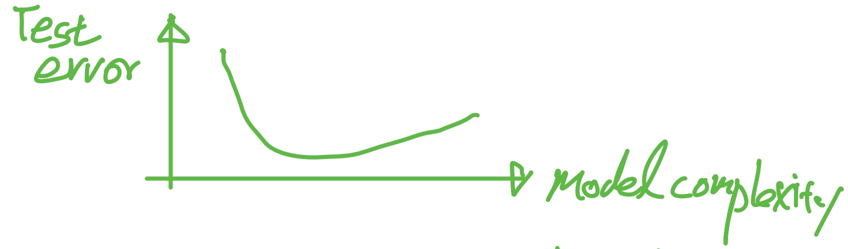
Lecture 5: Regularization

- how to avoid overfitting.

Bias-Variance Tradeoff



• polynomial degree

• # of features.

↑

human engineered.

Ridge-regression ← Regularization

How to avoid overfitting automatically.

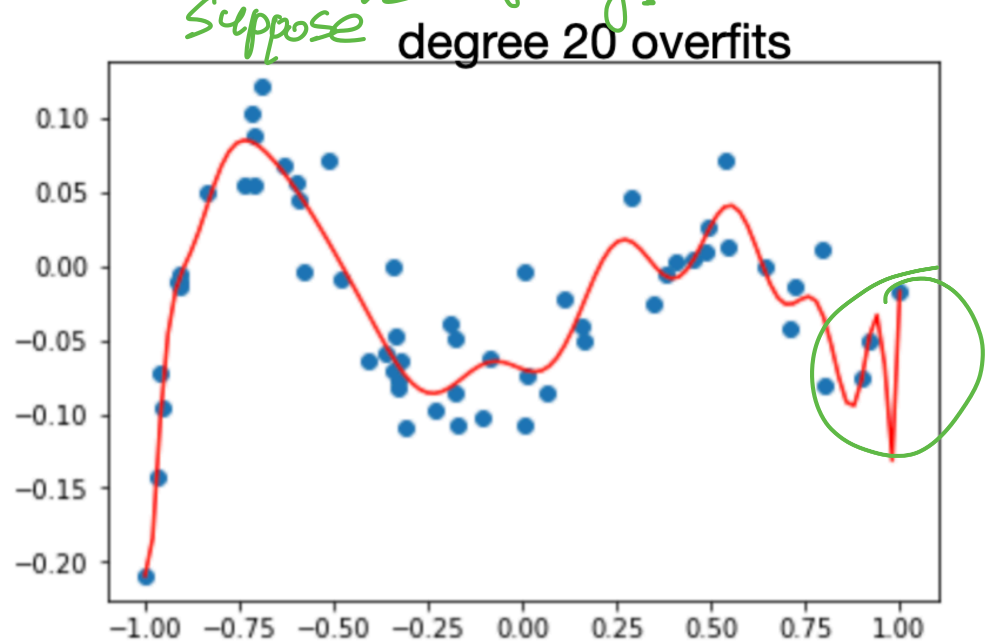
Sensitivity: how much prediction changes as we change the input

- For a linear model,
  $$y \simeq b + w_1x_1 + w_2x_2 + \cdots + w_dx_d$$
  if $|w_j|$ is large then the prediction is sensitive to small changes in x_j

the train set   test error ≠ train error

- Large ***sensitivity*** leads to overfitting and poor generalization, and equivalently models that overfit tend to have large weights
- Note that b is a constant and hence there is no sensitivity for the offset b

Suppose we are fitting.



Sensitivity: how much prediction changes as we change the input

- For a linear model,
  $$y \simeq b + w_1 x_1 + w_2 x_2 + \cdots + w_d x_d$$
  if $|w_j|$ is large then the prediction is sensitive to small changes in x_j
- Large ***sensitivity*** leads to overfitting and poor generalization, and equivalently models that overfit tend to have large weights
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first algorithm to use regularization

$= w_1^2 + w_2^2 + \cdots + w_d^2$

- In ***Ridge Regression***, we use a regularizer $\|w\|_2^2$ to measure and control the sensitivity of the predictor
- And optimize for small loss and small sensitivity, by adding a ***regularizer*** in the objective (assume no offset for now)

$$\hat{w}_{\text{ridge}} = \arg\min_{w} \left\{ \sum_{i=1}^{n} \underbrace{(y_i - x_i^T w)^2}_{\text{error}} + \overbrace{\underset{\mathbb{R}^+}{\lambda} \underbrace{\|w\|_2^2}_{\text{sensitivity}}}^{\text{regularizer}} \right\}$$

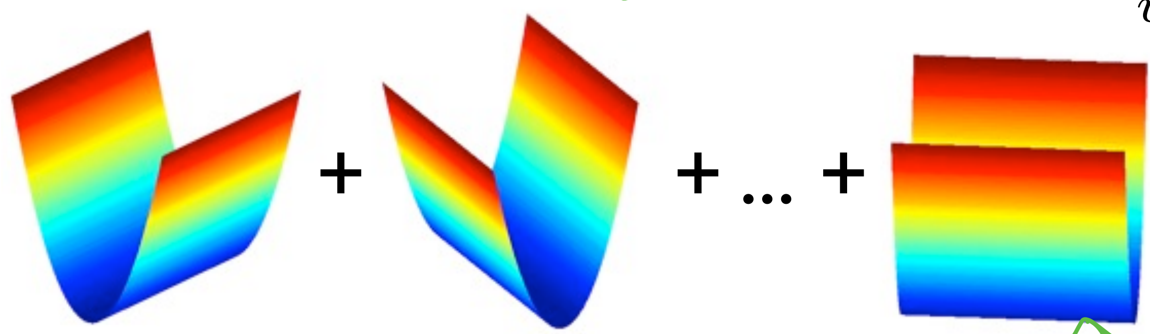
regularization coefficient

Ridge Regression

mean squared error

- (Original) $\boxed{\text{Least squares}}$ objective:

$$\hat{w}_{MLE} = \hat{w}_{LS} = \arg\min_w \sum_{i=1}^{n} \underbrace{\left(y_i - x_i^T w\right)^2}_{\substack{\text{strictly} \\ \text{1-direction: Quadratic} \\ \text{d-1 directions: flat}}}$$

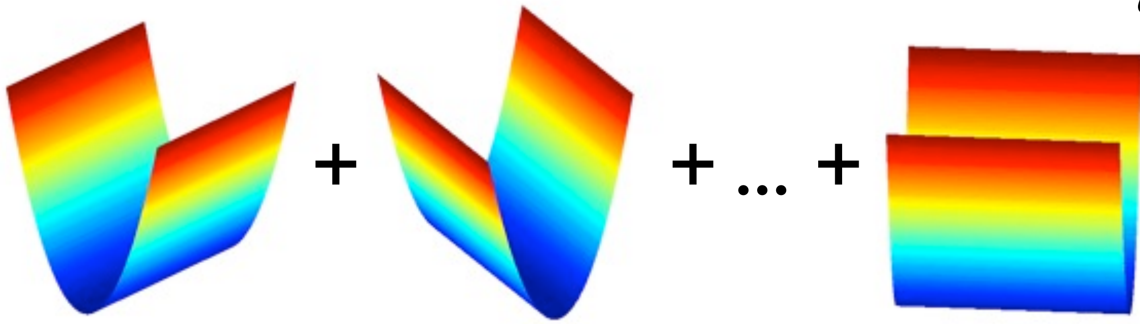


$$\text{e.g., } f(w_1, w_2) = \underbrace{(\underset{y}{1} - \overset{\overset{x^T}{[x_1, x_2]}}{[1,0]} \begin{bmatrix} w_1 \\ w_2 \end{bmatrix})^2}_{f_1(w_1,w_2) = (1-w_1)^2} + \underbrace{(2 - [0,1] \begin{bmatrix} w_1 \\ w_2 \end{bmatrix})^2}_{f_2(w_1,w_2) = (2-w_2)^2}$$

