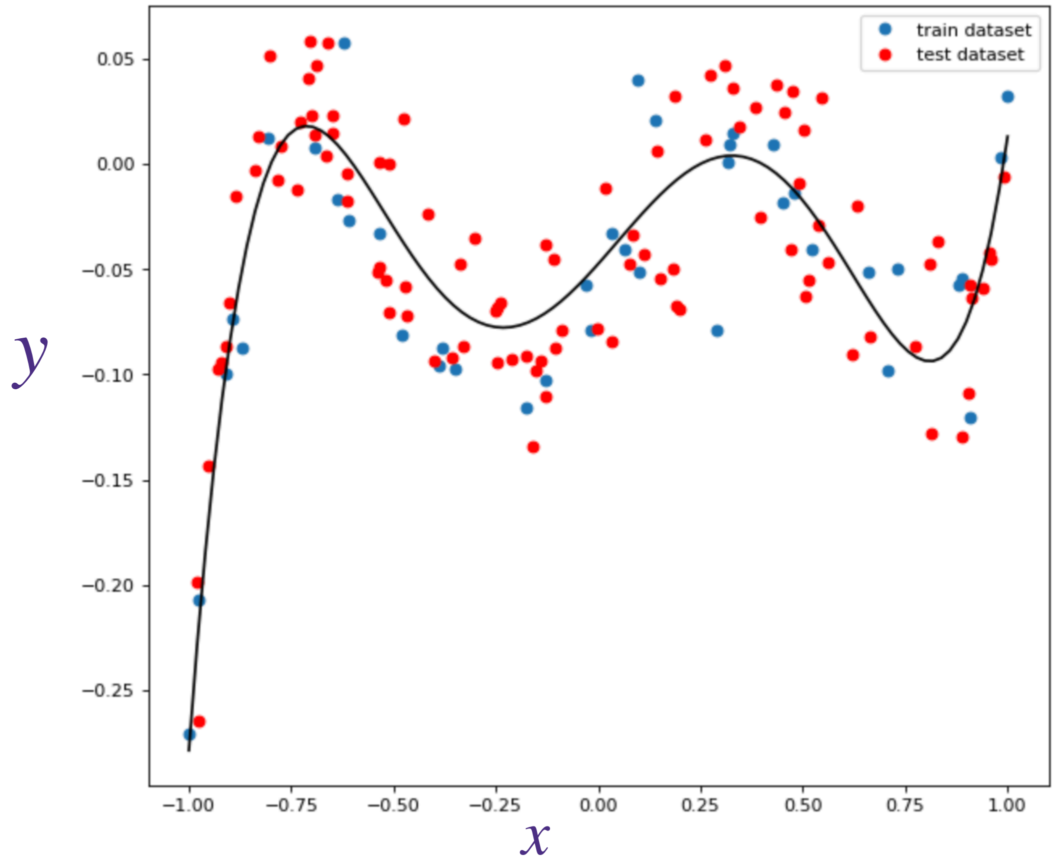
Lecture 7: Regularization

Recap: bias-variance tradeoff

- Consider 40 training examples and 100 test examples i.i.d.drawn from degree-5 polynomial features $x_i \sim \text{Uniform}[-1,1]$, $y_i \sim f_{w*}(x_i) + \epsilon_i$, $\epsilon_i \sim \mathcal{N}(0,\sigma^2)$

$$f_{w*}(x_i) = b^* + w_1^* x_i + w_2^*(x_i)^2 + w_3^*(x_i)^3 + w_4^*(x_i)^4 + w_5^*(x_i)^5$$



