Bias-Variance Tradeoff

Machine Learning – CSE446

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University of Washington

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Optimal Prediction

Goal: Predict $Y \in \mathbb{R}^d$ given $X \in \mathbb{R}^d$ if $(X, Y) \sim P_{XY}$

Find function η that minimizes

n(X) takes in an X value and predicts a value of Y. Has no idea what Y is, only knows the value of X.

$$\mathbb{E}_{XY}[(Y - \eta(X))^2] = \mathbb{E}_X\left[\mathbb{E}_{Y|X}[(Y - \eta(x))^2 | X = x]\right]$$

(Hint: for any x, $\eta(x) = c_x$ where c_x minimizes $\mathbb{E}_{Y|X}[(Y - c_x)^2 | X = x]$)

$$0 = \frac{d}{dc_x}\mathbb{E}_{Y|X}[(Y - c_x)^2 | X = x]$$

$$= \mathbb{E}_{Y|X}[\frac{d}{dc_x}(Y - c_x)^2 | X = x]$$

$$= \mathbb{E}_{Y|X}[-2(Y - c_x) | X = x] = -2\mathbb{E}_{Y|X}[Y | X = x] + 2c_x$$

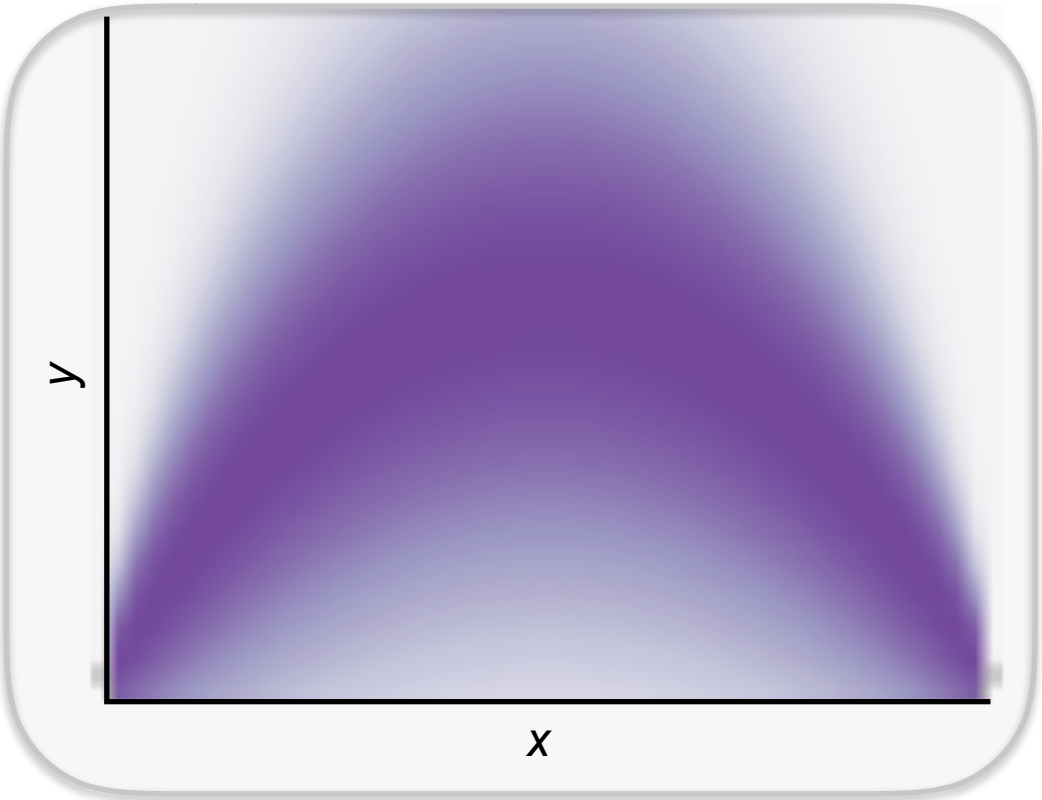
NOTE: n(X) minimizes the error over all possible values of Y! does NOT give the most likely choice of Y

Squared Error Optimal Predictor: $\eta(x) = \mathbb{E}_{Y|X}[Y | X = x]$

optimal estimation that will minimize the squared error.

Statistical Machine Learning

$$P_{XY}(X = x, Y = y)$$



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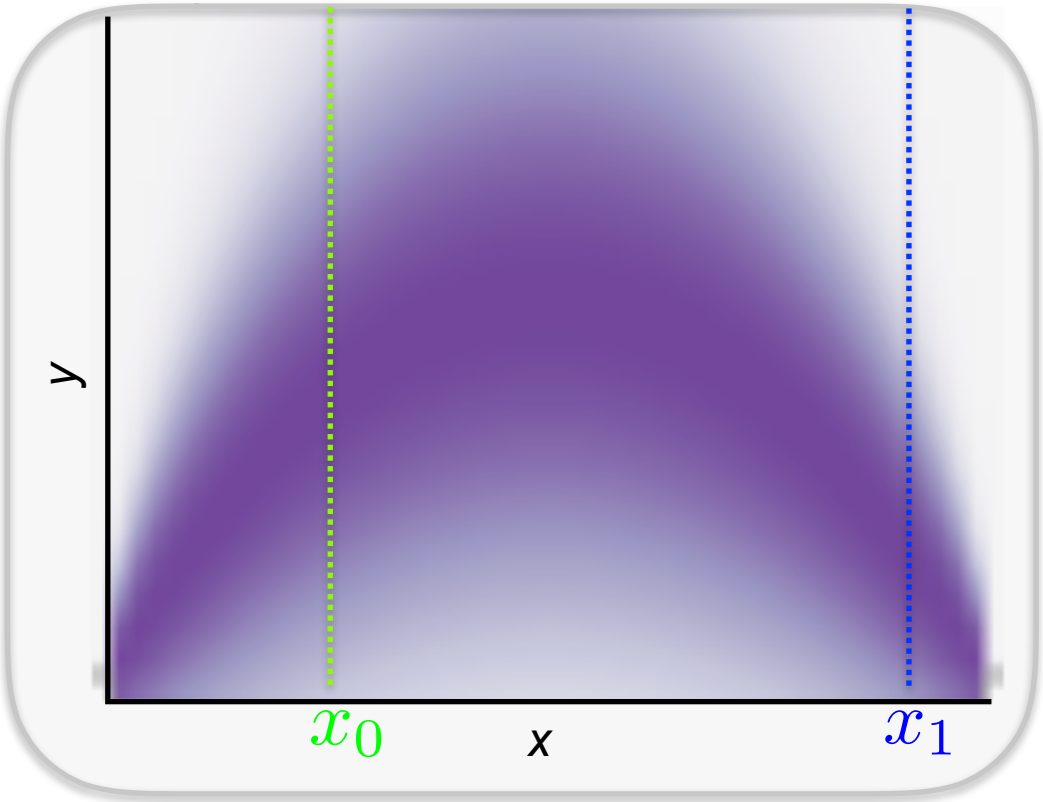
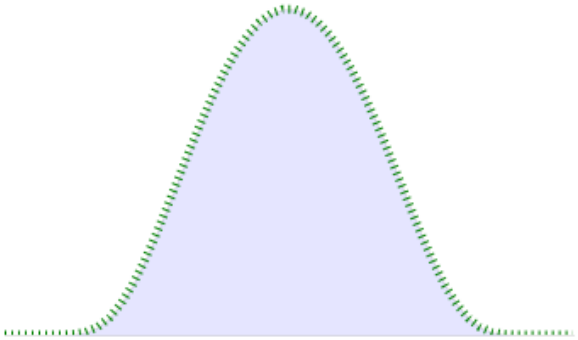
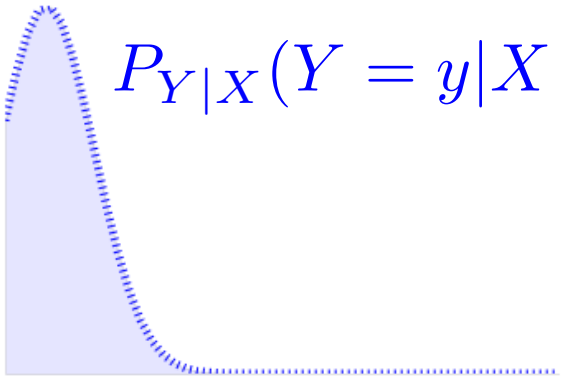


conditional distribution of Y given X = x0

$$P_{Y|X}(Y = y|X = x_0)$$

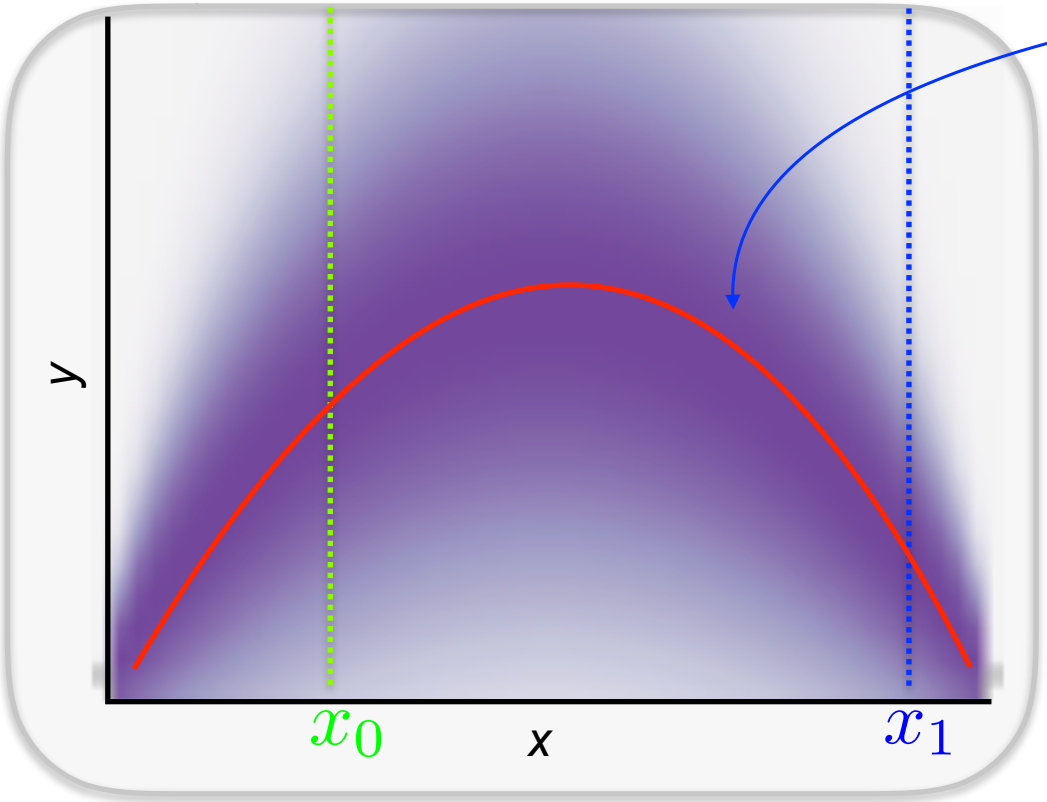




$$P_{Y|X}(Y = y|X = x_1)$$

Statistical Machine Learning

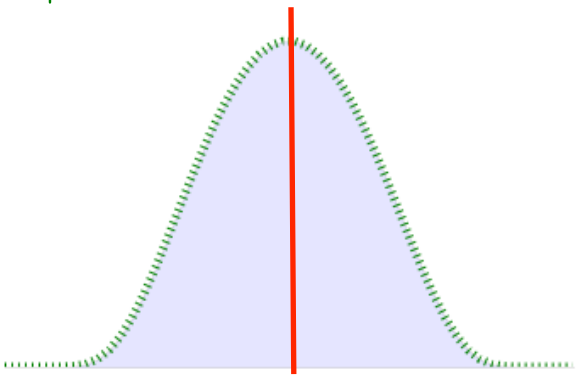
$P_{XY}(X = x, Y = y)$

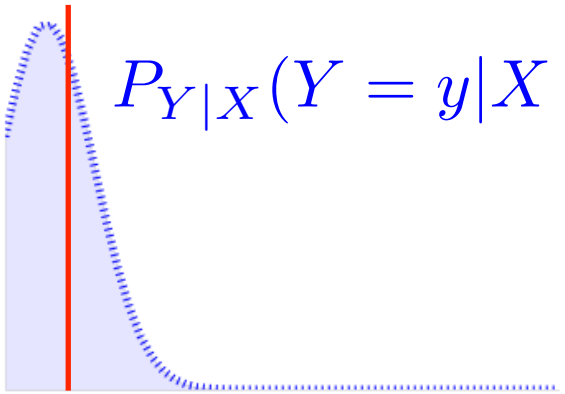


Ideally, we want to find:

