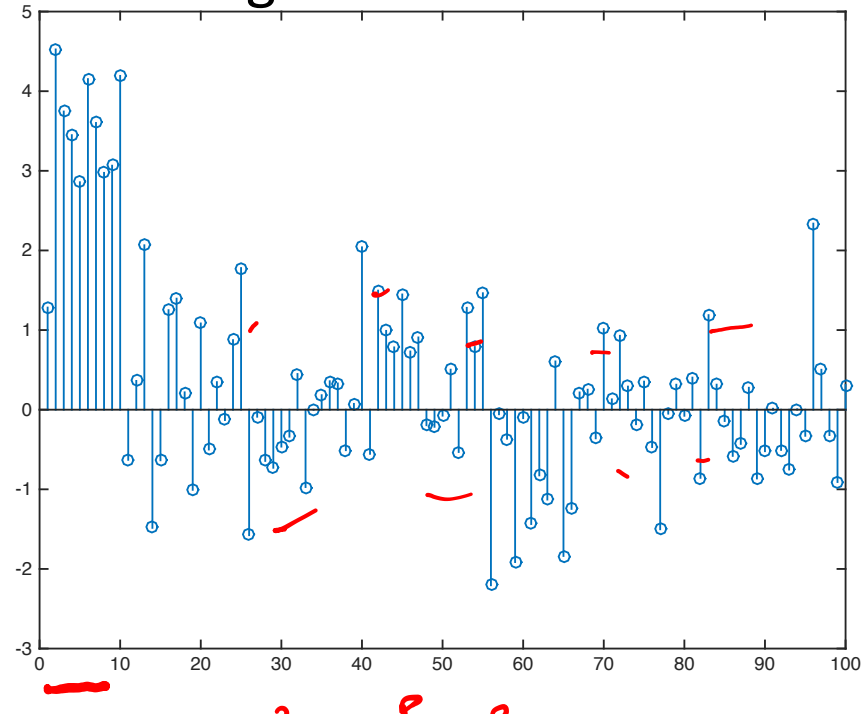
Test MSE = 33.7997 ✓

## Lasso Coefficients



Test MSE = 185.9948 ✓

## Ridge Coefficients



$$\|\beta\|_2^2 = \sum_{j=1}^p \beta_j^2$$

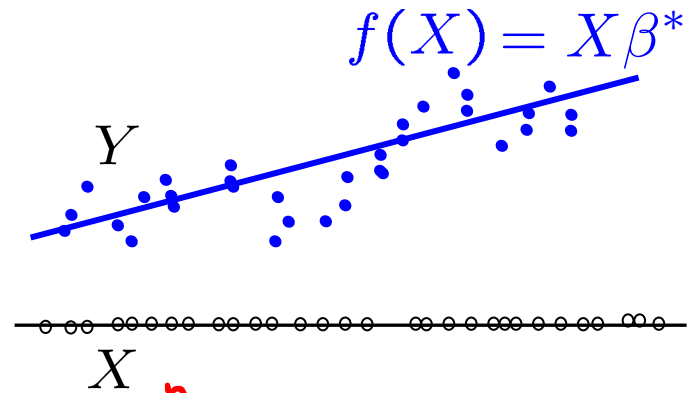
# Least Squares and M(C)LE

$E[Y|X]$  ✓

Intuition: Signal plus (zero-mean) Noise model

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

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



$$\hat{\beta}_{\text{MLE}} = \arg \max_{\beta} \log p(\{Y_i\}_{i=1}^n | \beta, \sigma^2, \{X_i\}_{i=1}^n) \sim \log \prod_{i=1}^n \mathcal{N}(X_i \beta^*, \sigma^2 \mathbf{I})$$

Conditional log likelihood

$$= \arg \max_{\beta} \sum_{i=1}^n \log \left( \frac{1}{(\sqrt{2\pi\sigma^2})^d} \exp\left(-\frac{(Y_i - X_i \beta)^2}{2\sigma^2}\right) \right)$$

$\log(ab) = \log a + \log b$

$$= \arg \max_{\beta} \sum_{i=1}^n -\frac{(Y_i - X_i \beta)^2}{2\sigma^2}$$

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

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?