Ridge Regression

- (Original) Least squares objective:

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

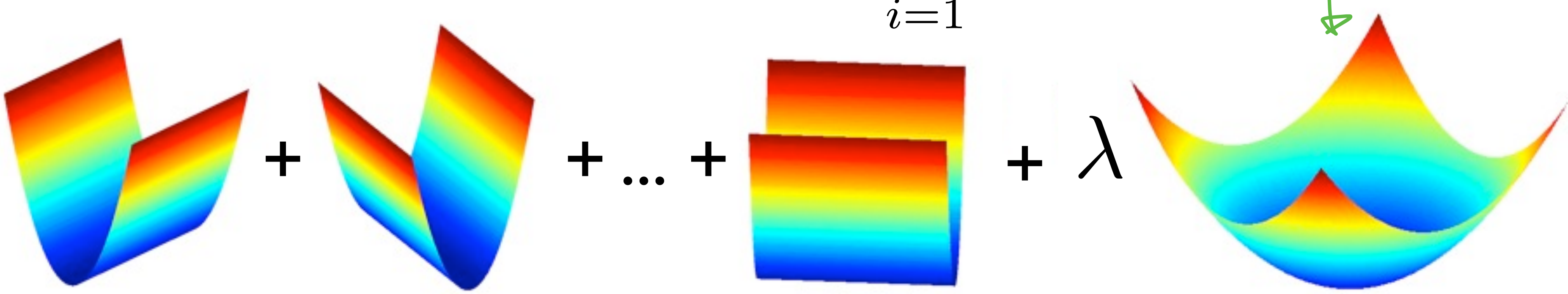


- Ridge Regression objective:

$w_1^2 + w_2^2$

$\|$

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



Minimizing the Ridge Regression Objective

$$\hat{w}_{\text{ridge}} = \arg\min_{w} \|y - Xw\|_2^2 + \lambda \|w\|_2^2$$

$$= (y-Xw)^T(y-Xw) + \lambda \cdot w^T w$$

$$= -2X^T(y-Xw) + 2\lambda \cdot w = 0$$

$$X^TXw + \lambda \cdot w = X^Ty$$

$$(X^TX + \lambda \mathbb{I}_{d\times d})\, w = X^Ty$$

$$\begin{bmatrix} 1 & & 0 \\ & \ddots & \\ 0 & & 1 \end{bmatrix}$$

$$\hat{w}_{\text{ridge}} = \underline{(X^TX + \lambda \mathbb{I}_{d\times d})}^{-1} \cdot X^Ty.$$

$$\hat{w}_{MLE} = (X^TX)^{-1} X^Ty$$

for Symmetric B

Scalar derivative			vector gradient		
$f(x)$	$\rightarrow$	$\frac{df}{dx}$	$f(\mathbf{x})$	$\rightarrow$	$\nabla_x f(x)$
bx	$\rightarrow$	b	$\mathbf{x}^T\mathbf{B}$	$\rightarrow$	$\mathbf{B}$
bx	$\rightarrow$	b	$\mathbf{x}^T\mathbf{b}$	$\rightarrow$	$\mathbf{b}$
x^2	$\rightarrow$	$2x$	$\mathbf{x}^T\mathbf{x}$	$\rightarrow$	$2\mathbf{x}$
bx^2	$\rightarrow$	$2bx$	$\mathbf{x}^T\mathbf{B}\mathbf{x}$	$\rightarrow$	$2\mathbf{B}\mathbf{x}$

Shrinkage Properties

$$\hat{w}_{\text{ridge}} = \arg\min_w \|y - Xw\|_2^2 + \lambda\|w\|_2^2$$
$$= (\mathbf{X}^T\mathbf{X} + \lambda I)^{-1}\mathbf{X}^T\mathbf{y}$$

$\hat{w}_{MLE} = (X^TX)^{-1}X^Ty$

To get some intuition, suppose input X satisfies $\boxed{X^TX = n\mathbf{I}_{d\times d},}$

$\hat{w}_{ridge} = (n\mathbb{I} + \lambda\mathbb{I})^{-1}X^Ty$

$= \left(\frac{1}{n+\lambda}\right)X^Ty$

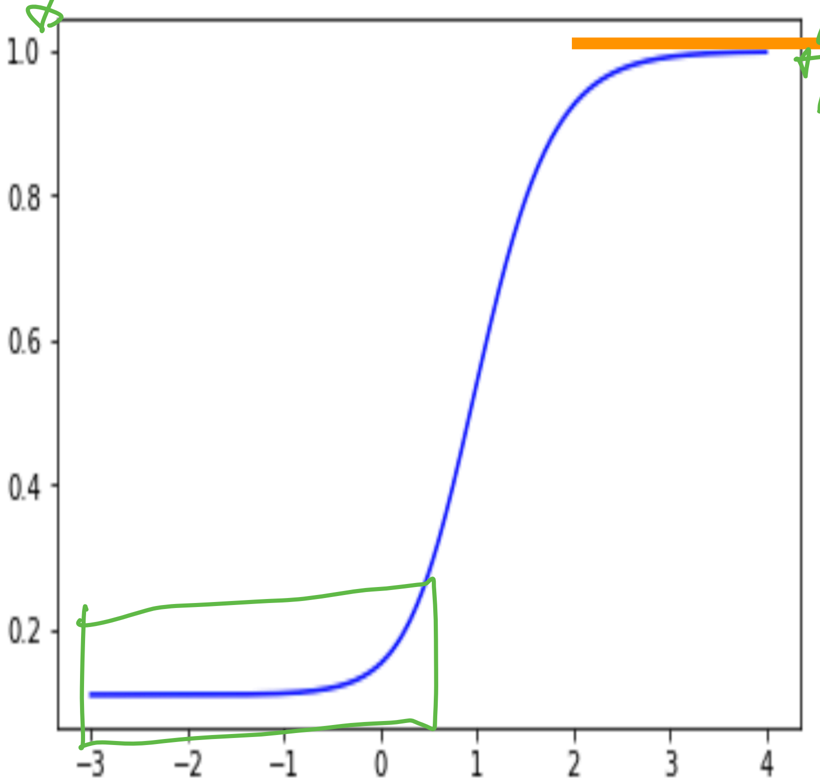
- When $\lambda = 0$, this recovers the least squares model, as a special case
- This defines a family of models hyper-parametrized by λ
- Large λ means more regularization and simpler model with smaller $|w_j|$
- Small λ means less regularization and more complex model with larger $|w_j|$