$$\eta(x) = \mathbb{E}_{Y|X}[Y|X = x]$$

$P_{Y|X}(Y = y|X = x_0)$

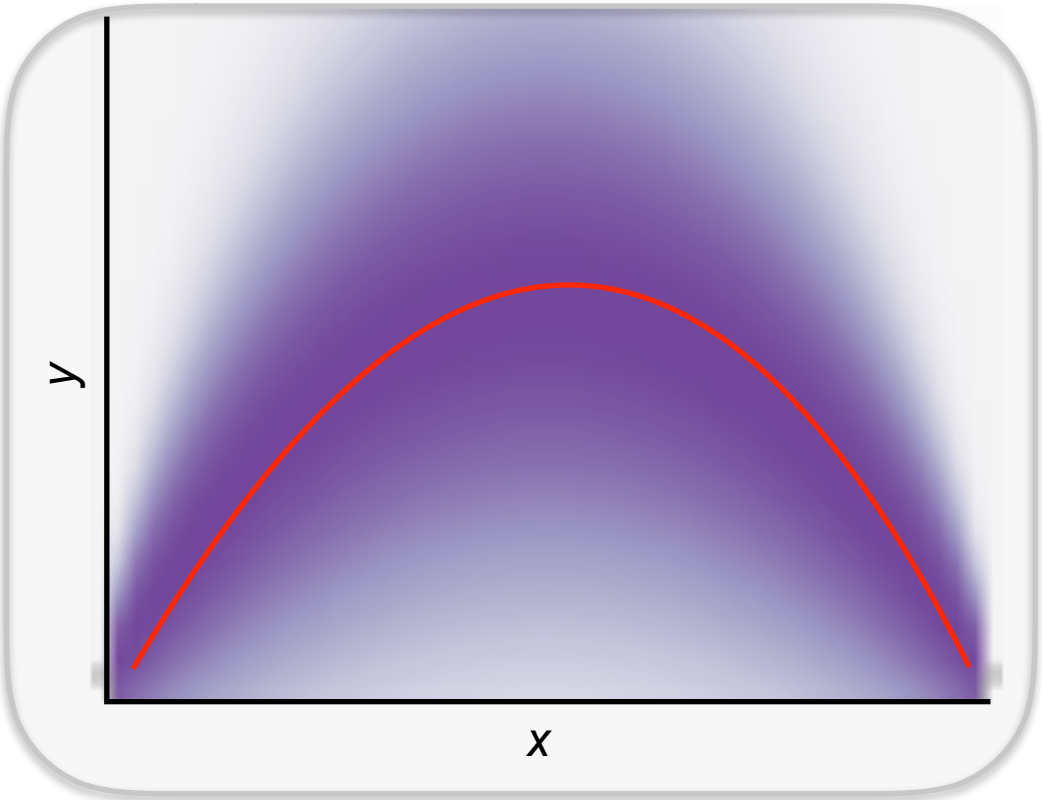




$P_{Y|X}(Y = y|X = x_1)$

Statistical Machine Learning

$P_{XY}(X = x, Y = y)$



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Statistical Machine Learning

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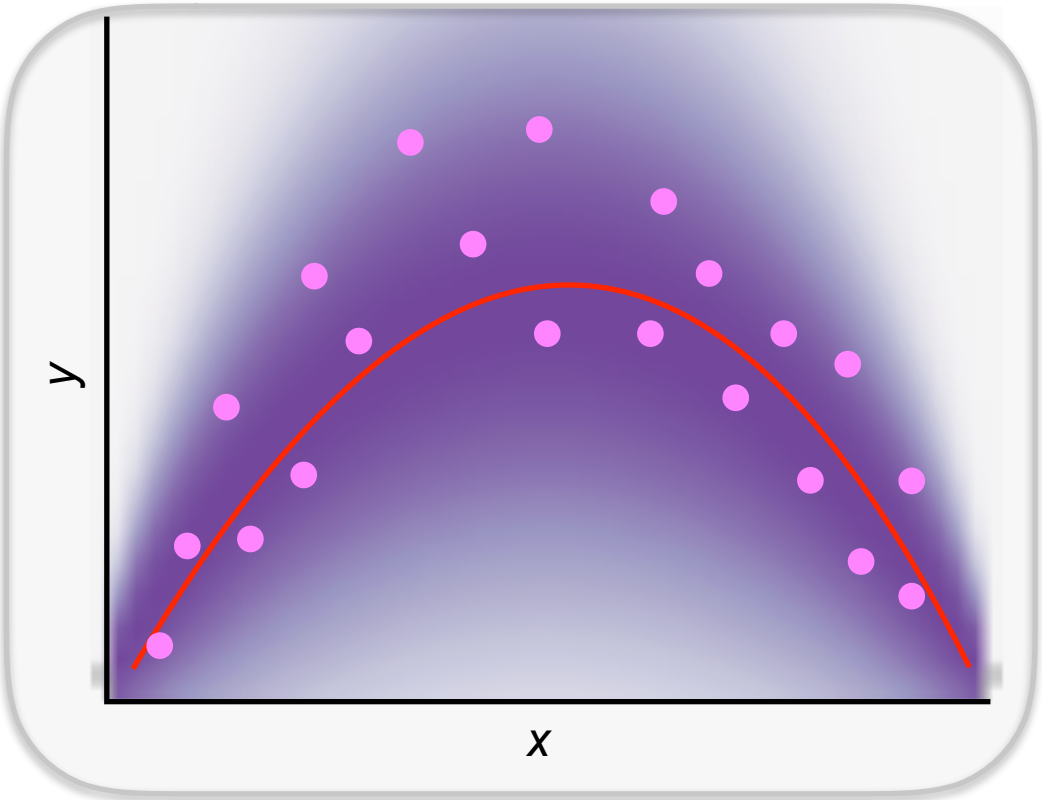


Ideally, we want to find:

$$\eta(x) = \mathbb{E}_{Y|X}[Y|X = x]$$

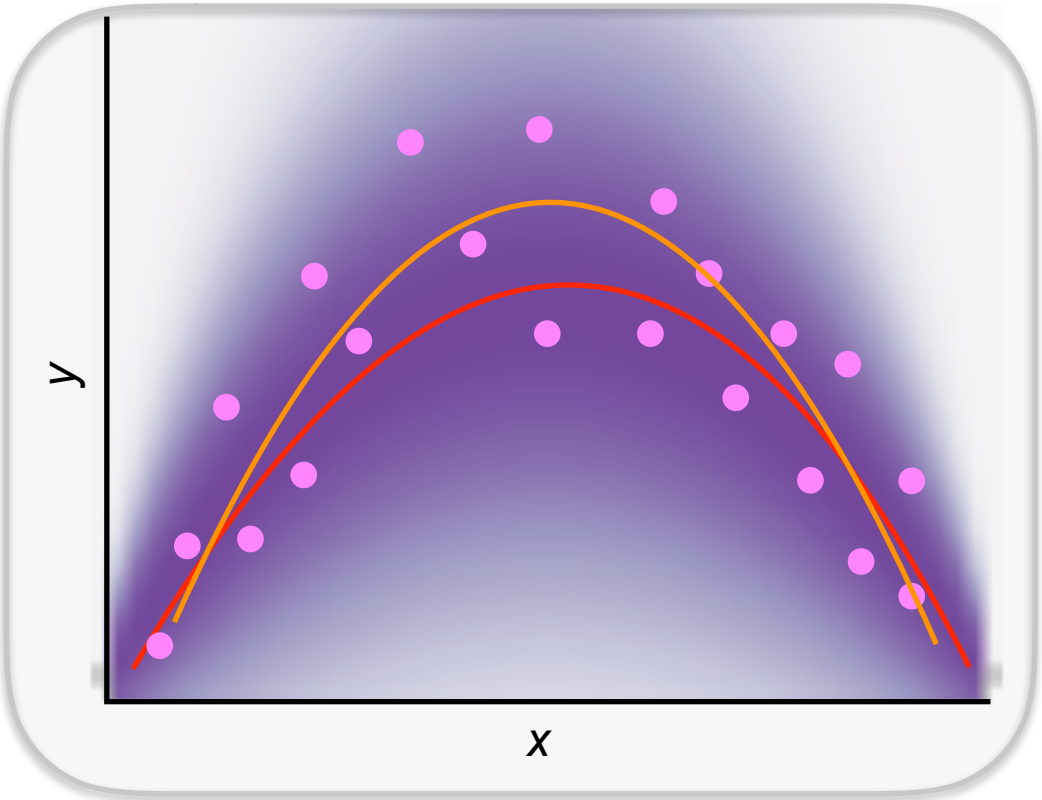
But we only have samples:

$$\mathcal{D} = \{(x_i, y_i)\}_{i=1}^{n} \overset{iid}{\sim} P_{XY}$$

do NOT know the true distributions. Only have a series of samples from P_xy

Statistical Machine Learning

$P_{XY}(X = x, Y = y)$



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and are restricted to a function class (e.g., linear) so we compute:

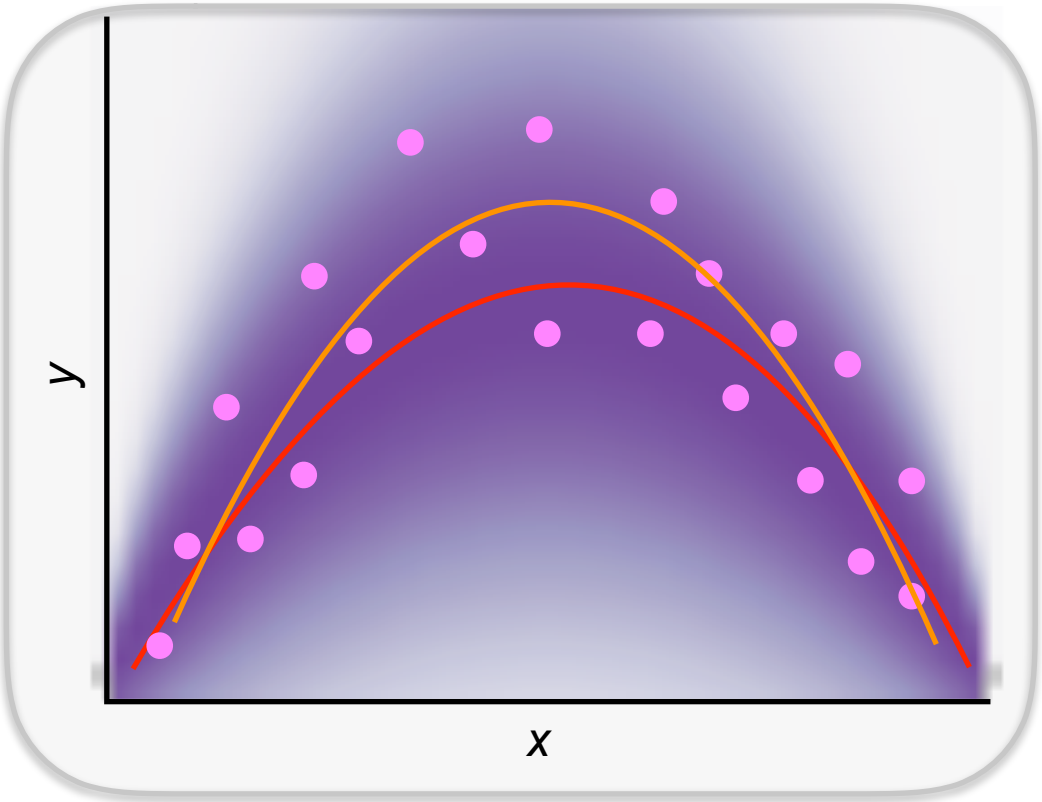
$$\widehat{f}_{\mathcal{D}} = \arg\min_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^{n} (y_i - f(x_i))^2$$

minimize the squared error in the OBSERVED data

this is an approximation of n(X).

Statistical Machine Learning

$P_{XY}(X = x, Y = y)$



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What about future predictions? $\mathbb{E}_{Y|X,\mathcal{D}}[(Y - \widehat{f}_{\mathcal{D}}(x))^2 | X = x]$

how does this model that the data trained perform on future predictions for Y?