$p(\beta)$  - prior  
 $p(\beta | \text{Data}) \propto p(\text{Data} | \beta) \cdot p(\beta)$

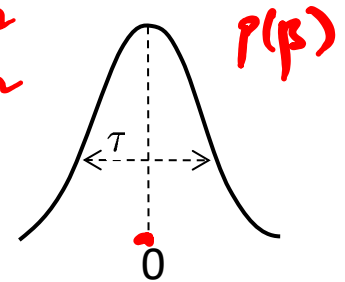
$$\hat{\beta}_{\text{MAP}} = \arg \max_{\beta} \underbrace{\log p(\{Y_i\}_{i=1}^n | \beta, \sigma^2, \{X_i\}_{i=1}^n)}_{\text{Conditional log likelihood}} + \underbrace{\log p(\beta)}_{\text{log prior}}$$

1) Gaussian Prior

$$\beta \sim \mathcal{N}(0, \tau^2 \mathbf{I})$$

$$\log p(\beta) \propto -\frac{\beta^T \beta}{2\tau^2} = -\frac{\|\beta\|^2}{2\tau^2}$$

$$p(\beta) \propto e^{-\beta^T \beta / 2\tau^2}$$



$$\hat{\beta}_{\text{MAP}} = \arg \min_{\beta} \sum_{i=1}^n \underbrace{(Y_i - X_i \beta)^2}_{2\sigma^2} + \underbrace{\lambda \|\beta\|_2^2}_{\text{constant}(\sigma^2, \tau^2)}$$

Ridge Regression

Prior belief that  $\beta$  is Gaussian with zero-mean biases solution to “small”  $\beta$

# Regularized Least Squares and M(C)AP

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

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

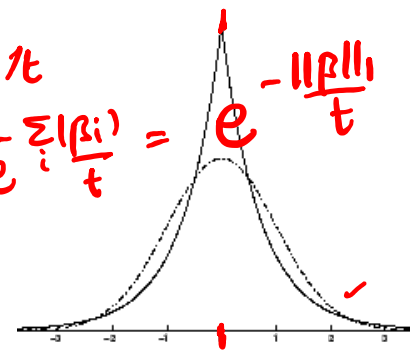
$= \|\beta\|_1$

II) Laplace Prior

$\beta_i \stackrel{iid}{\sim} \text{Laplace}(0, t)$

$p(\beta) = \prod_i p(\beta_i) \propto \prod_i e^{-|\beta_i|/t} = e^{-\sum_i |\beta_i|/t} = e^{-\frac{\|\beta\|_1}{t}}$

$p(\beta_i) \propto e^{-|\beta_i|/t}$



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

↓  
constant( $\sigma^2, t$ )

Lasso

Prior belief that  $\beta$  is Laplace with zero-mean biases solution to "sparse"  $\beta$



# Polynomial Regression

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

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

$$\hat{\beta} = (\mathbf{A}^T \mathbf{A})^{-1} \mathbf{A}^T \mathbf{Y} \quad \checkmark$$