Ridge regression: minimize $\sum_{i=1}^{n}(w^T x_i - y_i)^2 + \lambda \|w\|_2^2$

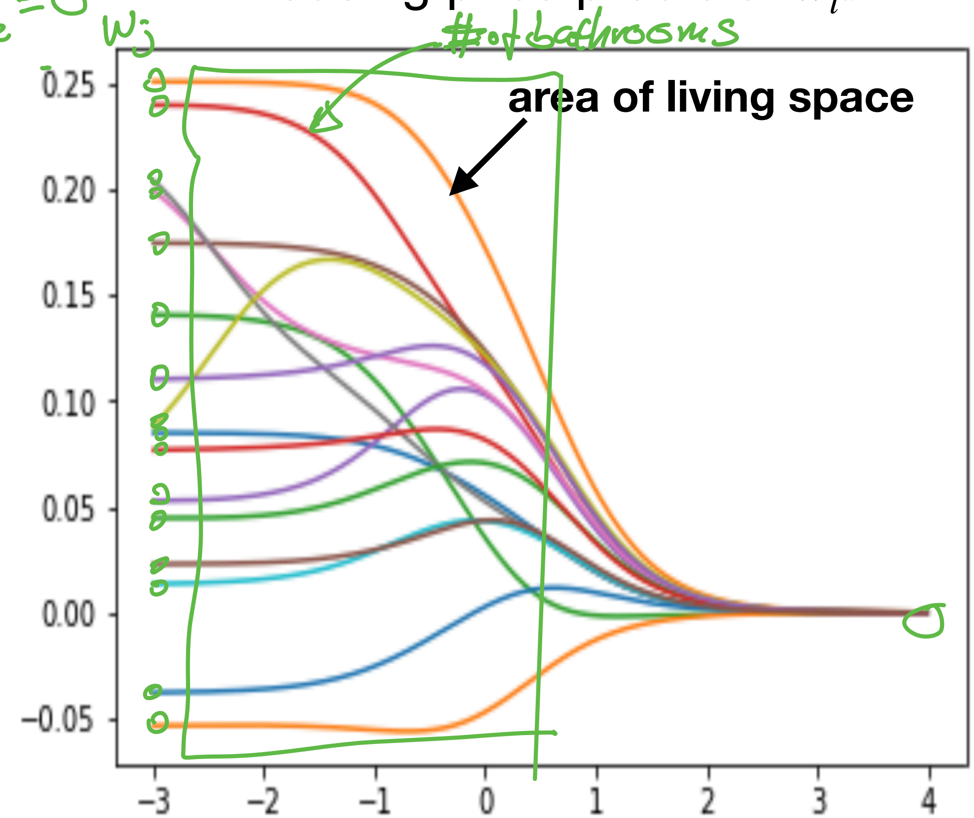
training MSE $\frac{1}{n}\sum_{i=1}^{n}(y_i - x_i^T \hat{w}^{(\lambda)}_{\text{ridge}})^2$

$\hat{w}^{(\infty)}_{\text{ridge}} = 0$

$\frac{1}{n}\sum_{i=1}^{n} y_i^2$



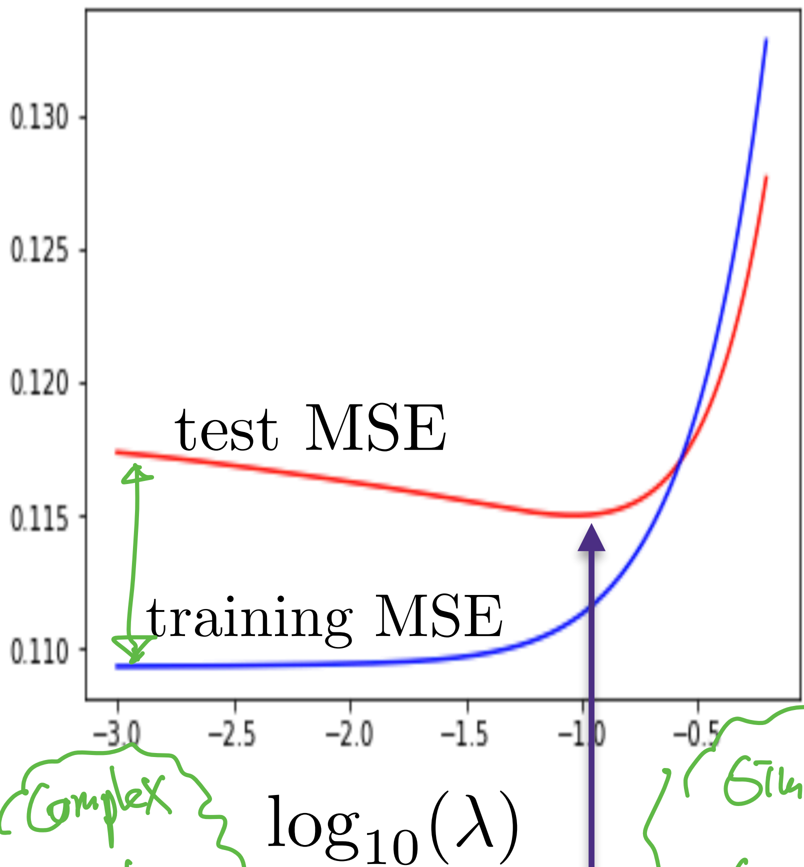
Housing price predictor $w_i's$



which model is more complex?

- Left plot: leftmost training error is with no regularization: 0.1093
- Left plot: rightmost training error is variance of the training data: 0.9991
- Right plot: called **regularization path**