This is a linear model with features

$$h(x_i) = (x_i, (x_i)^2, (x_i)^3, (x_i)^4, (x_i)^5)$$

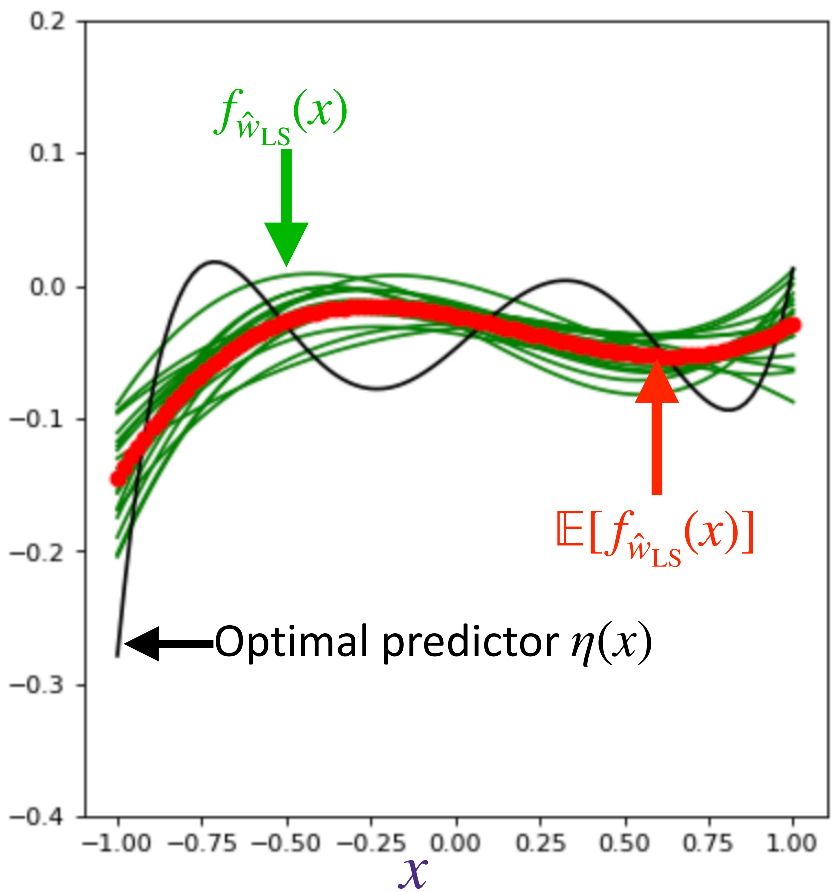
$$f_w(x_i) = h(x_i)^T w + b$$

$$\widehat{w}_{\text{LS}} = \arg \min_{b \in \mathbb{R}, w \in \mathbb{R}^5} \sum_{i=1}^{N} \left(y_i - (h_w(x_i) + b) \right)^2$$

Recap: bias-variance tradeoff

With degree-3 polynomials, we underfit

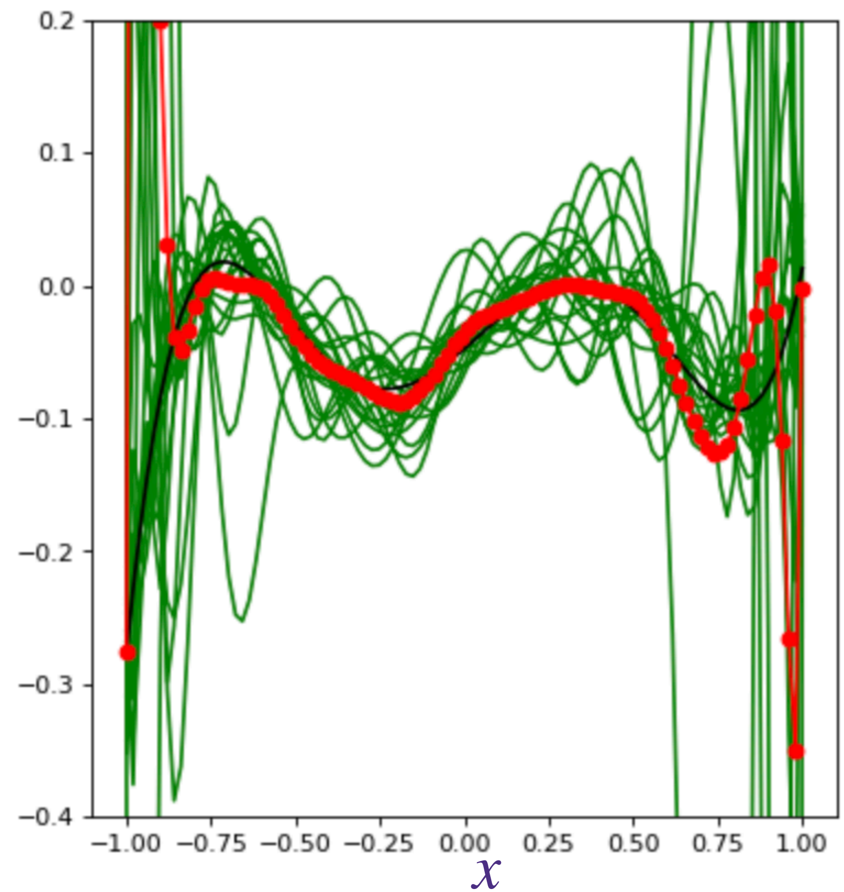
$\hat{f}_{\hat{w}_{\mathrm{LS}}}(x)$




```
current train error = 0.0036791644380554187
current test error  = 0.0037962529988410953
```