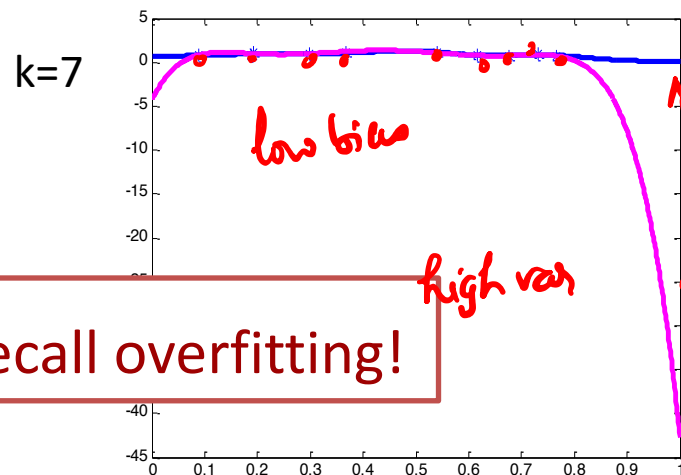
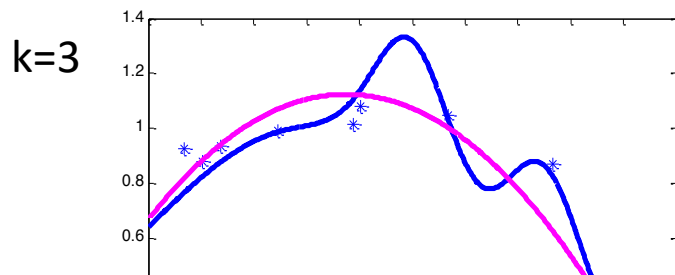
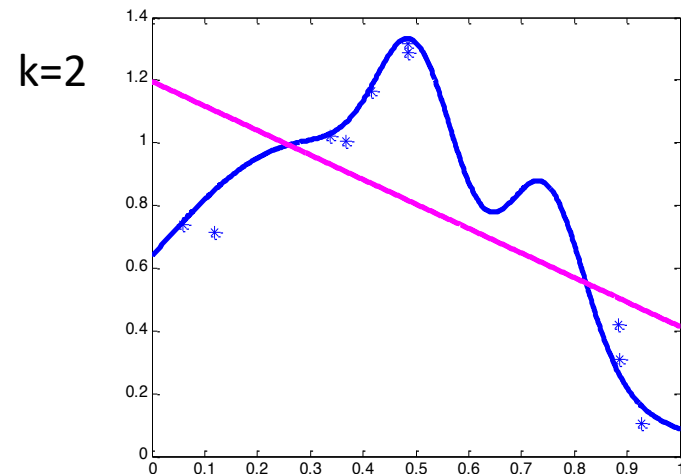
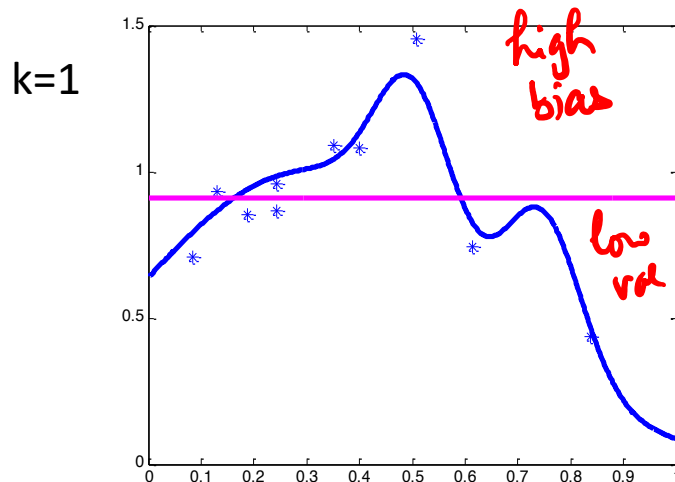
$$\hat{f}_n(X) = \mathbf{X}\hat{\beta}$$

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

Multivariate (p-dim)  $f(X) = \beta_0 + \beta_1 X^{(1)} + \beta_2 X^{(2)} + \dots + \beta_p X^{(p)}$   
 case:  
 $+ \sum_{i=1}^p \sum_{j=1}^p \beta_{ij} X^{(i)} X^{(j)} + \sum_{i=1}^p \sum_{j=1}^p \sum_{k=1}^p X^{(i)} X^{(j)} X^{(k)}$   
 $+ \dots$  terms up to degree m