Bias-Variance Tradeoff

$$\eta(x) = \mathbb{E}_{Y|X}[Y|X = x] \qquad \widehat{f}_{\mathcal{D}} = \arg\min_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^{n} (y_i - f(x_i))^2$$

data is a random variable

$$\mathbb{E}_{Y|X}[\mathbb{E}_{\mathcal{D}}[(Y - \widehat{f}_{\mathcal{D}}(x))^2]\big|X = x] = \mathbb{E}_{Y|X}[\mathbb{E}_{\mathcal{D}}[(Y - \eta(x) + \eta(x) - \widehat{f}_{\mathcal{D}}(x))^2]\big|X = x]$$

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$$= \mathbb{E}_{Y|X}\Big[\mathbb{E}_{\mathcal{D}}[(Y - \eta(x))^2 + 2(Y - \eta(x))(\eta(x) - \widehat{f}_{\mathcal{D}}(x)) + (\eta(x) - \widehat{f}_{\mathcal{D}}(x))^2]|X = x\Big]$$

the expectation of this is zero when X is given by the definition of n(X)

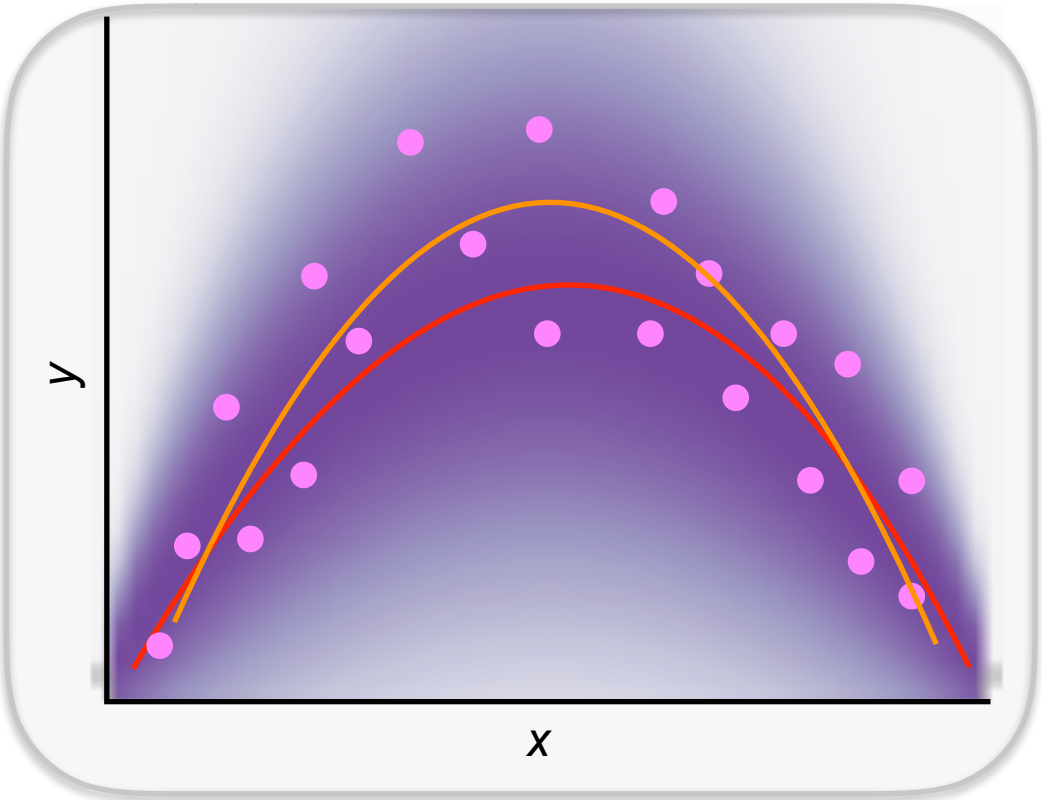
$$= \mathbb{E}_{Y|X}[(Y - \eta(x))^2|X = x] + \mathbb{E}_{\mathcal{D}}[(\eta(x) - \widehat{f}_{\mathcal{D}}(x))^2]$$

irreducible error
Caused by stochastic label noise

learning error
Caused by either using too "simple" of a model or not enough data to learn the model accurately

Statistical Machine Learning

$P_{XY}(X = x, Y = y)$



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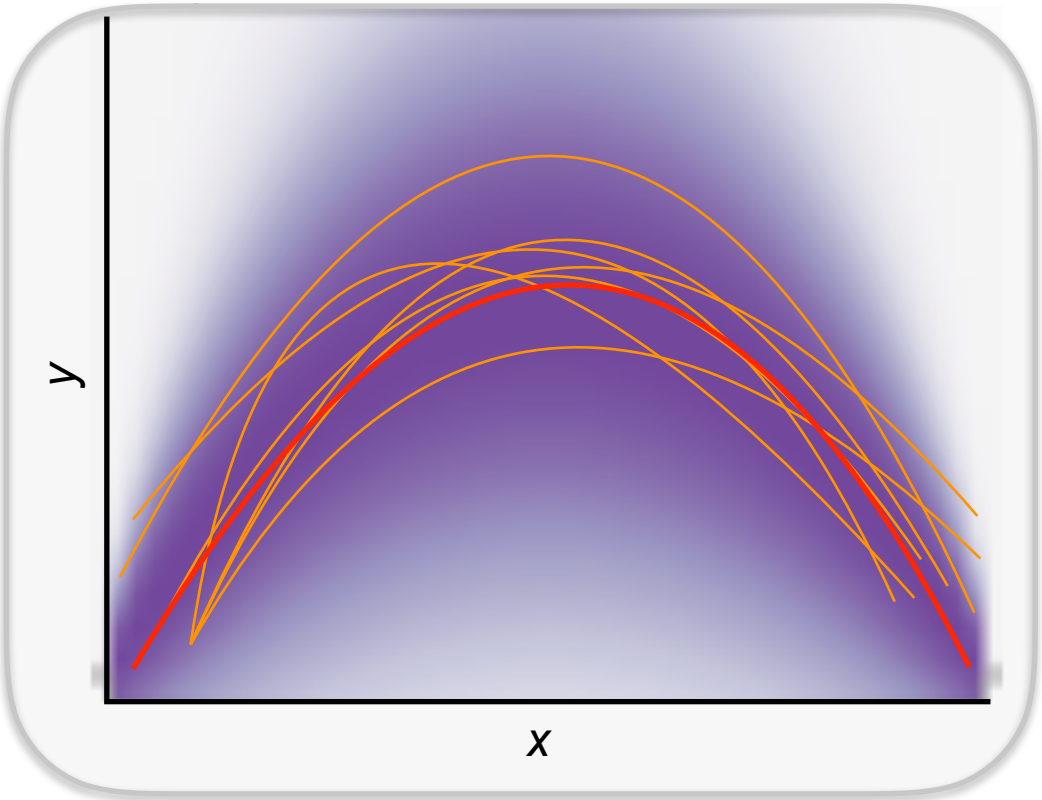

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Each draw $\mathcal{D} = \{(x_i, y_i)\}_{i=1}^{n}$ results in different $\widehat{f}$

Statistical Machine Learning

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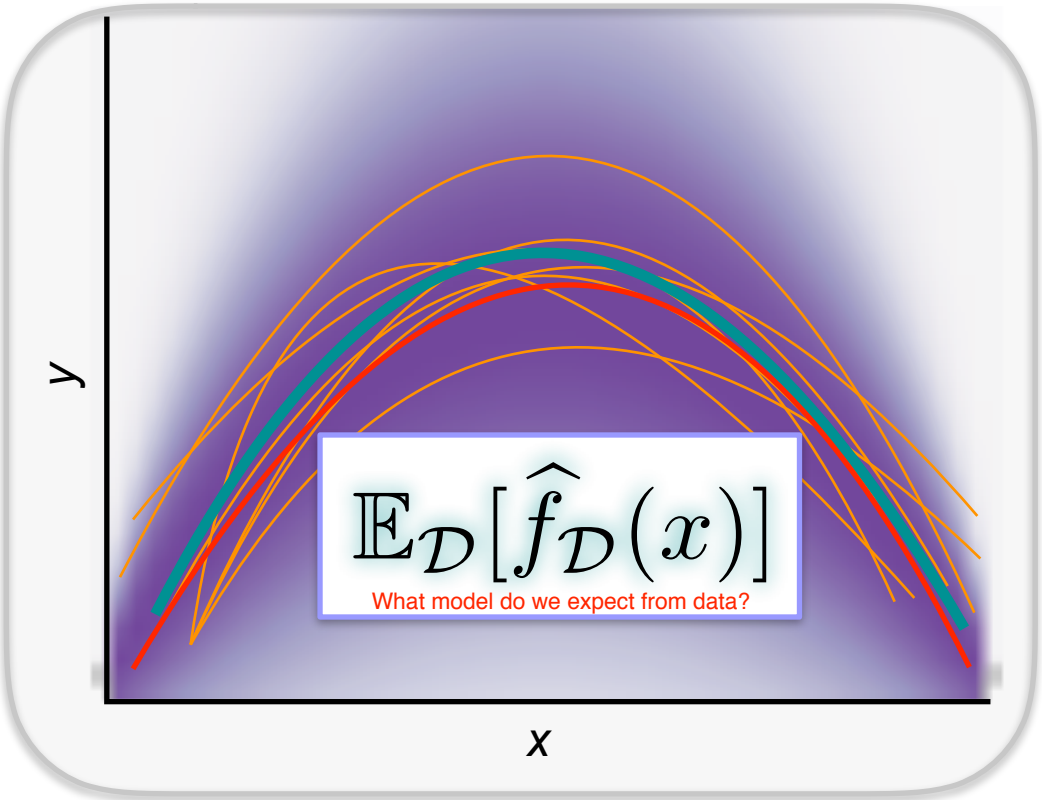

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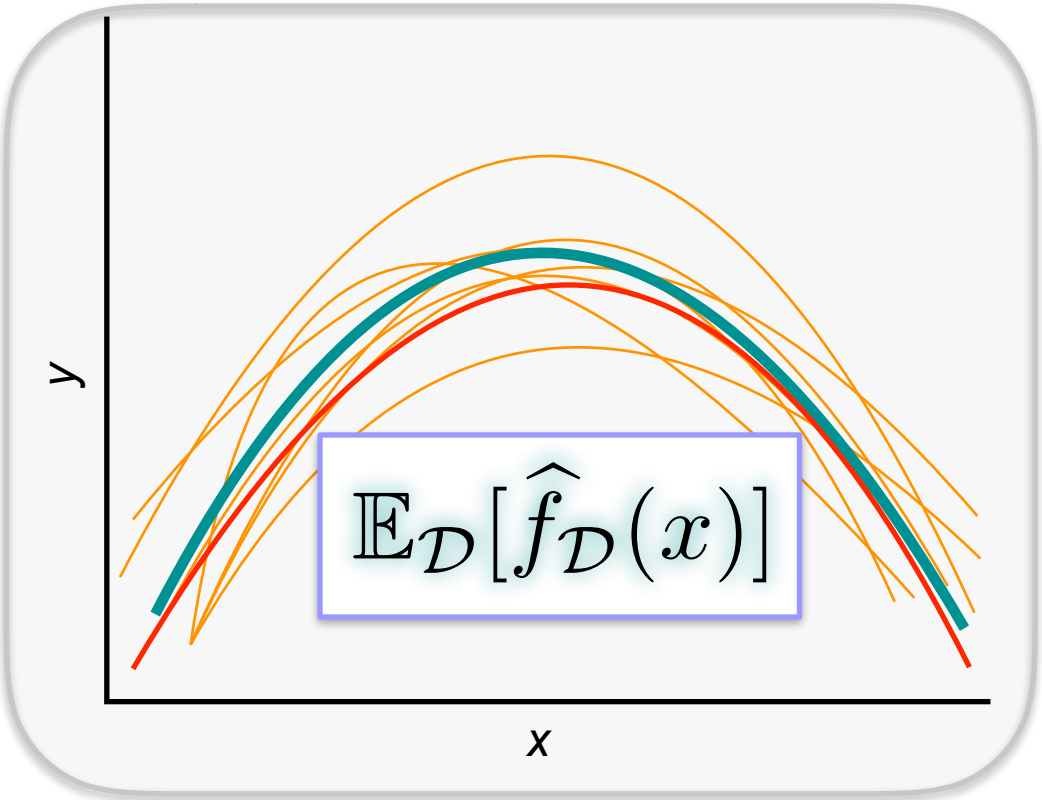

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Bias-Variance Tradeoff

$$\eta(x) = \mathbb{E}_{Y|X}[Y|X = x]$$

$$\mathbb{E}_{\mathcal{D}}[\widehat{f}_{\mathcal{D}}(x)]$$

$$\widehat{f}_{\mathcal{D}} = \arg\min_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^{n} (y_i - f(x_i))^2$$

$$\mathbb{E}_{\mathcal{D}}[(\eta(x) - \widehat{f}_{\mathcal{D}}(x))^2] = \mathbb{E}_{\mathcal{D}}[(\eta(x) - \mathbb{E}_{\mathcal{D}}[\widehat{f}_{\mathcal{D}}(x)] + \mathbb{E}_{\mathcal{D}}[\widehat{f}_{\mathcal{D}}(x)] - \widehat{f}_{\mathcal{D}}(x))^2]$$

Bias-Variance Tradeoff

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$$\mathbb{E}_{\mathcal{D}}[\widehat{f}_{\mathcal{D}}(x)]$$