Ridge regression: minimize $\sum_{i=1}^{n}(w^T x_i - y_i)^2 + \lambda\|w\|_2^2$

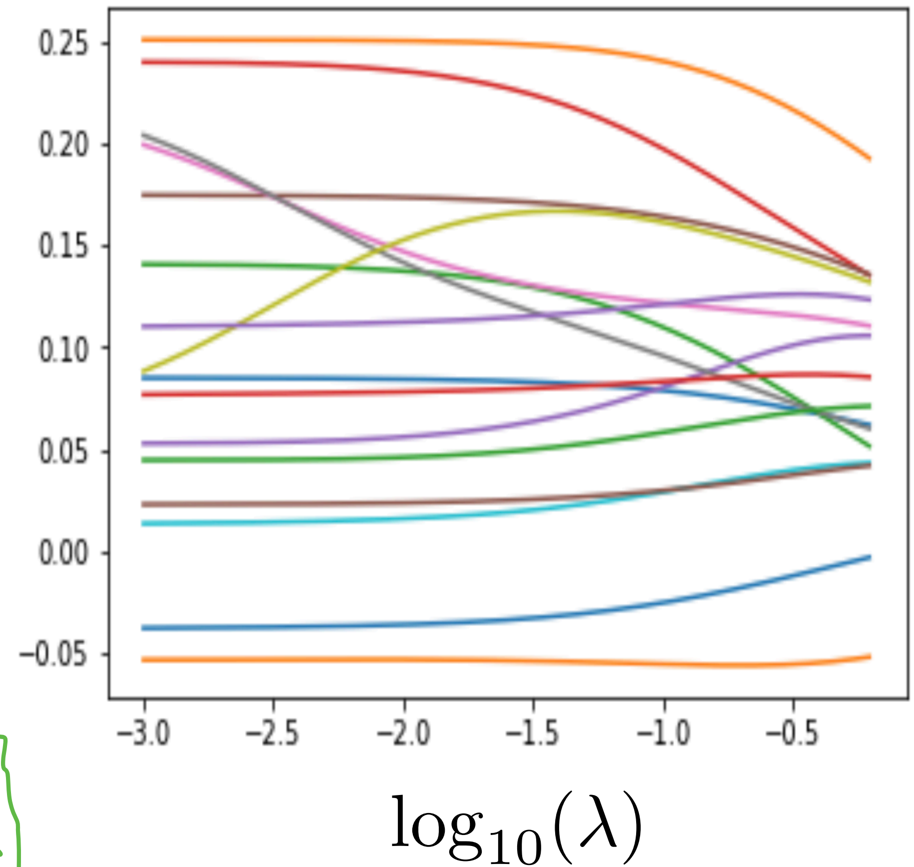


Complex
Bias ↓
Fit data ↑

model complexity

Simple
Generalize ↑
Variance ↓

Housing price predictor $w_i's$



- as we increase λ, this gain in test MSE comes from shrinking w's to get a less sensitive predictor (which in turn reduces the variance)
- this is the role of regularizer

Bias-Variance Properties

role λ.

- Recall: $\hat{w}_{\text{ridge}} = (\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I})^{-1}\mathbf{X}^T\mathbf{y}$
- To analyze bias-variance tradeoff, we need to assume probabilistic generative model: $x_i \sim P_X$, $\mathbf{y} = \mathbf{X}w + \epsilon$, $\epsilon \sim \mathcal{N}(0,\sigma^2\mathbf{I})$ for some ground truth model parameter w
- The true error at a sample with feature x is

$$\mathbb{E}_{y,\mathcal{D}_{\text{train}}|x}[(y - x^T\hat{w}_{\text{ridge}})^2 \,|\, x] = \mathbb{E}\Big[\big(\underbrace{y - \mathbb{E}[y|x]}_{A} + \underbrace{\mathbb{E}[y|x] - x^T\hat{w}_{\text{ridge}}}_{B} \big)^2 \Big]$$

$$= \underbrace{\mathbb{E}\big[(y - \overbrace{\mathbb{E}[y|x]}^{\eta(x)})^2 \big]}_{\text{irreducible error}} + \underbrace{\mathbb{E}\big[(\mathbb{E}[y|x] - x^T\hat{w}_{\text{ridge}})^2 \big]}_{\text{learning error}}$$

Bias-Variance Properties

- Recall: $\hat{w}_{\text{ridge}} = (\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I})^{-1}\mathbf{X}^T\mathbf{y}$
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$$\mathbb{E}_{y,\mathcal{D}_{\text{train}}|x}[(y - x^T\hat{w}_{\text{ridge}})^2 \,|\, x]$$

$$= \underbrace{\mathbb{E}_{y|x}[(y - \mathbb{E}[y\,|\,x])^2 \,|\, x]}_{\text{Irreducible Error}} + \underbrace{\mathbb{E}_{\mathcal{D}_{\text{train}}}[(\mathbb{E}[y\,|\,x] - x^T\hat{w}_{\text{ridge}})^2 \,|\, x]}_{\text{Learning Error}}$$

$$\mathbb{E}[(x^Tw + \varepsilon - x^Tw)^2]$$

$$= \mathbb{E}\varepsilon^2 = \sigma^2$$

$$\underbrace{\mathbb{E}[(x^T\hat{w}_{\text{ridge}} - \mathbb{E}[x^T\hat{w}_{\text{ridge}}])^2]}_{\text{Variance}} + \mathbb{E}[(\mathbb{E}[x^T\hat{w}_{\text{ridge}}] - \underbrace{\mathbb{E}[y|x]}_{= x^Tw})^2]$$

Bias-Variance Properties

- Recall: $\hat{w}_{\text{ridge}} = (\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I})^{-1}\mathbf{X}^T\mathbf{y}$
- To analyze bias-variance tradeoff, we need to assume probabilistic generative model: $x_i \sim P_X, \;\; \mathbf{y} = \mathbf{X}w + \epsilon, \;\; \epsilon \sim \mathcal{N}(0, \sigma^2\mathbf{I})$
- The true error at a sample with feature x is

$$\mathbb{E}_{y,\mathcal{D}_{\text{train}}|x}[(y - x^T\hat{w}_{\text{ridge}})^2 \mid x]$$

$$= \mathbb{E}_{y|x}[(y - \mathbb{E}[y \mid x])^2 \mid x] + \mathbb{E}_{\mathcal{D}_{\text{train}}}[(\mathbb{E}[y \mid x] - x^T\hat{w}_{\text{ridge}})^2 \mid x]$$

$$= \mathbb{E}_{y|x}[(y - x^Tw)^2 \mid x] + \mathbb{E}_{\mathcal{D}_{\text{train}}}[(x^Tw - x^T\hat{w}_{\text{ridge}})^2 \mid x]$$

Bias-Variance Properties

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$$= \mathbb{E}_{y|x}[(y - x^Tw)^2 \,|\, x] + \mathbb{E}_{\mathcal{D}_{\text{train}}}[(x^Tw - x^T\hat{w}_{\text{ridge}})^2 \,|\, x]$$

$$= \underbrace{\sigma^2}_{\text{Irreduc. Error}} + \underbrace{(x^Tw - \mathbb{E}_{\tilde{\mathcal{D}}_{\text{train}}}[x^T\hat{w}_{\text{ridge}}\,|\,x])^2}_{\text{Bias-squared}} + \underbrace{\mathbb{E}_{\mathcal{D}_{\text{train}}}[(\mathbb{E}_{\tilde{\mathcal{D}}_{\text{train}}}[x^T\hat{w}_{\text{ridge}}\,|\,x] - x^T\hat{w}_{\text{ridge}})^2 \,|\, x]}_{\text{Variance}}$$

Bias-Variance Properties

- Recall: $\hat{w}_{\text{ridge}} = (\mathbf{X}^T\mathbf{X} + \lambda \mathbf{I})^{-1}\mathbf{X}^T\mathbf{y}$ $= \frac{1}{n+\lambda} \cdot X^T(Xw + \varepsilon)$
  $= \frac{1}{n+\lambda}(n \cdot w + x^T\varepsilon)$
- To analyze bias-variance tradeoff, we need to assume probabilistic generative model: $x_i \sim P_X$, $\mathbf{y} = \mathbf{X}w + \epsilon$, $\epsilon \sim \mathcal{N}(0,\sigma^2\mathbf{I})$
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$$= \mathbb{E}_{y|x}[(y - x^Tw)^2 \mid x] + \mathbb{E}_{\mathcal{D}_{\text{train}}}[(x^Tw - x^T\hat{w}_{\text{ridge}})^2 \mid x]$$

$$= \underbrace{\sigma^2}_{\text{Irreduc. Error}} + \underbrace{(x^Tw - \mathbb{E}_{\mathcal{D}_{\text{train}}}[x^T\hat{w}_{\text{ridge}} \mid x])^2}_{\text{Bias-squared}} + \underbrace{\mathbb{E}_{\mathcal{D}_{\text{train}}}[(\mathbb{E}_{\tilde{\mathcal{D}}_{\text{train}}}[x^T\hat{w}_{\text{ridge}} \mid x] - x^T\hat{w}_{\text{ridge}})^2 \mid x]}_{\text{Variance}}$$