With degree-20 polynomials, we overfit

$\hat{f}_{\hat{w}_{\mathrm{LS}}}(x)$




```
0.0005421686349568773
0.14210029429557927
```

Sensitivity: how to detect overfitting

- 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
- Note that b is a constant and hence there is no sensitivity for the offset b
- 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) with **regularization coefficient** $\lambda > 0$

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

- The regularization encourages solution w with smaller norm $\|w\|_2^2$, hence encouraging less overfitting.
- The first term encourages fitting the training data

Minimizing the Ridge Regression Objective

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

Shrinkage Properties

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

For example, if $\mathbf{X}^T\mathbf{X} = n\mathbf{I}$, then

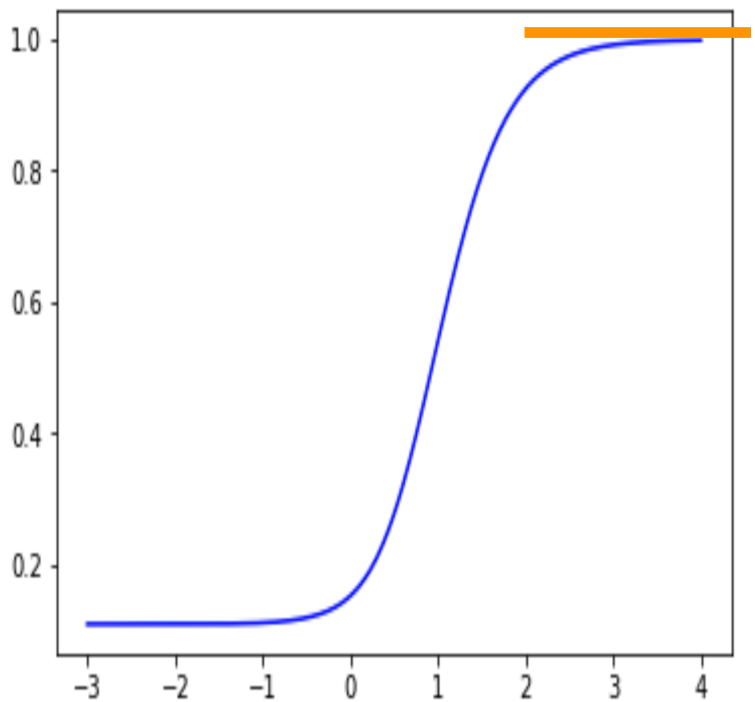
Similar shrinking effect for general $\mathbf{X}^T\mathbf{X}$, which we do not go into details in class (come to my OH id interested).

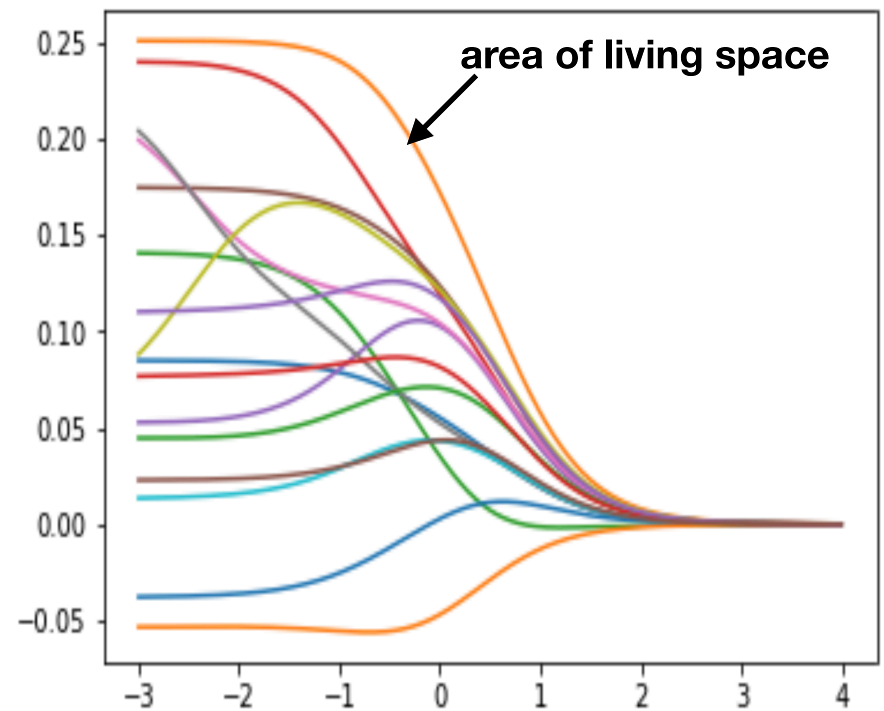
- When $\lambda = 0$, this gives the least squares model
- This defines a family of models hyper-parametrized by λ
- Large λ means more regularization and simpler model
- Small λ means less regularization and more complex model