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$$= \mathbb{E}_{\mathcal{D}}[(\eta(x) - \mathbb{E}_{\mathcal{D}}[\widehat{f}_{\mathcal{D}}(x)])^2 + 2(\eta(x) - \mathbb{E}_{\mathcal{D}}[\widehat{f}_{\mathcal{D}}(x)])(\mathbb{E}_{\mathcal{D}}[\widehat{f}_{\mathcal{D}}(x)] - \widehat{f}_{\mathcal{D}}(x))$$
$$+ (\mathbb{E}_{\mathcal{D}}[\widehat{f}_{\mathcal{D}}(x)] - \widehat{f}_{\mathcal{D}}(x))^2]$$

goes to zero

$$= (\eta(x) - \mathbb{E}_{\mathcal{D}}[\widehat{f}_{\mathcal{D}}(x)])^2 + \mathbb{E}_{\mathcal{D}}[(\mathbb{E}_{\mathcal{D}}[\widehat{f}_{\mathcal{D}}(x)] - \widehat{f}_{\mathcal{D}}(x))^2]$$

biased squared **variance**

Bias-Variance Tradeoff

$$\mathbb{E}_{Y|X}[\mathbb{E}_{\mathcal{D}}[(Y - \widehat{f}_{\mathcal{D}}(x))^2]\big|X = x] = \mathbb{E}_{Y|X}[(Y - \eta(x))^2\big|X = x]$$

irreducible error

$$+(\eta(x) - \mathbb{E}_{\mathcal{D}}[\widehat{f}_{\mathcal{D}}(x)])^2 + \mathbb{E}_{\mathcal{D}}[(\mathbb{E}_{\mathcal{D}}[\widehat{f}_{\mathcal{D}}(x)] - \widehat{f}_{\mathcal{D}}(x))^2]$$

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Bias-Variance Tradeoff

$$\mathbb{E}_{Y|X}[\mathbb{E}_{\mathcal{D}}[(Y - \widehat{f}_{\mathcal{D}}(x))^2]\big|X = x] = \mathbb{E}_{Y|X}[(Y - \eta(x))^2\big|X = x]$$

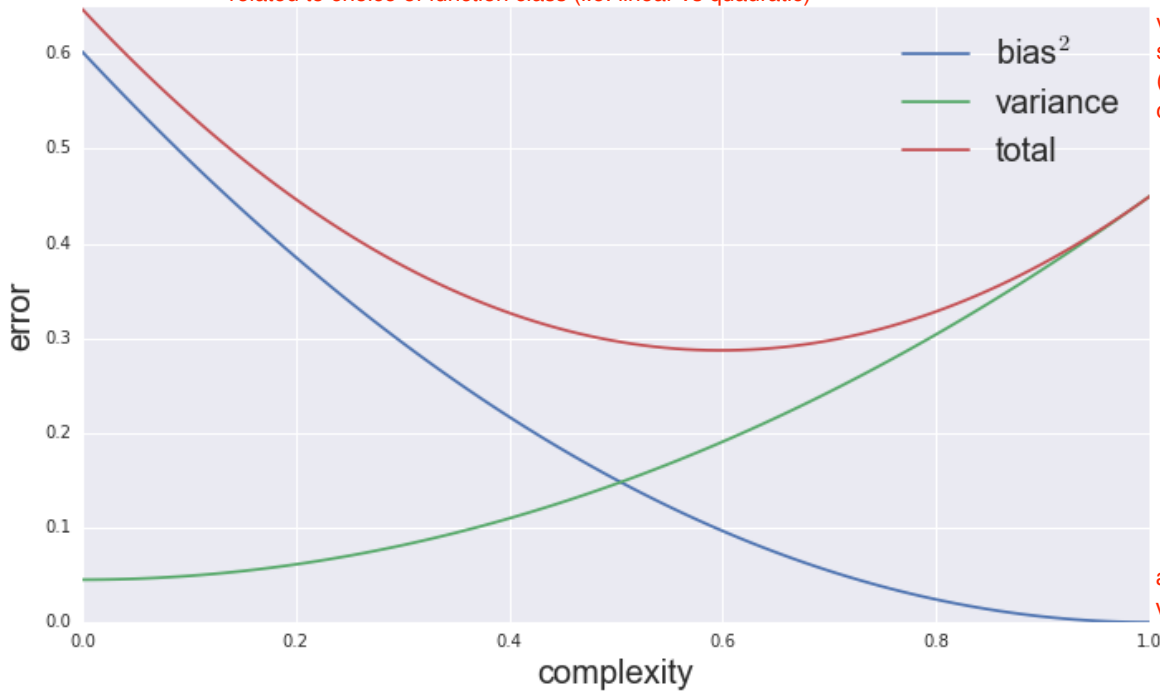
irreducible error

How well our choice of function class can capture the true function n(X). i.e. if n(X) is quadratic than no way a linear function could capture all its dynamics so I will have a nonzero bias. But if I choose a quadratic function class then I could possibly get the true function n(X)

$$+(\eta(x) - \mathbb{E}_{\mathcal{D}}[\widehat{f}_{\mathcal{D}}(x)])^2 + \mathbb{E}_{\mathcal{D}}[(\mathbb{E}_{\mathcal{D}}[\widehat{f}_{\mathcal{D}}(x)] - \widehat{f}_{\mathcal{D}}(x))^2]$$

biased squared **variance**

related to choice of function class (i.e. linear vs quadratic)



variation in model parameters sample to sample (i.e. how much our parameters change when we resample our data)

as function becomes more complicated variance increases and bias decreases.

Regularization

Machine Learning – CSE546

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April 15, 2019

Regularization in Linear Regression

find w that minimizes the error ll Xw - y ll^2

y is a vector so y_i is a number

x_i is a vector

Recall Least Squares: $\widehat{w}_{LS} = \arg\min_w \sum_{i=1}^{n} \left(y_i - x_i^T w\right)^2$

$= \arg\min_w (\mathbf{y} - \mathbf{X}w)^T(\mathbf{y} - \mathbf{X}w)$

when $(\mathbf{X}^T\mathbf{X})^{-1}$ exists.... $= (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$

this inverse does not always exist.

Regularization in Linear Regression

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$= \arg\min_w (\mathbf{y} - \mathbf{X}w)^T (\mathbf{y} - \mathbf{X}w)$

In general: $= \arg\min_w w^T (\mathbf{X}^T \mathbf{X}) w - 2y^T \mathbf{X} w$

Regularization in Linear Regression

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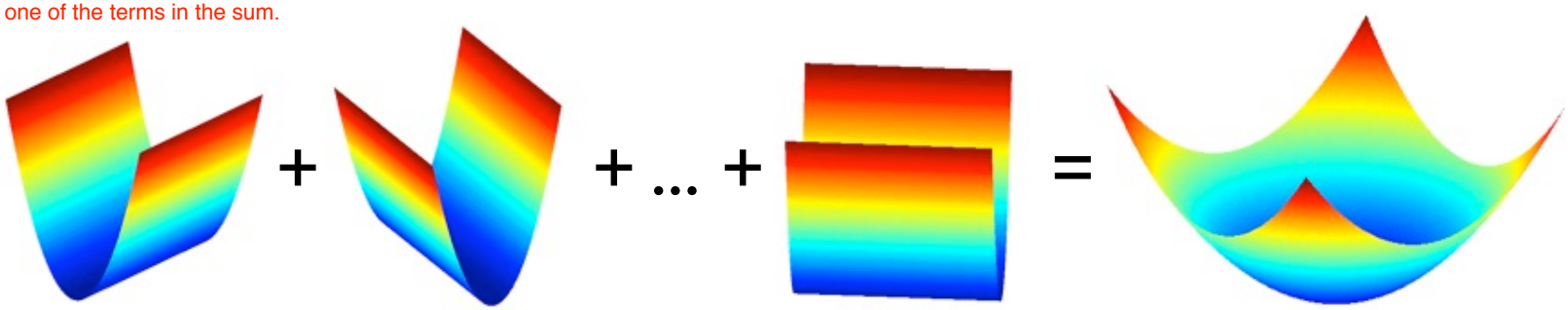
$= \arg\min_w (\mathbf{y} - \mathbf{X}w)^T (\mathbf{y} - \mathbf{X}w)$

In general: $= \arg\min_w w^T (\mathbf{X}^T \mathbf{X}) w - 2y^T \mathbf{X} w$

Each one of the terms in the sum.



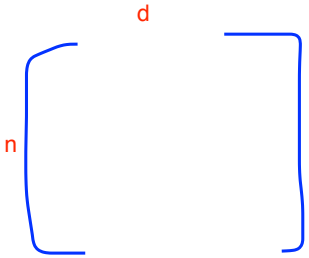
$$(y_1 - x_1^T w)^2 + (y_2 - x_2^T w)^2 + \cdots + (y_n - x_n^T w)^2 = \sum_{i=1}^{n} (y_i - x_i^T w)^2$$

Regularization in Linear Regression

Recall Least Squares: $\widehat{w}_{LS} = \arg\min_w \sum_{i=1}^{n} \left(y_i - x_i^T w\right)^2$

When $x_i \in \mathbb{R}^d$ and $d > n$ the objective function is flat in some directions:

X = [x1 x2 … xn] ^T –>



No unique solution to least squares solution

Changing data a little bit can alter which one of these possible solutions is chosen.

Regularization in Linear Regression

Recall Least Squares: $\widehat{w}_{LS} = \arg\min_w \sum_{i=1}^{n} \left(y_i - x_i^T w\right)^2$

When $x_i \in \mathbb{R}^d$ and $d > n$ the objective function is flat in some directions:

Implies optimal solution is *underconstrained* and unstable due to lack of curvature:

- small changes in training data result in large changes in solution
- often the *magnitudes* of *w* are "very large"

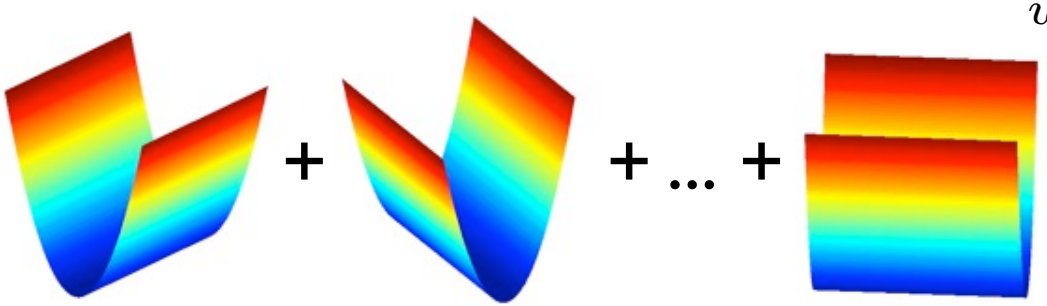
If the entries in w have large magnitude, a small change in one of the inputs can have a drastic change in the prediction made by the model. Not ideal

Regularization imposes "simpler" solutions by a "complexity" penalty

Ridge Regression

- Old Least squares objective:

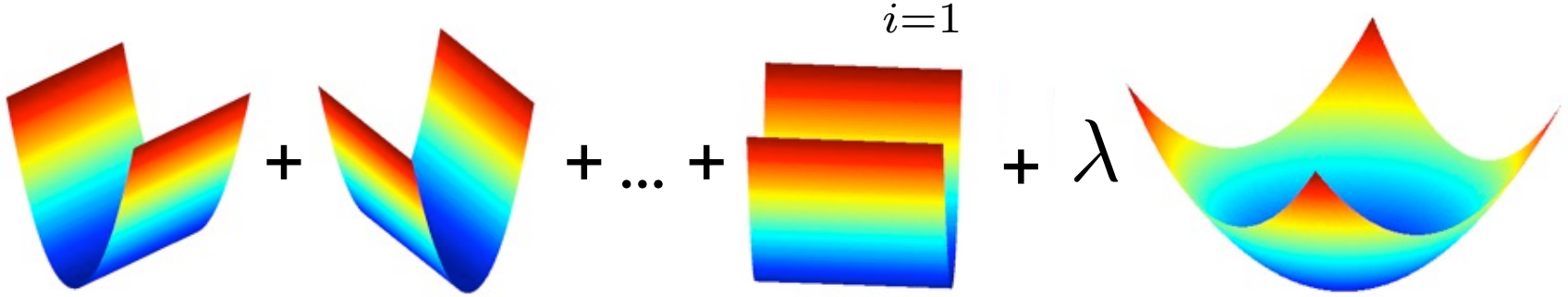
$$\widehat{w}_{LS} = \arg\min_w \sum_{i=1}^{n} \left(y_i - x_i^T w\right)^2$$



- Ridge Regression objective:

adds in curvature to our solution space; prevents the flat areas we saw were an issue earlier

$$\widehat{w}_{ridge} = \arg\min_w \sum_{i=1}^{n} \left(y_i - x_i^T w\right)^2 + \lambda ||w||_2^2$$



Minimizing the Ridge Regression Objective

$$\widehat{w}_{ridge} = \arg\min_{w} \sum_{i=1}^{n} \left(y_i - x_i^T w\right)^2 + \lambda ||w||_2^2$$

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$$\widehat{w}_{ridge} = \arg\min_w \sum_{i=1}^{n} \left(y_i - x_i^T w\right)^2 + \lambda ||w||_2^2$$

$$0 = \nabla_w \left(\sum_{i=1}^{n} \left(y_i - x_i^T w\right)^2 + \lambda ||w||_2^2 \right)$$

$$= -\sum_{i=1}^{n} 2x_i \left(y_i - x_i^T w\right) + 2\lambda w$$

$$= -2\left(\sum_{i=1}^{n} x_i y_i\right) + 2\left(\sum_{i=1}^{n} x_i x_i^T + \lambda I\right) w$$

$$\widehat{w}_{ridge} = \left(\sum_{i=1}^{n} x_i x_i^T + \lambda I\right)^{-1} \left(\sum_{i=1}^{n} x_i y_i\right)$$

$$= (\mathbf{X}^T\mathbf{X} + \lambda I)^{-1}\mathbf{X}^T\mathbf{y}$$

Matrix is always invertible for lambda > 0
XX^T is positive semi-definite

Shrinkage Properties

$$\widehat{w}_{ridge} = (\mathbf{X}^T\mathbf{X} + \lambda I)^{-1}\mathbf{X}^T\mathbf{y}$$

- ***Assume:*** $\mathbf{X}^T\mathbf{X} = nI$ why is this a valid assumption?

$$\begin{aligned}
\widehat{w}_{ridge} &= (\mathbf{X}^T\mathbf{X} + \lambda I)^{-1}\mathbf{X}^T\mathbf{y} \\
&= (\mathbf{X}^T\mathbf{X} + \lambda\frac{1}{n}\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y} \\
&= (1 + \lambda\frac{1}{n})^{-1}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y} \\
&= \frac{n}{n+\lambda}\widehat{w}_{LS}
\end{aligned}$$

Shrinking \hat{w} towards the origin

In this special case, Ridge is a "shrunk" Least squares!