$\boxed{\text{Suppose } \mathbf{X}^T\mathbf{X} = n\mathbf{I},}$ then $\hat{w}_{\text{ridge}} = (\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I})^{-1}\mathbf{X}^T(\mathbf{X}w + \epsilon)$

$$= \frac{n}{n+\lambda}w + \frac{1}{n+\lambda}\mathbf{X}^T\epsilon$$

Bias-Variance Properties

Suppose $\boxed{\mathbf{X}^T\mathbf{X} = n\mathbf{I},}$ then

$$\hat{w}_{\text{ridge}} = \frac{n}{n+\lambda}w + \frac{1}{n+\lambda}\mathbf{X}^T\epsilon$$

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$$= \mathbb{E}_{y|x}[(y - x^Tw)^2 \,|\, x] + \mathbb{E}_{\mathcal{D}_{\text{train}}}[(x^Tw - x^T\hat{w}_{\text{ridge}})^2 \,|\, x]$$

$$= \sigma^2 + (x^Tw - \mathbb{E}_{\mathcal{D}_{\text{train}}}[x^T\hat{w}_{\text{ridge}} \,|\, x])^2 + \mathbb{E}_{\mathcal{D}_{\text{train}}}[(\mathbb{E}_{\tilde{\mathcal{D}}_{\text{train}}}[x^T\hat{w}_{\text{ridge}} \,|\, x] - x^T\hat{w}_{\text{ridge}})^2 \,|\, x]$$

$\frac{n}{n+\lambda} x^Tw$

(verify at home)

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

The missing calculation from previous slide

Claim: $(x^T w - \mathbb{E}_{\mathcal{D}_{\text{train}}}[x^T \hat{w}_{\text{ridge}} \,|\, x])^2 = \frac{\lambda^2}{(n+\lambda)^2}(w^T x)^2$

proof: $(x^T w - \mathbb{E}_{\mathcal{D}_{\text{train}}}[x^T \hat{w}_{\text{ridge}} \,|\, x])^2 = \left(x^T w - \mathbb{E}\Big[\frac{n}{n+\lambda} x^T w + \frac{1}{n+\lambda} x^T X \epsilon\Big]\right)^2$

using $\mathbb{E}[\epsilon] = 0$

$$= \left(x^T w - \frac{n}{n+\lambda} x^T w\right)^2$$

$$= \frac{\lambda^2}{(n+\lambda)^2}(w^T x)^2$$

$\boxed{\text{Suppose } \mathbf{X}^T\mathbf{X} = n\mathbf{I},}$ then

$$\hat{w}_{\text{ridge}} = \frac{n}{n+\lambda} w + \frac{1}{n+\lambda} \mathbf{X}^T \epsilon$$

The missing calculation from previous slide

Claim: $\mathbb{E}_{\mathcal{D}_{\text{train}}}[(\mathbb{E}_{\tilde{\mathcal{D}}_{\text{train}}}[x^T\hat{w}_{\text{ridge}}\,|\,x] - x^T\hat{w}_{\text{ridge}})^2\,|\,x] = \frac{\sigma^2 n}{(n+\lambda)^2}\|x\|_2^2$

proof: $\mathbb{E}_{\mathcal{D}_{\text{train}}}[(\mathbb{E}_{\tilde{\mathcal{D}}_{\text{train}}}[x^T\hat{w}_{\text{ridge}}\,|\,x] - x^T\hat{w}_{\text{ridge}})^2\,|\,x]$

$$= \mathbb{E}\Big[\Big(\mathbb{E}\Big[\frac{n}{n+\lambda}x^T w + \frac{1}{n+\lambda}x^T X^T \epsilon\Big] - x^T\hat{w}_{\text{ridge}}\Big)^2\Big]$$

using $\mathbb{E}[\epsilon] = 0$
$$= \mathbb{E}\Big[\Big(\frac{n}{n+\lambda}x^T w - x^T\hat{w}_{\text{ridge}}\Big)^2\Big]$$

$$= \mathbb{E}\Big[\Big(\frac{1}{n+\lambda}x^T X^T \epsilon\Big)^2\Big]$$

$$= \frac{1}{(n+\lambda)^2}\mathbb{E}\Big[x^T X^T \epsilon\epsilon^T X x\Big]$$

using $\mathbb{E}[\epsilon\epsilon^T] = \sigma^2\mathbf{I}$.
$$= \frac{\sigma^2}{(n+\lambda)^2}\mathbb{E}\Big[x^T X^T X x\Big]$$

using $\mathbf{X}^T\mathbf{X} = n\mathbf{I}$.
$$= \frac{\sigma^2 n}{(n+\lambda)^2}\mathbb{E}\Big[x^T x\Big]$$

$$= \frac{\sigma^2 n}{(n+\lambda)^2}\|x\|_2^2$$

$\boxed{\text{Suppose } \mathbf{X}^T\mathbf{X} = n\mathbf{I},}$ then

$$\hat{w}_{\text{ridge}} = \frac{n}{n+\lambda}w + \frac{1}{n+\lambda}\mathbf{X}^T\epsilon$$

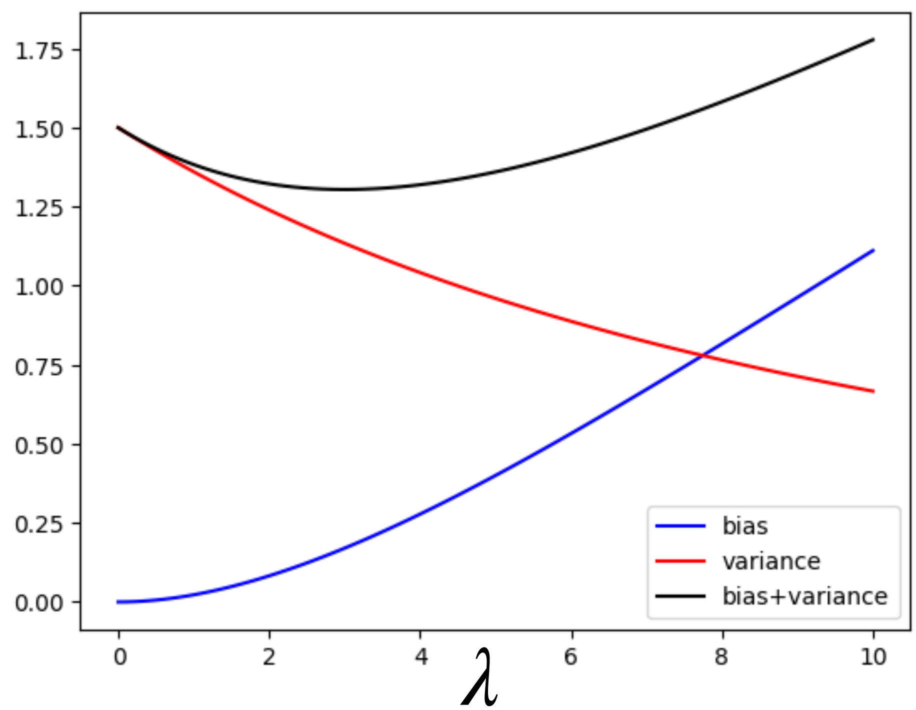
Bias-Variance Properties

Suppose $\mathbf{X}^T\mathbf{X} = n\mathbf{I}$,

- Ridge regressor: $\hat{w}_{\text{ridge}} = \arg\min_w \|y - Xw\|_2^2 + \lambda\|w\|_2^2$
- True error