# Polynomial Regression

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



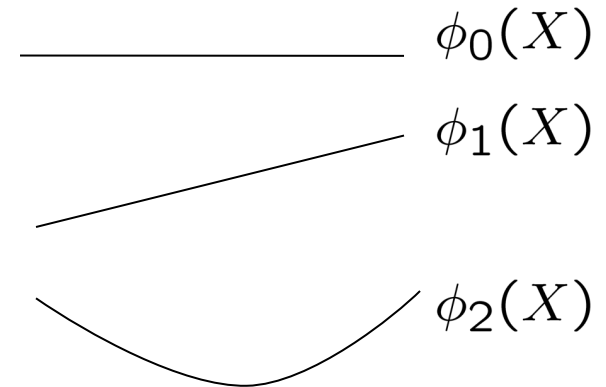
What is the right order? Recall overfitting!

# 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.  $e^X$ ,  $\log X$ ,  $1/X$ ,  $\sin(X)$ , ...

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

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

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

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

# Poll

- The maximum likelihood estimate of model parameter  $\alpha$  for the random variable  $y \sim N(\alpha x_1 x_2^3, \sigma^2)$ , where  $x_1$  and  $x_2$  are random variables, can be learned using linear regression on  $n$  iid samples of  $(x_1, x_2, y)$

- True
- False

$$y \sim N(\alpha x_1 x_2, \sigma^2) \checkmark$$

$$y \sim N(\alpha x_1 + x_2, \sigma^2) \checkmark$$

$$\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \rightarrow x_1 x_2^3 = z$$
$$y \sim N(\alpha z, \sigma^2)$$

**Can we kernelize linear regression?**

# Linear (Ridge) regression

$$\min_{\beta} \sum_{i=1}^n (Y_i - X_i \beta)^2 + \lambda \|\beta\|_2^2 \quad \hat{\beta} = (\underbrace{\mathbf{A}^T \mathbf{A} + \lambda \mathbf{I}}_{p \times p})^{-1} \mathbf{A}^T \mathbf{Y}$$

Recall

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

$$\begin{aligned} x_i \cdot x_j &= x_i^T x_j \\ \phi(x_i) \cdot \phi(x_j) \\ \underline{K(x_i, x_j)} \end{aligned}$$

Hence  $\mathbf{A}^T \mathbf{A}$  is a  $p \times p$  matrix whose entries denote the (sample) correlation between the features

NOT inner products between the data points – the inner product matrix would be  $\mathbf{A} \mathbf{A}^T$  which is  $n \times n$  (also known as Gram matrix)

Using dual formulation, we can write the solution in terms of  $\mathbf{A} \mathbf{A}^T$

# Ridge regression

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

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

## Similarity with SVMs

Primal problem:

$$\min_{\beta, z_i} \sum_{i=1}^n z_i^2 + \lambda \|\beta\|_2^2$$

$$\text{s.t. } z_i = Y_i - X_i \beta$$

SVM Primal problem:

$$\min_{w, \xi_i} C \sum_{i=1}^n \xi_i + \frac{1}{2} \|w\|_2^2$$

$$\text{s.t. } \xi_i = \max(1 - Y_i X_i w, 0)$$

Lagrangian:

$$\sum_{i=1}^n z_i^2 + \lambda \|\beta\|_2^2 + \sum_{i=1}^n \alpha_i (z_i - Y_i + X_i \beta)$$

$\alpha_i$  – Lagrange parameter, one per training point

# Ridge regression (dual)

$$\min_{\beta} \sum_{i=1}^n (Y_i - X_i\beta)^2 + \lambda \|\beta\|_2^2 \quad \hat{\beta} = (\mathbf{A}^T \mathbf{A} + \lambda \mathbf{I})^{-1} \mathbf{A}^T \mathbf{Y}$$

Dual problem:

$$\max_{\alpha} \min_{\beta, z_i} \sum_{i=1}^n z_i^2 + \lambda \|\beta\|_2^2 + \sum_{i=1}^n \alpha_i (z_i - Y_i + X_i\beta)$$