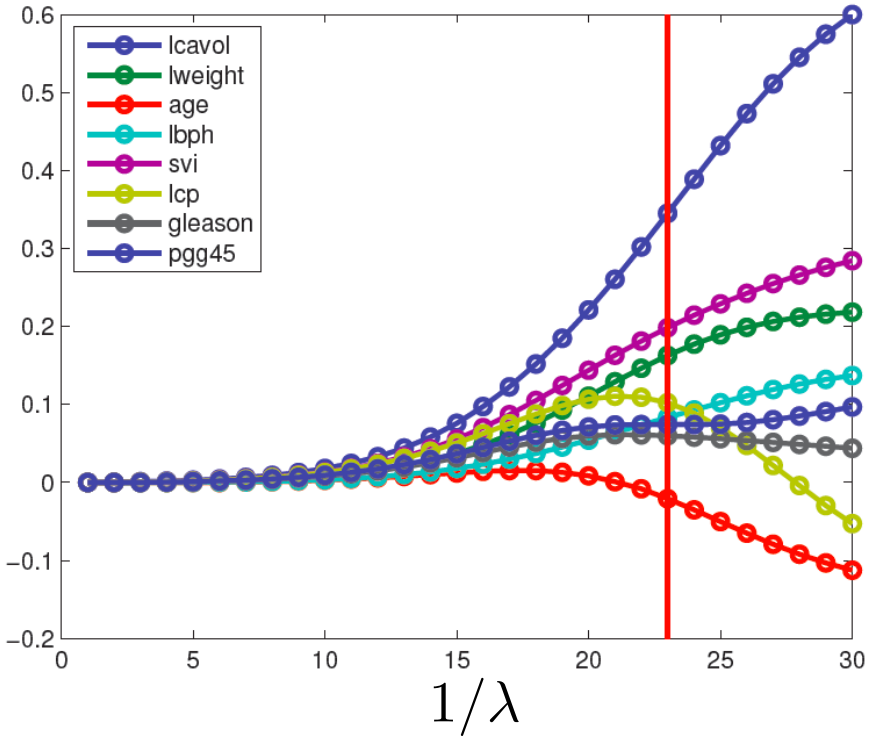
Ridge Coefficient Path

$\mathbf{X}^T\mathbf{X}$ in general

plotted individual components in the solution vector w

As lambda —> 0 we get the least squares solution.

Note: NOT monotonic like in the case we studied above using our assumption. Changes solutions in a nontrivial way.



From Kevin Murphy textbook

- Typical approach: select λ using cross validation, up next

Bias-Variance Properties

$$\widehat{w}_{ridge} = (\mathbf{X}^T\mathbf{X} + \lambda I)^{-1}\mathbf{X}^T\mathbf{y}$$

our data points have zero mean gaussian error. Our model given by parameters in X would be enough to predict y, besides some noise.

- ***Assume:*** $\mathbf{X}^T\mathbf{X} = nI$ ***and*** $\mathbf{y} = \mathbf{X}w + \boldsymbol{\epsilon}$ $\quad \boldsymbol{\epsilon} \sim \mathcal{N}(0, \sigma^2 I)$

If $x \in \mathbb{R}^d$ and $Y \sim \mathcal{N}(x^T w, \sigma^2)$, what is $\mathbb{E}_{Y|x,\text{train}}[(Y - x^T\widehat{w}_{ridge})^2 | X = x]$?

D

how well does the ridge predictor estimate the true value that Y takes on?

Bias-Variance Properties

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- ***Assume:*** $\mathbf{X}^T\mathbf{X} = nI$ ***and*** $\mathbf{y} = \mathbf{X}w + \boldsymbol{\epsilon}$ $\quad \boldsymbol{\epsilon} \sim \mathcal{N}(0, \sigma^2 I)$

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$\mathbb{E}_{Y|X,\mathcal{D}}[(Y - x^T\widehat{w}_{ridge})^2 | X = x]$ Same math as before.

$= \mathbb{E}_{Y|X}[(Y - \mathbb{E}_{Y|X}[Y|X = x])^2 | X = x] + \mathbb{E}_{\mathcal{D}}[(\mathbb{E}_{Y|X}[Y|X = x] - x^T\widehat{w}_{ridge})^2]$

Irreducible Error — Learning Error

= sigma^2

Y ~ N(x^Tw, sigma^2)
so this is mu = x^Tw

Bias-Variance Properties

$$\widehat{w}_{ridge} = (\mathbf{X}^T\mathbf{X} + \lambda I)^{-1}\mathbf{X}^T\mathbf{y}$$

- ***Assume:*** $\mathbf{X}^T\mathbf{X} = nI$ ***and*** $\mathbf{y} = \mathbf{X}w + \boldsymbol{\epsilon}$ Text $\quad \epsilon \sim \mathcal{N}(0, \sigma^2 I)$

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&\mathbb{E}_{Y|X,\mathcal{D}}[(Y - x^T\widehat{w}_{ridge})^2 | X = x] \\
&\quad = \mathbb{E}_{Y|X}[(Y - \mathbb{E}_{Y|X}[Y|X = x])^2 | X = x] + \mathbb{E}_{\mathcal{D}}[(\mathbb{E}_{Y|X}[Y|X = x] - x^T\widehat{w}_{ridge})^2] \\
&\quad = \mathbb{E}_{Y|X}[(Y - x^T w)^2 | X = x] + \mathbb{E}_{\mathcal{D}}[(x^T w - x^T\widehat{w}_{ridge})^2] \\
&\quad = \underline{\sigma^2} + \underline{(x^T w - \mathbb{E}_{\mathcal{D}}[x^T\widehat{w}_{ridge}])^2} + \underline{\mathbb{E}_{\mathcal{D}}[(\mathbb{E}_{\mathcal{D}}[x^T\widehat{w}_{ridge}] - x^T\widehat{w}_{ridge})^2]}
\end{aligned}$$

Irreduc. Error — Bias-squared — Variance

Bias-Variance Properties

$$\widehat{w}_{ridge} = (\mathbf{X}^T\mathbf{X} + \lambda I)^{-1}\mathbf{X}^T\mathbf{y}$$

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&\mathbb{E}_{Y|X,\mathcal{D}}[(Y - x^T\widehat{w}_{ridge})^2 | X = x] \\
&= \mathbb{E}_{Y|X}[(Y - \mathbb{E}_{Y|X}[Y|X = x])^2 | X = x] + \mathbb{E}_{\mathcal{D}}[(\mathbb{E}_{Y|X}[Y|X = x] - x^T\widehat{w}_{ridge})^2] \\
&= \mathbb{E}_{Y|X}[(Y - x^T w)^2 | X = x] + \mathbb{E}_{\mathcal{D}}[(x^T w - x^T\widehat{w}_{ridge})^2] \\
&= \sigma^2 + (x^T w - \mathbb{E}_{\mathcal{D}}[x^T\widehat{w}_{ridge}])^2 + \mathbb{E}_{\mathcal{D}}[(\mathbb{E}_{\mathcal{D}}[x^T\widehat{w}_{ridge}] - x^T\widehat{w}_{ridge})^2]
\end{aligned}$$

Irreduc. Error — Bias-squared — Variance

plugging this in we can calc E_D(xTw_ridge)

E[epsilon] = 0 so the right term disappears

$$\begin{aligned}
\widehat{w}_{ridge} &= (\mathbf{X}^T\mathbf{X} + \lambda I)^{-1}\mathbf{X}^T(\mathbf{X}w + \boldsymbol{\epsilon}) \\
&= \frac{n}{n+\lambda}w + \frac{1}{n+\lambda}\mathbf{X}^T\boldsymbol{\epsilon}
\end{aligned}$$

Bias-Variance Properties

$$\widehat{w}_{ridge} = (\mathbf{X}^T\mathbf{X} + \lambda I)^{-1}\mathbf{X}^T\mathbf{y}$$

- ***Assume:*** $\mathbf{X}^T\mathbf{X} = nI$ ***and*** $\mathbf{y} = \mathbf{X}w + \boldsymbol{\epsilon}$ $\quad \boldsymbol{\epsilon} \sim \mathcal{N}(0, \sigma^2 I)$

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&\mathbb{E}_{Y|X,\mathcal{D}}[(Y - x^T\widehat{w}_{ridge})^2 | X = x] \\
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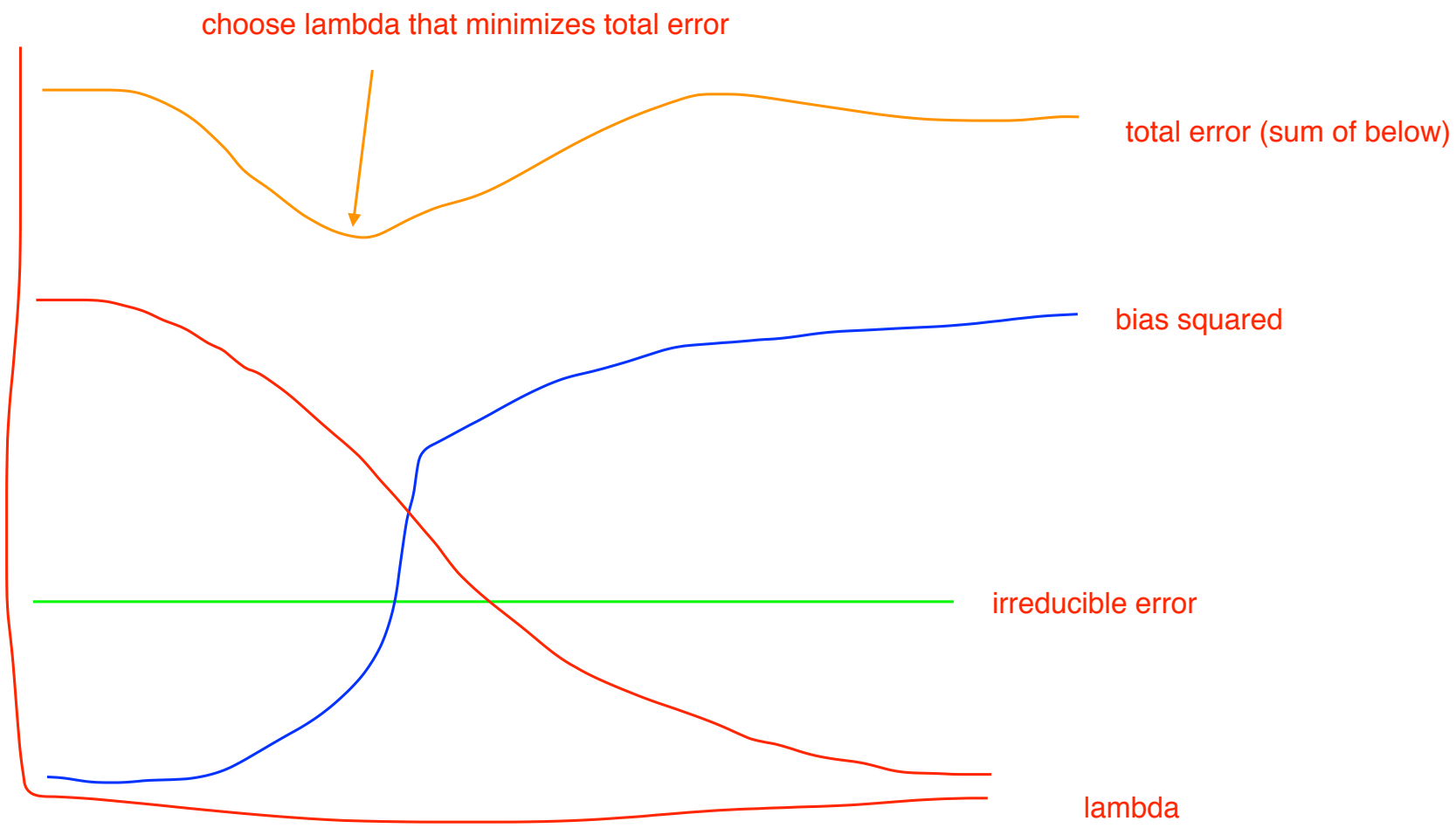
&\quad = \mathbb{E}_{Y|X}[(Y - x^T w)^2 | X = x] + \mathbb{E}_{\mathcal{D}}[(x^T w - x^T\widehat{w}_{ridge})^2] \\
&\quad = \sigma^2 + (x^T w - \mathbb{E}_{\mathcal{D}}[x^T\widehat{w}_{ridge}])^2 + \mathbb{E}_{\mathcal{D}}[(\mathbb{E}_{\mathcal{D}}[x^T\widehat{w}_{ridge}] - x^T\widehat{w}_{ridge})^2]
\end{aligned}$$

total error in predicting Y given X = x

$$= \underbrace{\sigma^2}_{\text{Irreduc. Error}} + \underbrace{\frac{\lambda^2}{(n+\lambda)^2}(w^T x)^2}_{\text{Bias-squared}} + \underbrace{\frac{d\sigma^2 n}{(n+\lambda)^2}\|x\|_2^2}_{\text{Variance}}$$