$$\mathbb{E}_{y,\mathcal{D}_{\text{train}}|x}[(y - x^T\hat{w}_{\text{ridge}})^2 \,|\, x] = \sigma^2 + \underbrace{\frac{\lambda^2}{(n+\lambda)^2}(w^Tx)^2}_{\text{Bias-squared}} + \underbrace{\frac{\sigma^2 n}{(n+\lambda)^2}\|x\|_2^2}_{\text{Variance}}$$

d=10, n=20, $\sigma^2 = 3.0, \|w\|_2^2 = 10$



as $\lambda \to 0$, $\hat{w}_{\text{ridge}} \to \hat{w}_{\text{MLE}}$

as $\lambda \to \infty$ $\hat{w}_{\text{ridge}} \to 0$

What you need to know…

- Regularization
  - Penalizes complex models towards preferred, simpler models
- Ridge regression
  - L_2 penalized least-squares regression
  - Regularization parameter trades off model complexity with training error
  - Never regularize the offset b, because b does not contribute to sensitivity of the input.

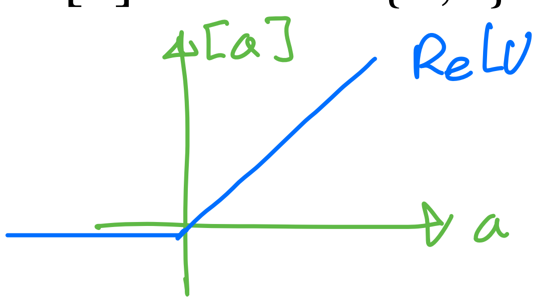
[Homework 1 Problem A5 implements Ridge regression on MNIST.]

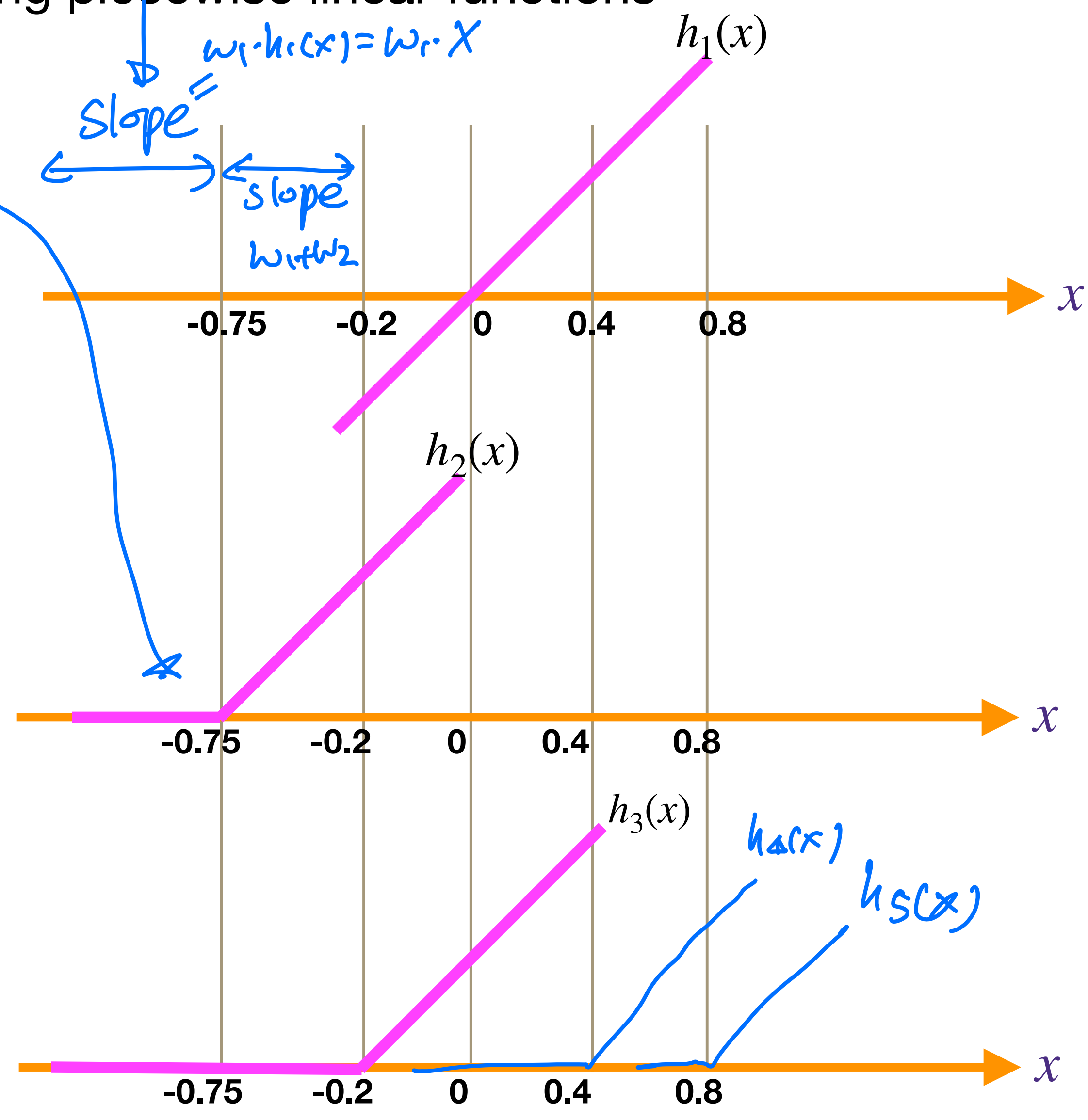
Example: piecewise linear fit

- we fit a linear model:
  $f(x) = b + w_1h_1(x) + w_2h_2(x) + w_3h_3(x) + w_4h_4(x) + w_5h_5(x)$
- with a specific choice of features using piecewise linear functions

$$h(x) = \begin{bmatrix} h_1(x) \\ h_2(x) \\ h_3(x) \\ h_4(x) \\ h_5(x) \end{bmatrix} = \begin{bmatrix} x \\ [x+0.75]^+ \\ [x+0.2]^+ \\ [x-0.4]^+ \\ [x-0.8]^+ \end{bmatrix}$$