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

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

$\widehat{w}_{\text{LS},i}$'s

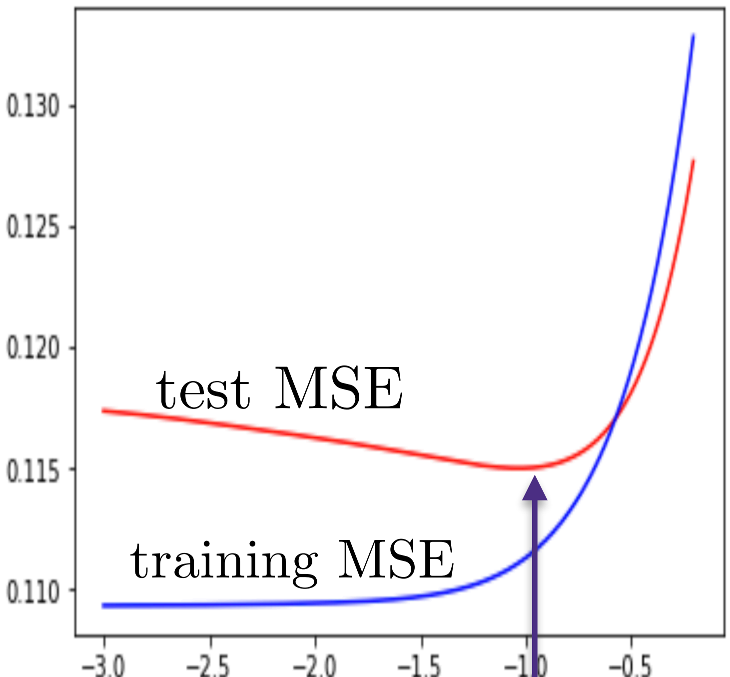




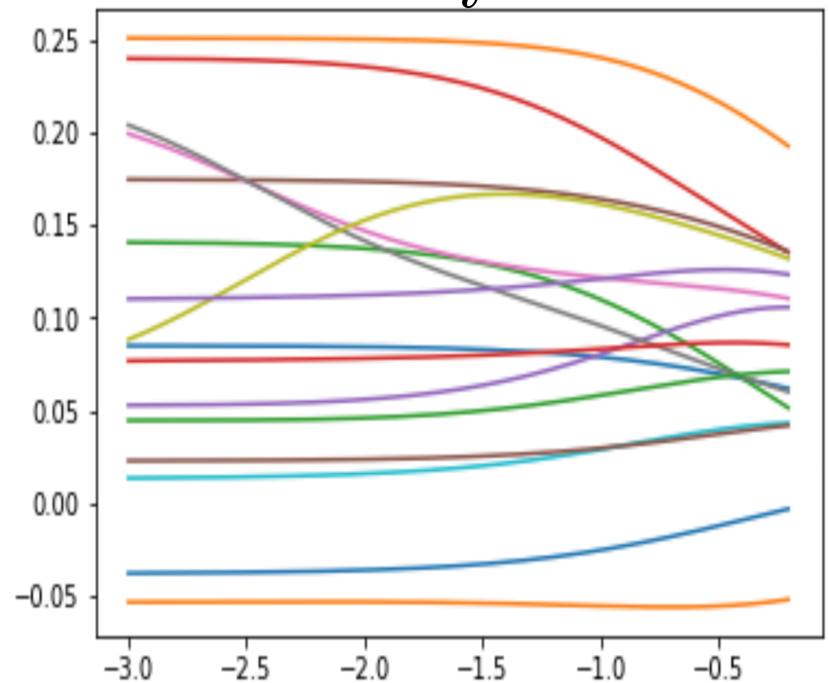
High model complexity | $\log_{10}(\lambda)$ | Low model complexity | $\log_{10}(\lambda)$

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



w_i's



- this gain in test MSE comes from shrinking w's to get a less sensitive predictor
(which in turn reduces the variance)