(verify at home)

can never predict Y better than the irreducible error —> error will never go to zero unless Irreducible error = 0


choose lambda that minimizes total error
total error (sum of below)
bias squared
irreducible error
lambda

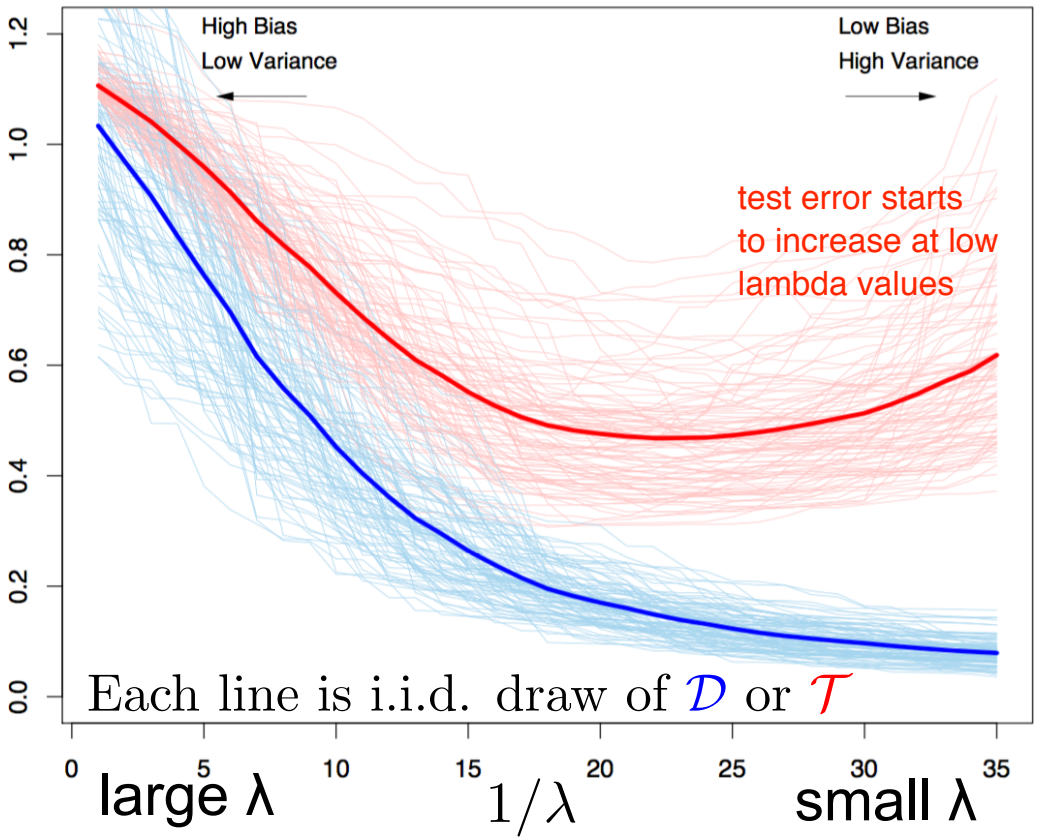
Ridge Regression: Effect of Regularization

$$\widehat{w}_{ridge} = \arg\min_{w} \sum_{i=1}^{n} \left(y_i - x_i^T w\right)^2 + \lambda ||w||_2^2$$

- Solution is indexed by the regularization parameter λ
- Larger λ Bias increases; Variance decreases
- Smaller λ
- As λ → 0, $\widehat{w}_{ridge} \longrightarrow$ w_LS = least squares solution
- As λ →∞, $\widehat{w}_{ridge} \longrightarrow$ zero vector

Ridge Regression: Effect of Regularization

$$\mathcal{D} \overset{i.i.d.}{\sim} P_{XY} \qquad \widehat{w}^{(\lambda)}_{\mathcal{D},ridge} = \arg\min_w \frac{1}{|\mathcal{D}|} \sum_{(x_i,y_i)\in\mathcal{D}} (y_i - x_i^T w)^2 + \lambda ||w||_2^2$$



TRAIN error:

$$\frac{1}{|\mathcal{D}|} \sum_{(x_i,y_i)\in\mathcal{D}} (y_i - x_i^T \widehat{w}^{(\lambda)}_{\mathcal{D},ridge})^2$$

TEST error:

$$\mathcal{T} \overset{i.i.d.}{\sim} P_{XY}$$

$$\frac{1}{|\mathcal{T}|} \sum_{(x_i,y_i)\in\mathcal{T}} (y_i - x_i^T \widehat{w}^{(\lambda)}_{\mathcal{D},ridge})^2$$

Important: $\mathcal{D} \cap \mathcal{T} = \emptyset$

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

Machine Learning – CSE546

Kevin Jamieson
University of Washington

April 15, 2016

How… How… How???????

- *How do we pick the regularization constant λ…*
- *How do we pick the number of basis functions…*

- We could use the test data, but…

How… How… How???????

- *How do we pick the regularization constant λ…*
- *How do we pick the number of basis functions…*

- We could use the test data, but…

- 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 train on the test data

(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 ($\mathbf{x}_j$,$\mathbf{y}_j$) moved to validation set
- **Learn classifier $f_{D\setminus j}$ with D\j dataset**
- **Estimate true error** as squared error on predicting $\mathbf{y}_j$:
  - Unbiased estimate of $\text{error}_{\text{true}}(f_{D\setminus j})$!

(LOO) Leave-one-out cross validation

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- **LOO cross validation**: Average over all data points j:
  - **For each data point you leave out, learn a new classifier $f_{D\setminus j}$**
  - **Estimate error** as:

$$\text{error}_{LOO} = \frac{1}{n}\sum_{j=1}^{n}\left(y_j - f_{\mathcal{D}\setminus j}(x_j)\right)^2$$

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! Use LOO error for model selection!!!**
  - **E.g., picking λ**

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!!!
  -

Use *k*-fold cross validation

- Randomly **divide training data into *k* equal parts**
  - $D_1,\ldots,D_k$
- For each *i*
  - **Learn classifier $f_{D\setminus Di}$ using data point not in D_i**
  - **Estimate error of $f_{D\setminus Di}$ on validation set D_i:**
- $$\text{error}_{\mathcal{D}_i} = \frac{1}{|\mathcal{D}_i|} \sum_{(x_j,y_j)\in\mathcal{D}_i} (y_j - f_{\mathcal{D}\setminus\mathcal{D}_i}(x_j))^2$$

1	2	3	4	5
Train	Train	Validation	Train	Train

Use *k*-fold cross validation

- Randomly **divide training data into *k* equal parts**
  - $D_1,\ldots,D_k$
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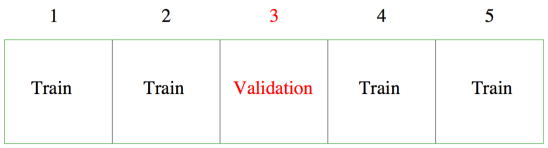

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- ***k*-fold cross validation error is average** over data splits:

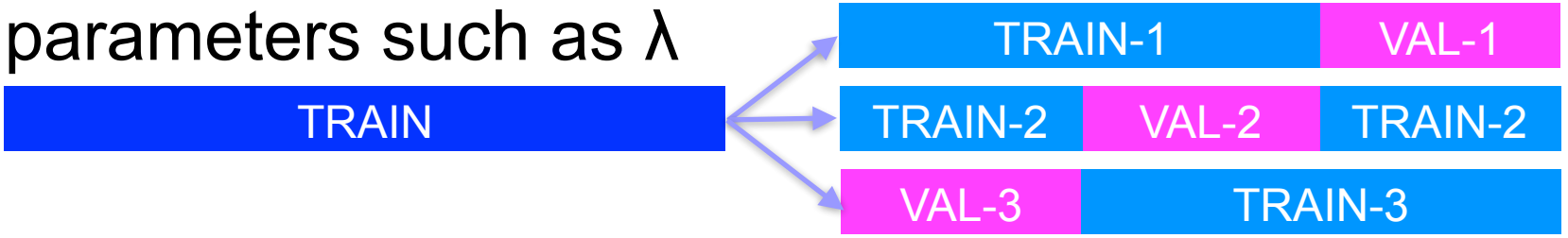
$$error_{k-fold} = \frac{1}{k}\sum_{i=1}^{k} error_{\mathcal{D}_i}$$

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

Recap

- Given a dataset, begin by splitting into

- **Model selection**: Use k-fold cross-validation on TRAIN to train predictor and choose magic parameters such as λ



- **Model assessment**: Use TEST to assess the accuracy of the model you output
  - Never ever ever ever ever train or choose parameters based on the test data

Example

- Given 10,000-dimensional data and n examples, we pick a subset of 50 dimensions that have the highest correlation with labels in the training set:

50 indices j that have largest $\frac{|\sum_{i=1}^{n} x_{i,j} y_i|}{\sqrt{\sum_{i=1}^{n} x_{i,j}^2}}$

- After picking our 50 features, we then use CV to train ridge regression with regularization λ
- What's wrong with this procedure?

Recap

- Learning is…
  - Collect some data
    - E.g., housing info and sale price
  - Randomly split dataset into TRAIN, VAL, and TEST
    - E.g., 80%, 10%, and 10%, respectively
  - Choose a hypothesis class or model
    - E.g., linear with non-linear transformations
  - Choose a loss function
    - E.g., least squares with ridge regression penalty on TRAIN
  - Choose an optimization procedure
    - E.g., set derivative to zero to obtain estimator, cross-validation on VAL to pick num. features and amount of regularization
  - Justifying the accuracy of the estimate
    - E.g., report TEST error

Warm up

Fix any $a, b, c > 0$.

1. What is the $x \in \mathbb{R}$ that minimizes $ax^2 + bx + c$

2. What is the $x \in \mathbb{R}$ that minimizes $\max\{-ax + b, cx\}$

Simple Variable Selection LASSO: Sparse Regression

Machine Learning – CSE546

Kevin Jamieson

University of Washington

April 15, 2019

Sparsity

$$\widehat{w}_{LS} = \arg\min_{w} \sum_{i=1}^{n} \left(y_i - x_i^T w\right)^2$$

- Vector **w** is sparse, if many entries are zero

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- Very useful for many tasks, e.g.,
  - **Efficiency**: If size(**w**) = 100 Billion, each prediction is expensive:
    - If **w** is sparse, prediction computation only depends on number of non-zeros
  - **Interpretability**: What are the relevant dimensions to make a prediction?
    - E.g., what are the parts of the brain associated with particular words?

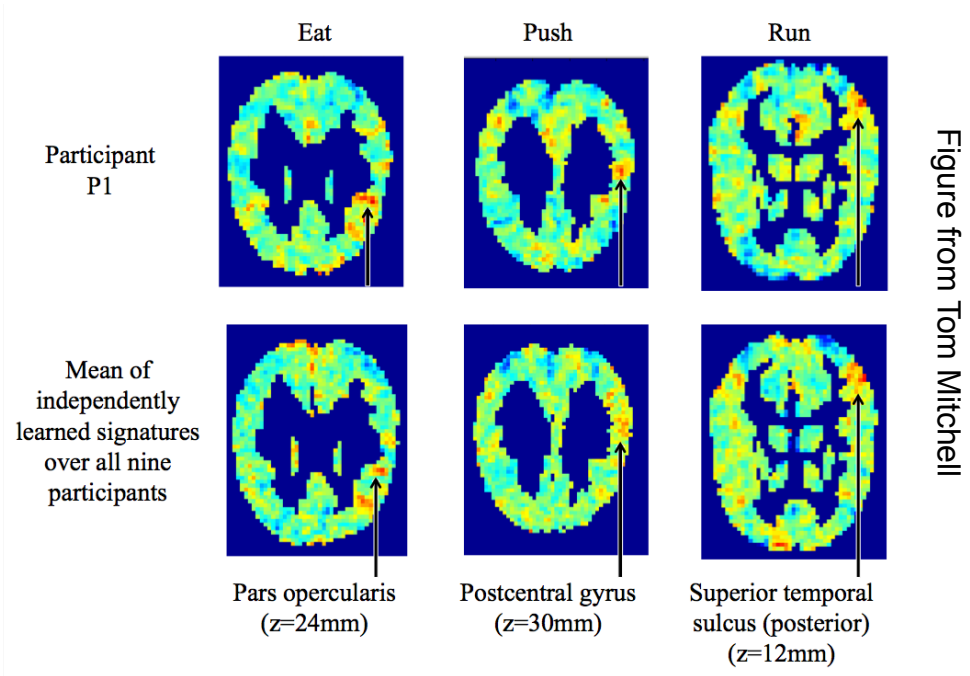

Figure from Tom Mitchell

Sparsity

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  - **Interpretability**: What are the relevant dimensions to make a prediction?
    - E.g., what are the parts of the brain associated with particular words?