$$[a]^+ \triangleq \max\{a, 0\}$$





Example: piecewise linear fit

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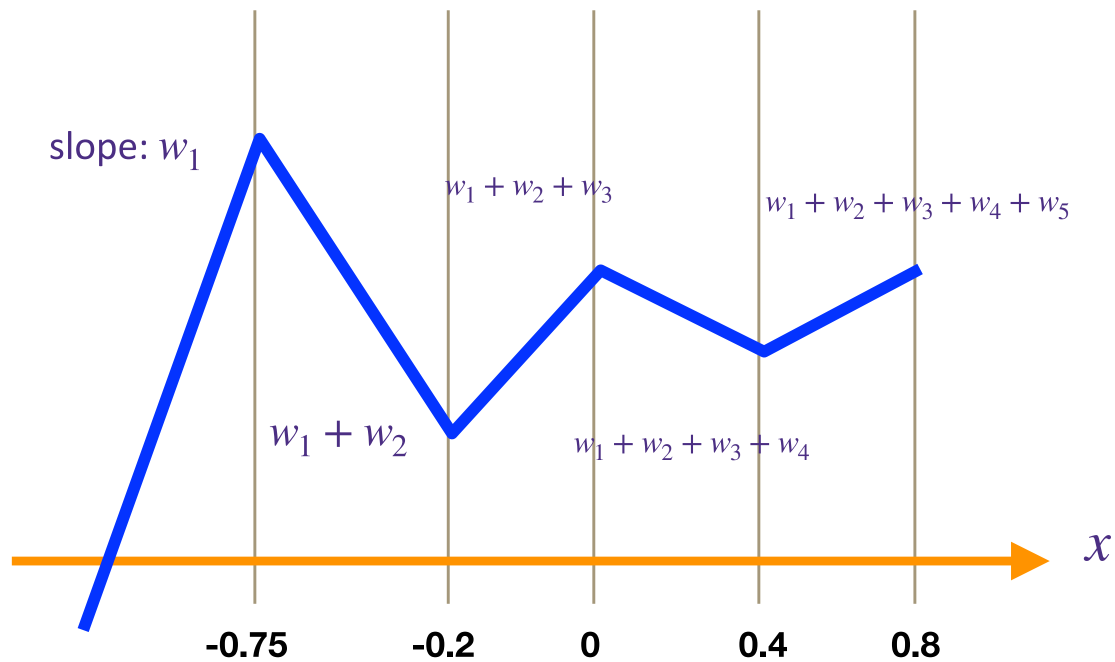
- with a specific choice of features using piecewise linear functions

$$h(x) = \begin{bmatrix} h_1(x) \\ h_2(x) \\ h_3(x) \\ h_4(x) \\ h_5(x) \end{bmatrix} = \begin{bmatrix} x \\ [x+0.75]^+ \\ [x+0.2]^+ \\ [x-0.4]^+ \\ [x-0.8]^+ \end{bmatrix}$$