Bias-variance tradeoff for ridge regression model

If $Y_i = X_i^T w^* + \epsilon_i$ and $\epsilon_i \sim \mathcal{N}(0, \sigma^2)$

$$\mathbf{y} = \mathbf{X} w^* + \epsilon$$

$$\eta(x) = \mathbb{E}_{Y|X}[Y \,|\, X = x] = x^T w^*$$

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

$$=$$

For example, if $\mathbf{X}^T \mathbf{X} = n\mathbf{I}$, then

$$\hat{w}_{\text{ridge}} =$$

Bias-variance tradeoff for ridge regression model

If $Y_i = X_i^T w^* + \epsilon_i$ and $\epsilon_i \sim \mathcal{N}(0,\sigma^2)$

$$\mathbf{y} = \mathbf{X}w^* + \epsilon$$

$$\eta(x) = \mathbb{E}_{Y|X}[Y \,|\, X = x] = x^T w^*$$

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

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

For example, if $\mathbf{X}^T\mathbf{X} = n\mathbf{I}$, then

$$\hat{w}_{\text{ridge}} = \underbrace{w^* - \frac{\lambda}{n+\lambda}w^*}_{\text{estimate is shrunk by regularizer}} + \underbrace{\frac{1}{n+\lambda}\mathbf{X}^T\epsilon}_{\text{error due to noise}}$$

$\rightarrow$ larger λ increases bias

$\rightarrow$ larger λ decreases variance

Bias-variance tradeoff for ridge regression model

If $Y_i = X_i^T w^* + \epsilon_i$ and $\epsilon_i \sim \mathcal{N}(0,\sigma^2)$

$$\mathbf{y} = \mathbf{X}w^* + \epsilon$$

$$\eta(x) = \mathbb{E}_{Y|X}[Y \,|\, X = x] = x^T w^*$$

For example, if $\mathbf{X}^T\mathbf{X} = n\mathbf{I}$, then

$$\hat{f}_{\mathcal{D}}(x) = x^T w^* - \frac{\lambda}{n+\lambda} x^T w^* + \frac{1}{n+\lambda} x^T \mathbf{X}^T \epsilon$$

- Irreducible error: $\mathbb{E}_{X,Y}[(Y - \eta(x))^2 \,|\, X = x] = \sigma^2$
- Bias squared: $\left(\eta(x) - \mathbb{E}_{\mathcal{D}}[\hat{f}_{\mathcal{D}}(x)] \right)^2 =$

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

  - Bias decreases with the sample size
  - Bias increases with λ

Bias-variance tradeoff for ridge regression model

If $Y_i = X_i^T w^* + \epsilon_i$ and $\epsilon_i \sim \mathcal{N}(0,\sigma^2)$

$$\mathbf{y} = \mathbf{X}w^* + \epsilon$$

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

For example, if $\mathbf{X}^T\mathbf{X} = n\mathbf{I}$, then

$$\hat{f}_{\mathcal{D}}(x) = x^T w^* - \frac{\lambda}{n+\lambda} x^T w^* + \frac{1}{n+\lambda} x^T \mathbf{X}^T \epsilon$$

- Variance: $\mathbb{E}_{\mathcal{D}}\left[\left(\hat{f}_{\mathcal{D}}(x) - \mathbb{E}_{\mathcal{D}}[\hat{f}_{\mathcal{D}}(x)]\right)^2\right] =$

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

  - Variance decreases with the sample size
  - Variance decrease with λ

Bias-Variance Properties

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

$$\mathbb{E}_{Y|X,\mathscr{D}}[(y - x^T \hat{w}_{\text{ridge}})^2 \,|\, x] = \sigma^2 + \frac{\lambda^2}{(n+\lambda)^2}(w^T x)^2 + \frac{\sigma^2 n}{(n+\lambda)^2}\|x\|_2^2$$