- How do we find "best" subset among all possible?

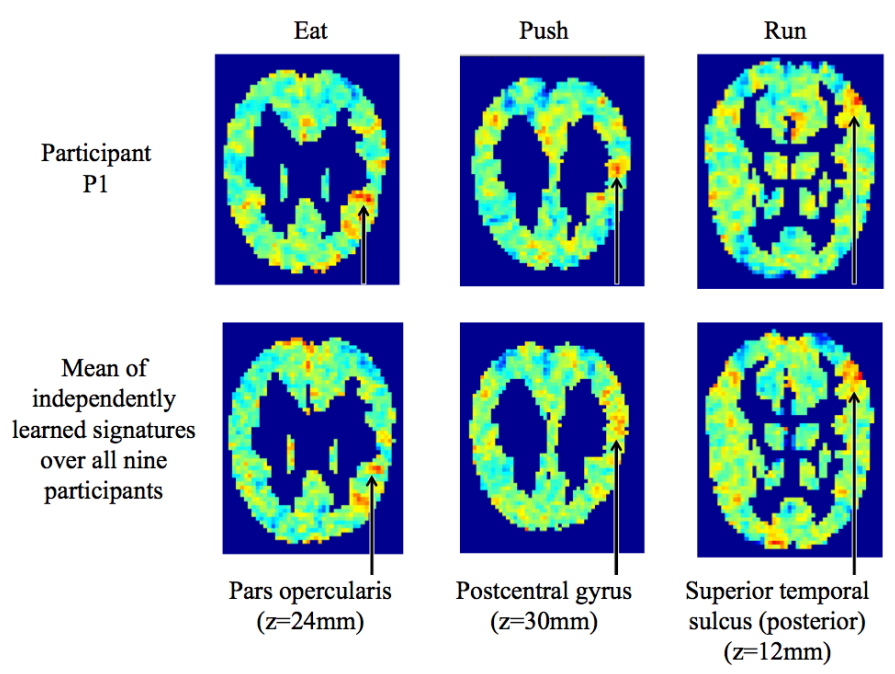


Figure from Tom Mitchell

Greedy model selection algorithm

- Pick a dictionary of features
  - e.g., cosines of random inner products
- Greedy heuristic:
  - Start from empty (or simple) set of features $F_0 = \varnothing$
  - Run learning algorithm for current set of features F_t
    - Obtain weights for these features
  - Select **next best feature $h_i(x)^*$**
    - e.g., $h_j(x)$ that results in lowest training error learner when using $F_t + \{h_j(x)^*\}$
  - $F_{t+1} \leftarrow F_t + \{h_i(x)^*\}$
  - Recurse

Greedy model selection

- Applicable in many other settings:
  - Considered later in the course:
    - Logistic regression: Selecting features (basis functions)
    - Naïve Bayes: Selecting (independent) features $P(X_i|Y)$
    - Decision trees: Selecting leaves to expand
- Only a heuristic!
  - **Finding the best set of k features is computationally intractable!**
  - Sometimes you can prove something strong about it…
-

When do we stop???

- Greedy heuristic:
  - …
  - Select **next best feature X_i^***
    - E.g. $h_j(x)$ that results in lowest training error learner when using $F_t + \{h_j(x)^*\}$
  - Recurse

When do you stop???

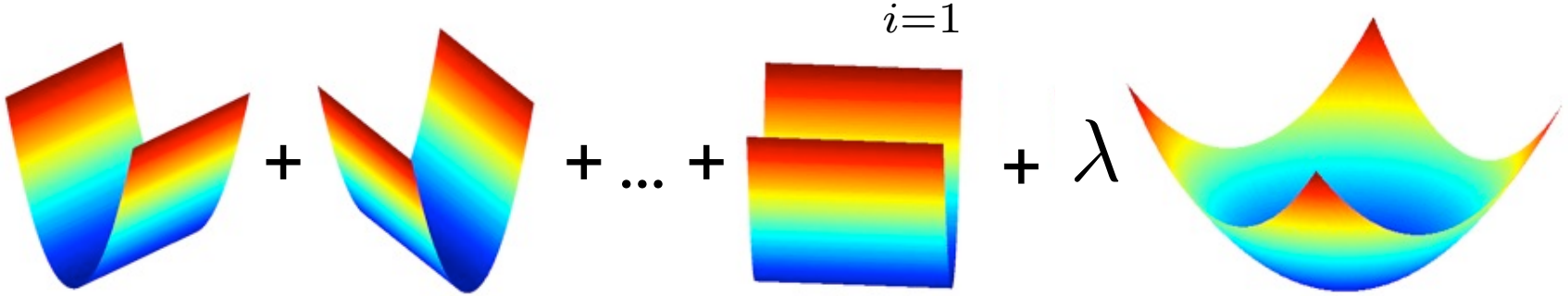
- When training error is low enough?
- When test set error is low enough?
- Using cross validation?

Is there a more principled approach?

Recall Ridge Regression

- Ridge Regression objective:

$$\widehat{w}_{ridge} = \arg\min_{w} \sum_{i=1}^{n} \left(y_i - x_i^T w\right)^2 + \lambda ||w||_2^2$$



Ridge vs. Lasso Regression

- Ridge Regression objective:

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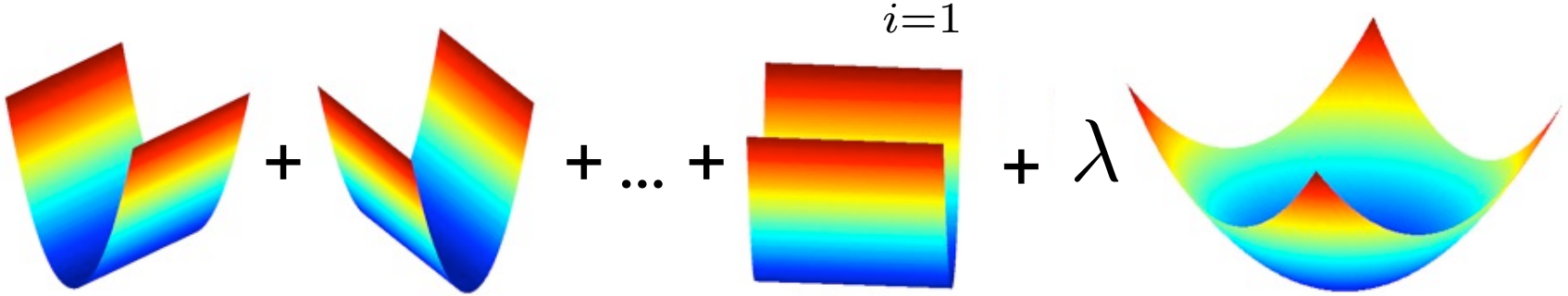
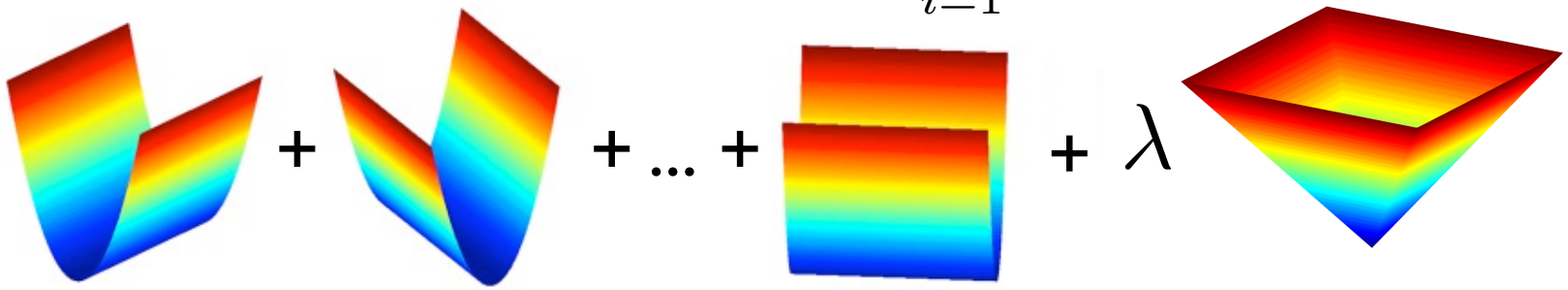


- Lasso objective:

$$\widehat{w}_{lasso} = \arg\min_{w} \sum_{i=1}^{n} \left(y_i - x_i^T w\right)^2 + \lambda ||w||_1$$



Penalized Least Squares

$$\text{Ridge} : r(w) = ||w||_2^2 \qquad \text{Lasso} : r(w) = ||w||_1$$

$$\widehat{w}_r = \arg\min_w \sum_{i=1}^{n} \left(y_i - x_i^T w\right)^2 + \lambda r(w)$$

Penalized Least Squares

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$$\widehat{w}_r = \arg\min_w \sum_{i=1}^{n} \left(y_i - x_i^T w\right)^2 + \lambda r(w)$$

For any $\lambda \geq 0$ for which $\widehat{w}_r$ achieves the minimum, there exists a $\nu \geq 0$ such that

$$\widehat{w}_r = \arg\min_w \sum_{i=1}^{n} \left(y_i - x_i^T w\right)^2 \qquad \text{subject to } r(w) \leq \nu$$

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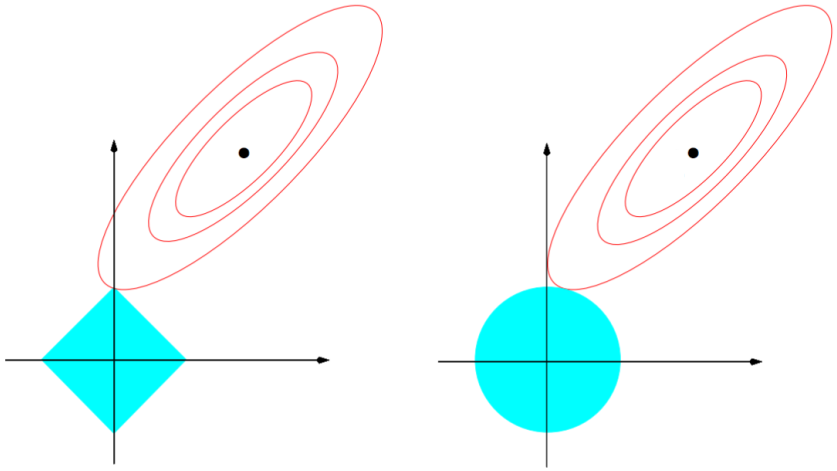

Optimizing the LASSO Objective

- LASSO solution:

$$\widehat{w}_{lasso}, \widehat{b}_{lasso} = \arg\min_{w,b} \sum_{i=1}^{n} \left(y_i - (x_i^T w + b)\right)^2 + \lambda ||w||_1$$

$$\widehat{b}_{lasso} = \arg\min_{w,b} \frac{1}{n} \sum_{i=1}^{n} \left(y_i - x_i^T \widehat{w}_{lasso}\right))$$

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$$\widehat{b}_{lasso} = \arg\min_{w,b} \frac{1}{n} \sum_{i=1}^{n} \left(y_i - x_i^T \widehat{w}_{lasso}\right)$$

So as usual, preprocess to make sure that $\frac{1}{n}\sum_{i=1}^{n} y_i = 0, \frac{1}{n}\sum_{i=1}^{n} x_i = \mathbf{0}$

so we don't have to worry about an offset.

Optimizing the LASSO Objective

- LASSO solution:

$$\widehat{w}_{lasso}, \widehat{b}_{lasso} = \arg\min_{w,b} \sum_{i=1}^{n} \left(y_i - (x_i^T w + b)\right)^2 + \lambda ||w||_1$$

$$\widehat{b}_{lasso} = \arg\min_{w,b} \frac{1}{n} \sum_{i=1}^{n} \left(y_i - x_i^T \widehat{w}_{lasso}\right)$$

So as usual, preprocess to make sure that $\frac{1}{n}\sum_{i=1}^{n} y_i = 0, \frac{1}{n}\sum_{i=1}^{n} x_i = \mathbf{0}$

so we don't have to worry about an offset.

$$\widehat{w}_{lasso} = \arg\min_{w} \sum_{i=1}^{n} \left(y_i - x_i^T w\right)^2 + \lambda ||w||_1$$

How do we solve this?