$\alpha = \{\alpha_i\}$  for  $i = 1, \dots, n$

Taking derivatives of Lagrangian wrt  $\beta$  and  $z_i$  we get:

$$\beta = -\frac{1}{2\lambda} \mathbf{A}^T \alpha \quad z_i = -\frac{\alpha_i}{2}$$

$$\text{Dual problem: } \max_{\alpha} -\frac{\alpha^T \alpha}{4} - \frac{1}{4\lambda} \alpha^T \mathbf{A} \mathbf{A}^T \alpha - \alpha^T \mathbf{Y}$$

n-dimensional optimization problem



# Ridge regression (dual)

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

$$\begin{aligned} \hat{\beta} &= (\mathbf{A}^T \mathbf{A} + \lambda \mathbf{I})^{-1} \mathbf{A}^T \mathbf{Y} \\ &= \mathbf{A}^T (\mathbf{A} \mathbf{A}^T + \lambda \mathbf{I})^{-1} \mathbf{Y} \end{aligned}$$

Dual problem:

$$\max_{\alpha} -\frac{\alpha^T \alpha}{4} - \frac{1}{4\lambda} \alpha^T \mathbf{A} \mathbf{A}^T \alpha - \alpha^T \mathbf{Y} \quad \Rightarrow \hat{\alpha} = -\left(\frac{\mathbf{A} \mathbf{A}^T}{\lambda} + \mathbf{I}\right)^{-1} 2 \mathbf{Y}$$

can get back  $\hat{\beta} = -\frac{1}{2\lambda} \mathbf{A}^T \hat{\alpha} = \mathbf{A}^T (\mathbf{A} \mathbf{A}^T + \lambda \mathbf{I})^{-1} \mathbf{Y}$

Weighted average of training points

Weight of each training point (but typically not sparse)

# Kernelized ridge regression

$$\hat{\beta} = (\mathbf{A}^T \mathbf{A} + \lambda \mathbf{I})^{-1} \mathbf{A}^T \mathbf{Y} \quad \checkmark$$

Using dual, can re-write solution as:

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

How does this help?

- Only need to invert  $n \times n$  matrix (instead of  $p \times p$  or  $m \times m$ )
- More importantly, kernel trick!

$\mathbf{A} \mathbf{A}^T$  involves only inner products between the training points  
BUT still have an extra  $\mathbf{A}^T$

$$\begin{aligned} \text{Recall the predicted label is } \hat{f}_n(X) &= \mathbf{X} \hat{\beta} \\ &= \mathbf{X} \mathbf{A}^T (\mathbf{A} \mathbf{A}^T + \lambda \mathbf{I})^{-1} \mathbf{Y} \\ &\quad \underbrace{\mathbf{X} \mathbf{A}^T}_{K_{\mathbf{x}, \mathbf{x}_i}} \underbrace{(\mathbf{A} \mathbf{A}^T + \lambda \mathbf{I})^{-1} \mathbf{Y}}_{K_{\mathbf{x}_i, \mathbf{x}_i}} \end{aligned}$$

$\mathbf{X} \mathbf{A}^T$  contains inner products between test point  $\mathbf{X}$  and training points!

# Kernelized ridge regression

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

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

Using dual, can re-write solution as:

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

How does this help?

- Only need to invert  $n \times n$  matrix (instead of  $p \times p$  or  $m \times m$ )
- More importantly, kernel trick!

$$\hat{f}_n(X) = \mathbf{K}_X (\mathbf{K} + \lambda \mathbf{I})^{-1} \mathbf{Y} \quad \text{where} \quad \begin{aligned} \mathbf{K}_X(i) &= \phi(X) \cdot \phi(X_i) \\ \mathbf{K}(i, j) &= \phi(X_i) \cdot \phi(X_j) \end{aligned}$$

Work with kernels, never need to write out the high-dim vectors

Ridge Regression with (implicit) nonlinear features  $\phi(X)$ !  $f(X) = \phi(X) \beta$