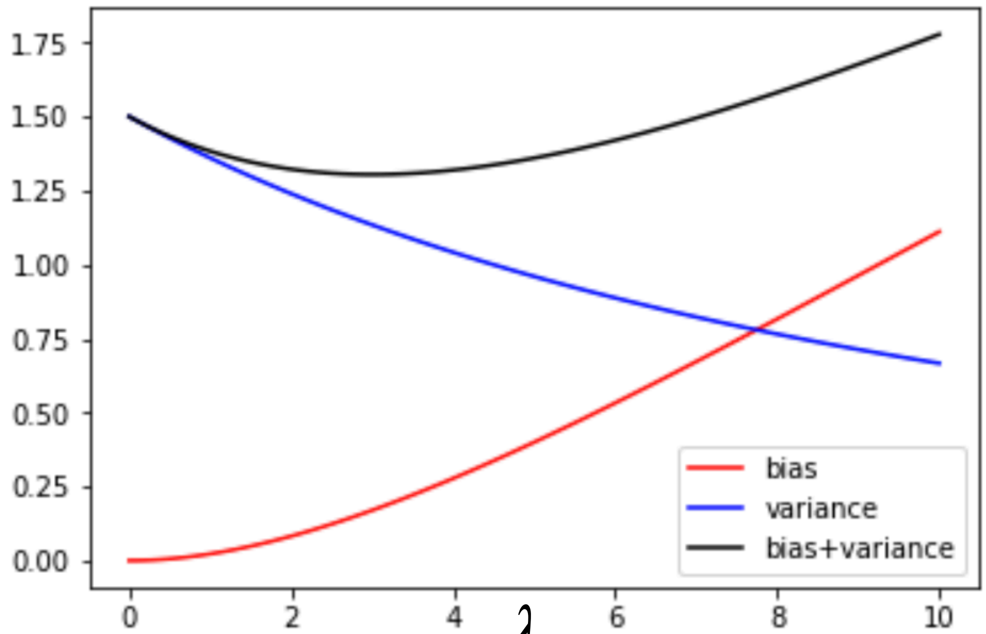
Bias-squared

Variance

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

as λ →0,

$\hat{w}_{\text{ridge}} \to \hat{w}_{\text{LS}}$



λ

as λ →∞

$\hat{w}_{\text{ridge}} \to 0$

What you need to know…

- Regularization
  - Penalizes complex models towards simpler models

- Ridge regression
  - L_2 penalized least-squares regression
  - Regularization parameter trades off model complexity with training error
  - Never regularize the offset!

Example: piecewise linear fit

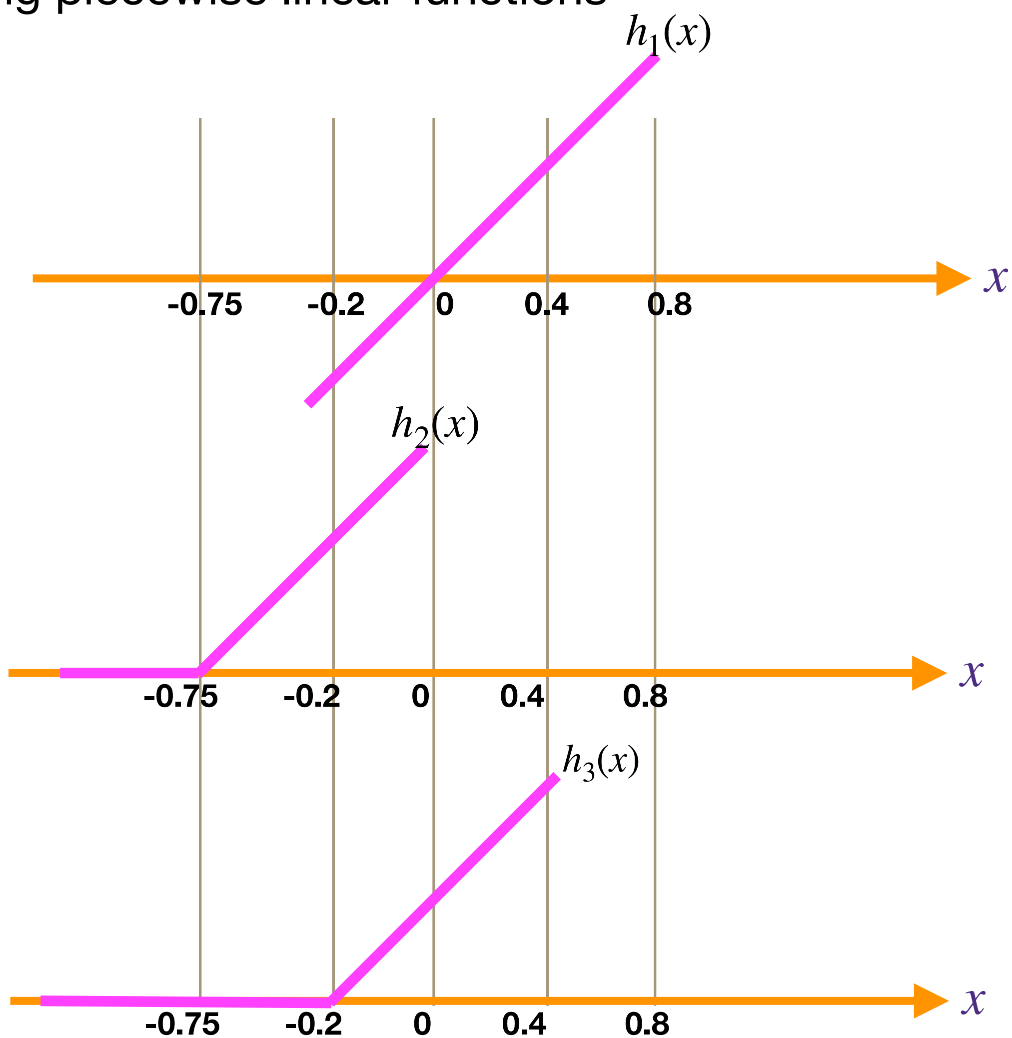
- we fit a linear model:

$$f(x) = b + w_1 h_1(x) + w_2 h_2(x) + w_3 h_3(x) + w_4 h_4(x) + w_5 h_5(x)$$

- with a specific choice of features using piecewise linear functions

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

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



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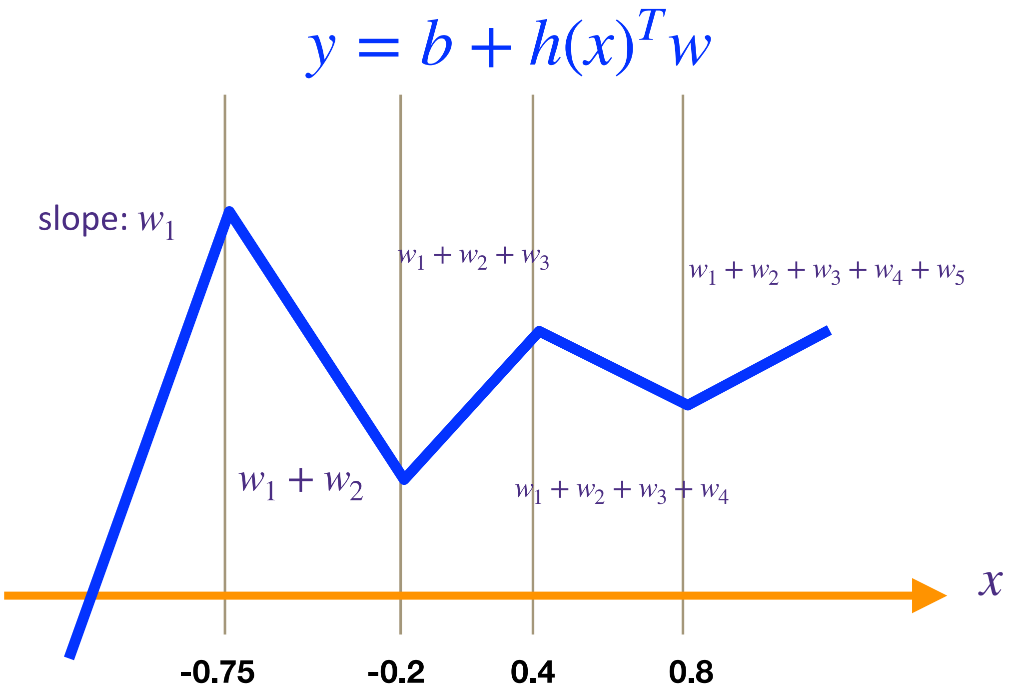