Coordinate Descent

- Given a function, we want to find minimum
- Often, it is easy to find minimum along a single coordinate:
- How do we pick next coordinate?
- Super useful approach for *many* problems
  - Converges to optimum in some cases, such as LASSO

Optimizing LASSO Objective One Coordinate at a Time

Fix any $j \in \{1, \ldots, d\}$

$$\sum_{i=1}^{n} \left(y_i - x_i^T w\right)^2 + \lambda ||w||_1 = \sum_{i=1}^{n} \left(y_i - \sum_{k=1}^{d} x_{i,k}\, w_k \right)^2 + \lambda \sum_{k=1}^{d} |w_k|$$

$$= \sum_{i=1}^{n} \left(\left(y_i - \sum_{k \neq j} x_{i,k}\, w_k \right) - x_{i,j}\, w_j \right)^2 + \lambda \sum_{k \neq j} |w_k| + \lambda |w_j|$$

Optimizing LASSO Objective One Coordinate at a Time

Fix any $j \in \{1, \ldots, d\}$

$$\sum_{i=1}^{n} \left(y_i - x_i^T w\right)^2 + \lambda ||w||_1 = \sum_{i=1}^{n} \left(y_i - \sum_{k=1}^{d} x_{i,k}\, w_k\right)^2 + \lambda \sum_{k=1}^{d} |w_k|$$

$$= \sum_{i=1}^{n} \left(\left(y_i - \sum_{k \neq j} x_{i,k}\, w_k\right) - x_{i,j}\, w_j\right)^2 + \lambda \sum_{k \neq j} |w_k| + \lambda |w_j|$$

Initialize $\widehat{w}_k = 0$ for all $k \in \{1, \ldots, d\}$

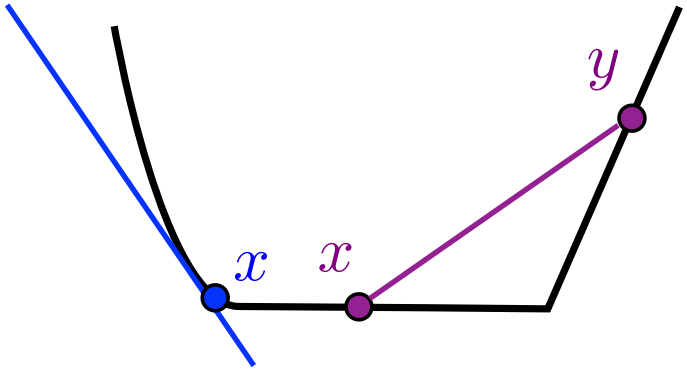
Loop over $j \in \{1, \ldots, n\}$:

$$r_i^{(j)} = \sum_{k \neq j} x_{i,j} \widehat{w}_k$$

$$\widehat{w}_j = \arg\min_{w_j} \sum_{i=1}^{n} \left(r_i^{(j)} - x_{i,j}\, w_j\right)^2 + \lambda |w_j|$$

Convex Functions

- Equivalent definitions of convexity:



f convex:

$$f(\lambda x + (1-\lambda)y) \leq \lambda f(x) + (1-\lambda) f(y) \qquad \forall x, y, \lambda \in [0,1]$$

$$f(y) \geq f(x) + \nabla f(x)^T (y - x) \qquad \forall x, y$$

- **Gradients** lower bound convex functions and are unique at **x** iff function differentiable at **x**
- **Subgradients** generalize gradients to non-differentiable points:
  - Any supporting hyperplane at **x** that lower bounds entire function

$$g \text{ is a subgradient at } x \text{ if } f(y) \geq f(x) + g^T (y - x)$$

Taking the Subgradient

$$\widehat{w}_j = \arg\min_{w_j} \sum_{i=1}^{n} \left(r_i^{(j)} - x_{i,j}\, w_j \right)^2 + \lambda |w_j|$$

g is a subgradient at x if $f(y) \geq f(x) + g^T(y - x)$

- Convex function is minimized at w if 0 is a sub-gradient at w.

$$\partial_{w_j} |w_j| =$$

$$\partial_{w_j} \sum_{i=1}^{n} \left(r_i^{(j)} - x_{i,j}\, w_j \right)^2 =$$

Setting Subgradient to 0

$$\partial_{w_j}\left(\sum_{i=1}^{n}\left(r_i^{(j)} - x_{i,j}\, w_j\right)^2 + \lambda|w_j|\right) = \begin{cases} a_j w_j - c_j - \lambda & \text{if } w_j < 0 \\ [-c_j - \lambda, -c_j + \lambda] & \text{if } w_j = 0 \\ a_j w_j - c_j + \lambda & \text{if } w_j > 0 \end{cases}$$

$$a_j = (\sum_{i=1}^{n} x_{i,j}^2) \qquad c_j = 2(\sum_{i=1}^{n} r_i^{(j)} x_{i,j})$$

Setting Subgradient to 0

$$\partial_{w_j}\left(\sum_{i=1}^{n}\left(r_i^{(j)}-x_{i,j}\,w_j\right)^2+\lambda|w_j|\right)=\begin{cases}a_jw_j-c_j-\lambda & \text{if } w_j<0\\ [-c_j-\lambda,-c_j+\lambda] & \text{if } w_j=0\\ a_jw_j-c_j+\lambda & \text{if } w_j>0\end{cases}$$

$$a_j=(\sum_{i=1}^{n}x_{i,j}^2)\qquad c_j=2(\sum_{i=1}^{n}r_i^{(j)}x_{i,j})$$

$$\widehat{w}_j=\arg\min_{w_j}\sum_{i=1}^{n}\left(r_i^{(j)}-x_{i,j}\,w_j\right)^2+\lambda|w_j|$$

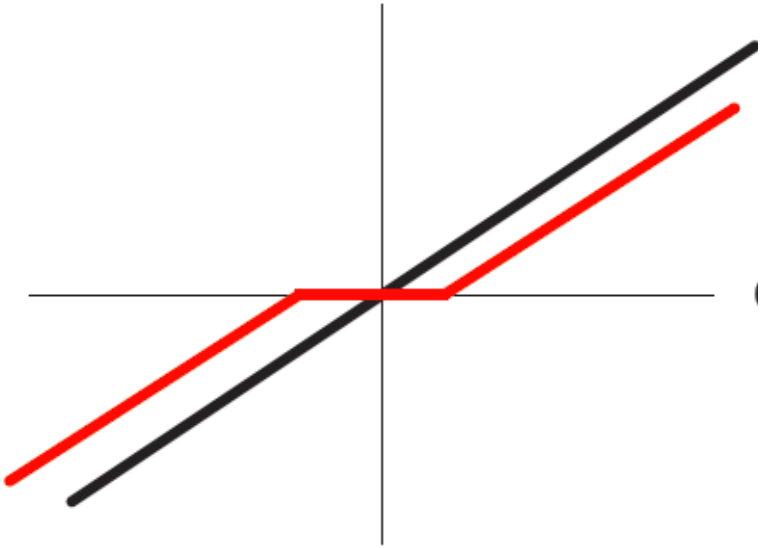
w is a minimum if
0 is a sub-gradient at w

$$\widehat{w}_j=\begin{cases}(c_j+\lambda)/a_j & \text{if } c_j<-\lambda\\ 0 & \text{if } |c_j|\le\lambda\\ (c_j-\lambda)/a_j & \text{if } c_j>\lambda\end{cases}$$

Soft Thresholding

$$\widehat{w}_j = \begin{cases} (c_j + \lambda)/a_j & \text{if } c_j < -\lambda \\ 0 & \text{if } |c_j| \leq \lambda \\ (c_j - \lambda)/a_j & \text{if } c_j > \lambda \end{cases}$$

$$a_j = \sum_{i=1}^{n} x_{i,j}^2 \qquad c_j = 2\sum_{i=1}^{n} \left(y_i - \sum_{k \neq j} x_{i,k}\, w_k \right) x_{i,j}$$



Coordinate Descent for LASSO (aka Shooting Algorithm)

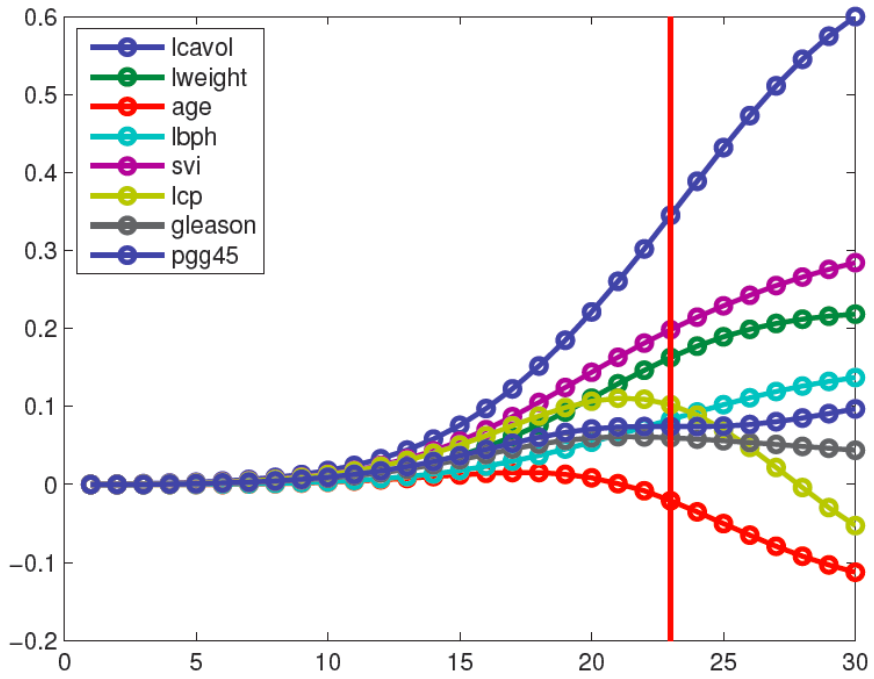
- Repeat until convergence
  - Pick a coordinate *l* at (random or sequentially)
    - Set:
    - Where:

$$\widehat{w}_j = \begin{cases} (c_j + \lambda)/a_j & \text{if } c_j < -\lambda \\ 0 & \text{if } |c_j| \leq \lambda \\ (c_j - \lambda)/a_j & \text{if } c_j > \lambda \end{cases}$$

$$a_j = \sum_{i=1}^{n} x_{i,j}^2 \qquad c_j = 2 \sum_{i=1}^{n} \left(y_i - \sum_{k \neq j} x_{i,k}\, w_k \right) x_{i,j}$$

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

Recall: *Ridge Coefficient Path*



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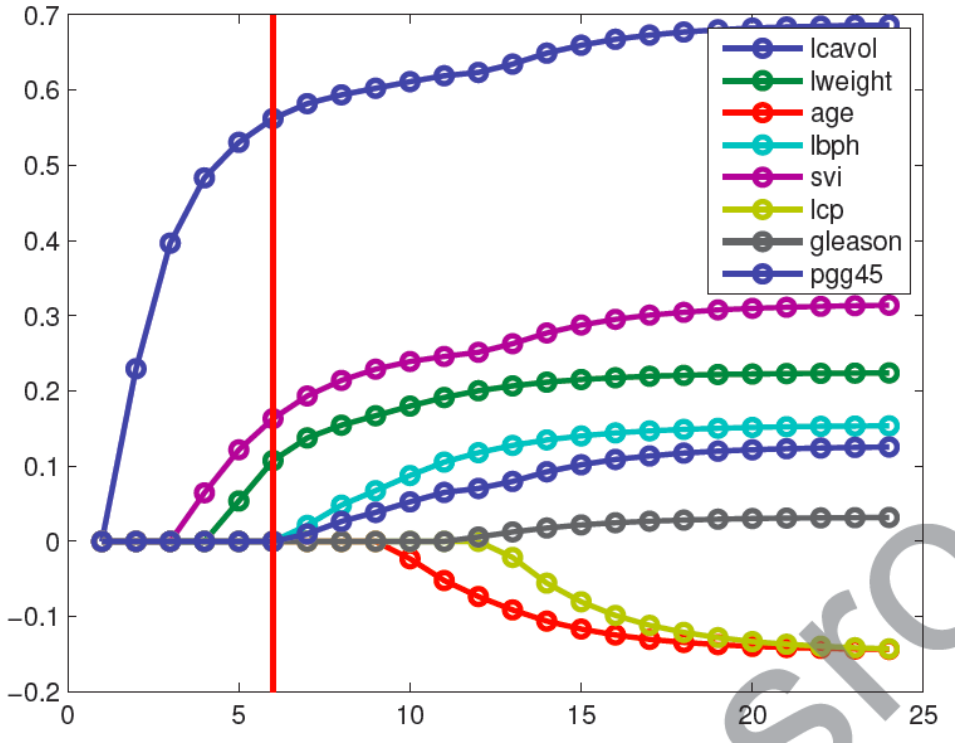
- Typical approach: select λ using cross validation

Now: *LASSO Coefficient Path*



From
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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 regression
  - 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 simple approach for solving LASSO