$$[a]^+ \triangleq \max\{a, 0\}$$

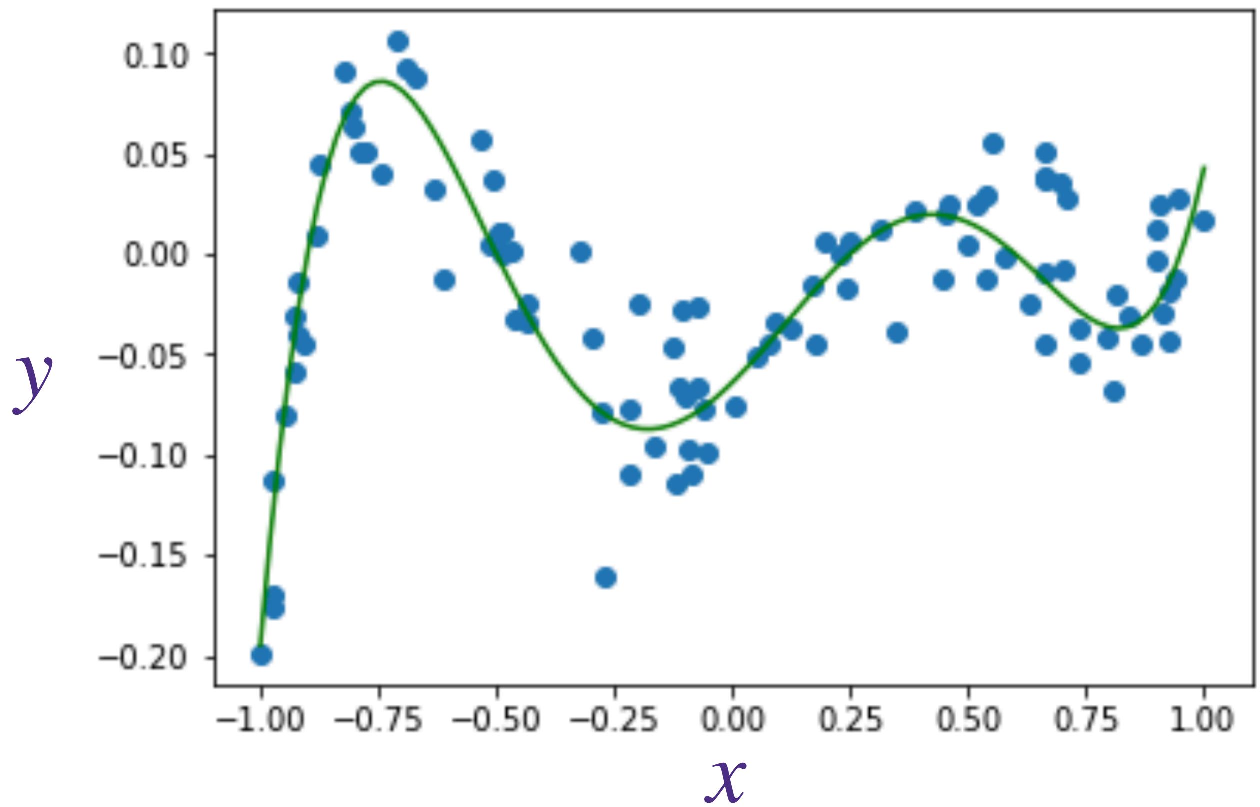
$$y = b + h(x)^T w$$



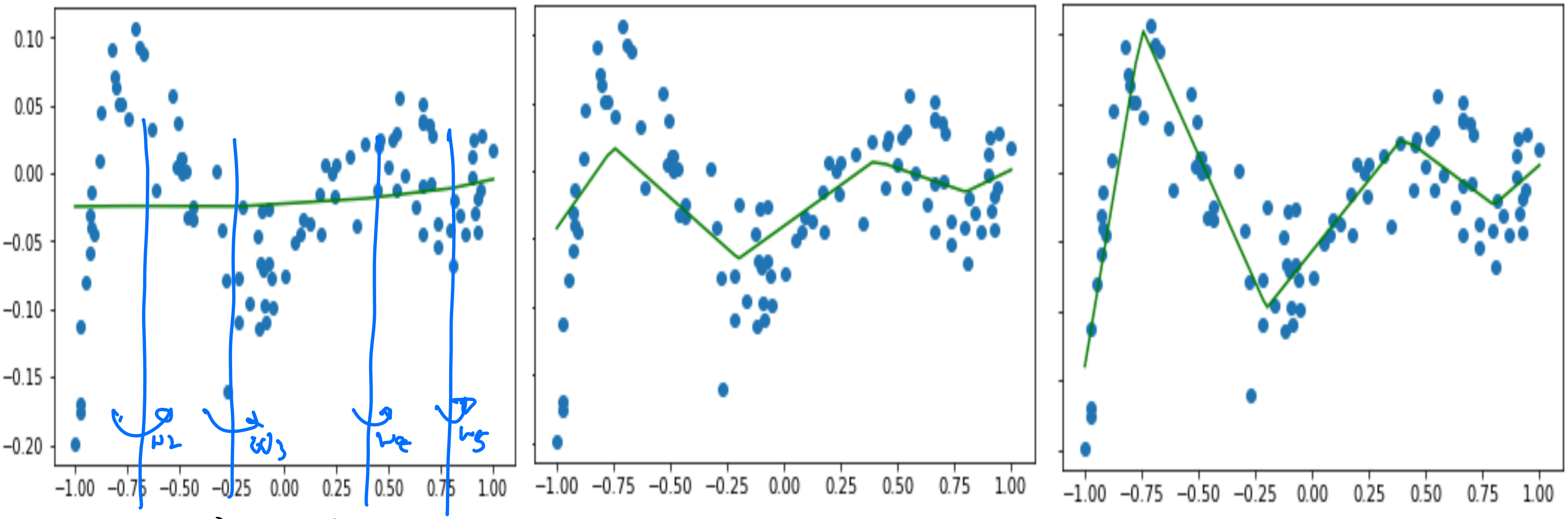
the weights capture the change in the slopes

Example: piecewise linear fit

- we fit a linear model:
  $f(x) = b + w_1 h_1(x) + w_2 h_2(x) + w_3 h_3(x) + w_4 h_4(x) + w_5 h_5(x)$
- with a specific choice of features using piecewise linear functions



Example: piecewise linear fit (ridge regression)



$\lambda = 1$ large

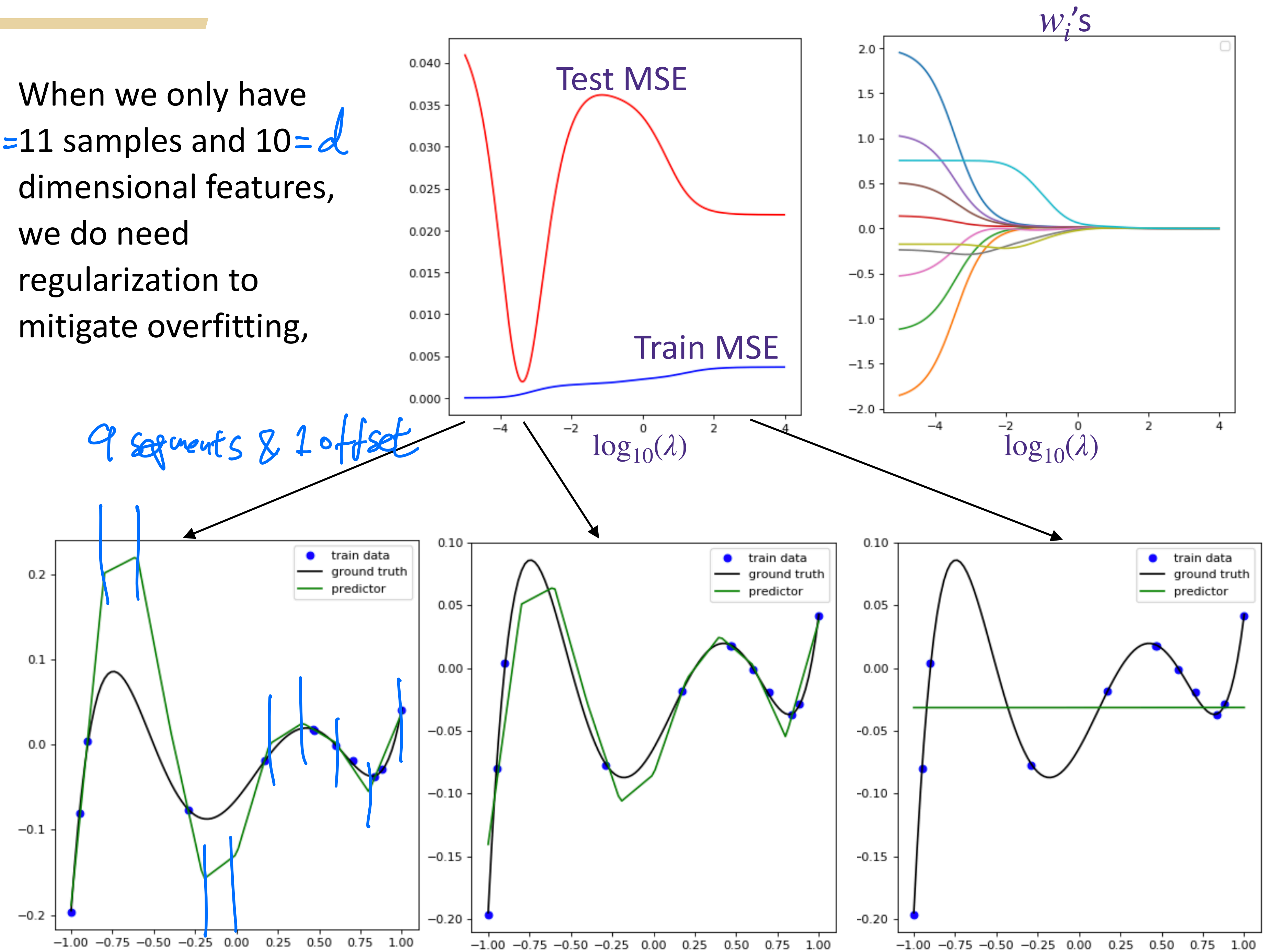
$\lambda = 0.005$

$\lambda = 0.000001$

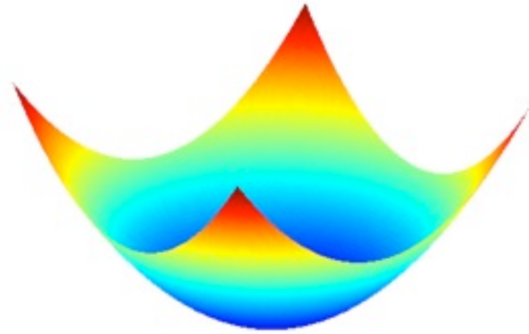
We do not observe overfitting, as d=5 << n=100

Piecewise linear with $w \in \mathbb{R}^{10}$ and n=11 samples

When we only have $n=$11 samples and 10$=d$ dimensional features, we do need regularization to mitigate overfitting,



What do we do if d<n?



$$\hat{w}_{\text{MLE}} = \arg\min_{w} \|y - X^T w\|^2$$

$$\hat{w}_{\text{MLE}} = \underbrace{(X^T X)}_{\text{not invertible}}{}^{-1} X^T y$$

$$\hat{w}_{\text{Ridge}} = \arg\min_{w} \|y - X^T w\|^2 + \lambda \|w\|^2$$

$$\hat{w}_{\text{Ridge}} = \underbrace{(X^T X + \lambda \mathbf{I})}_{\text{invertible}}{}^{-1} X^T y$$

Questions?