the weights capture the change in the slopes

Example: piecewise linear fit

- we fit a linear model:
  $f(x) = b + w_1 h_1(x) + w_2 h_2(x) + w_3 h_3(x) + w_4 h_4(x) + w_5 h_5(x)$
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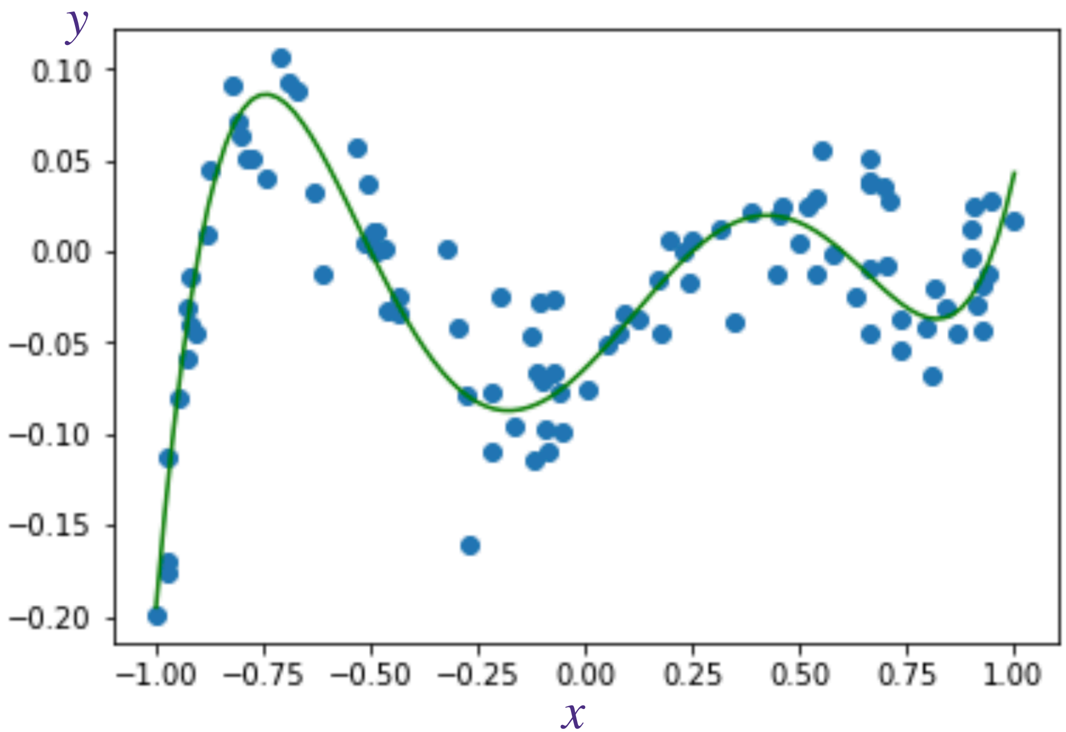
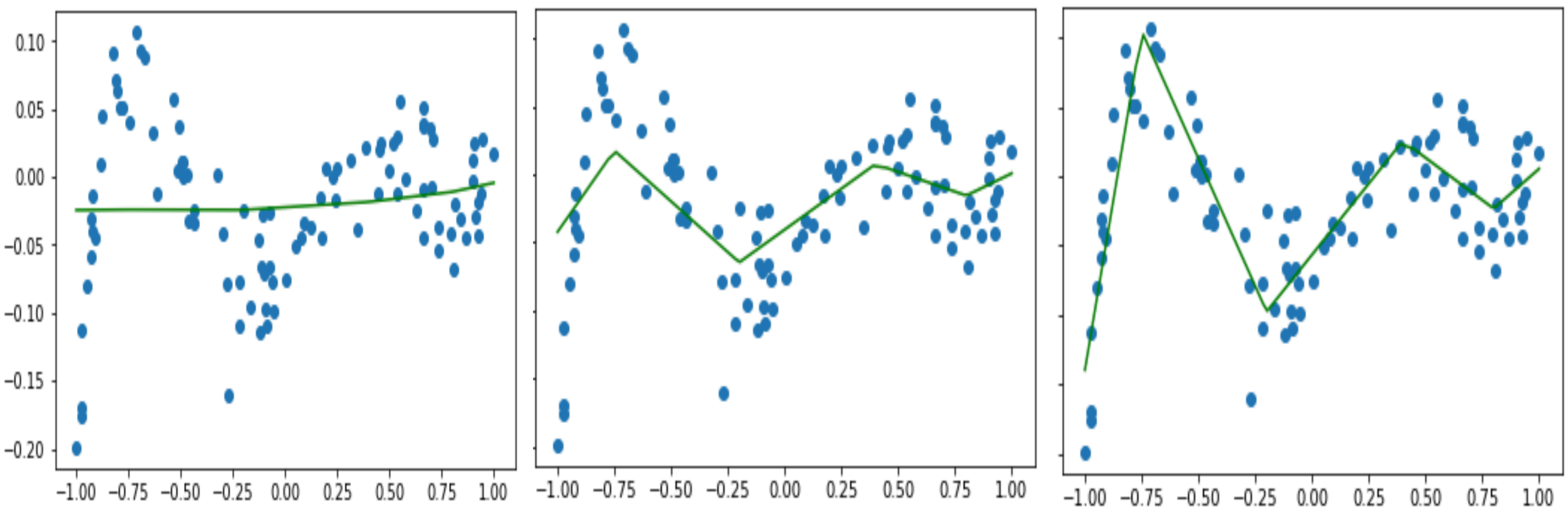


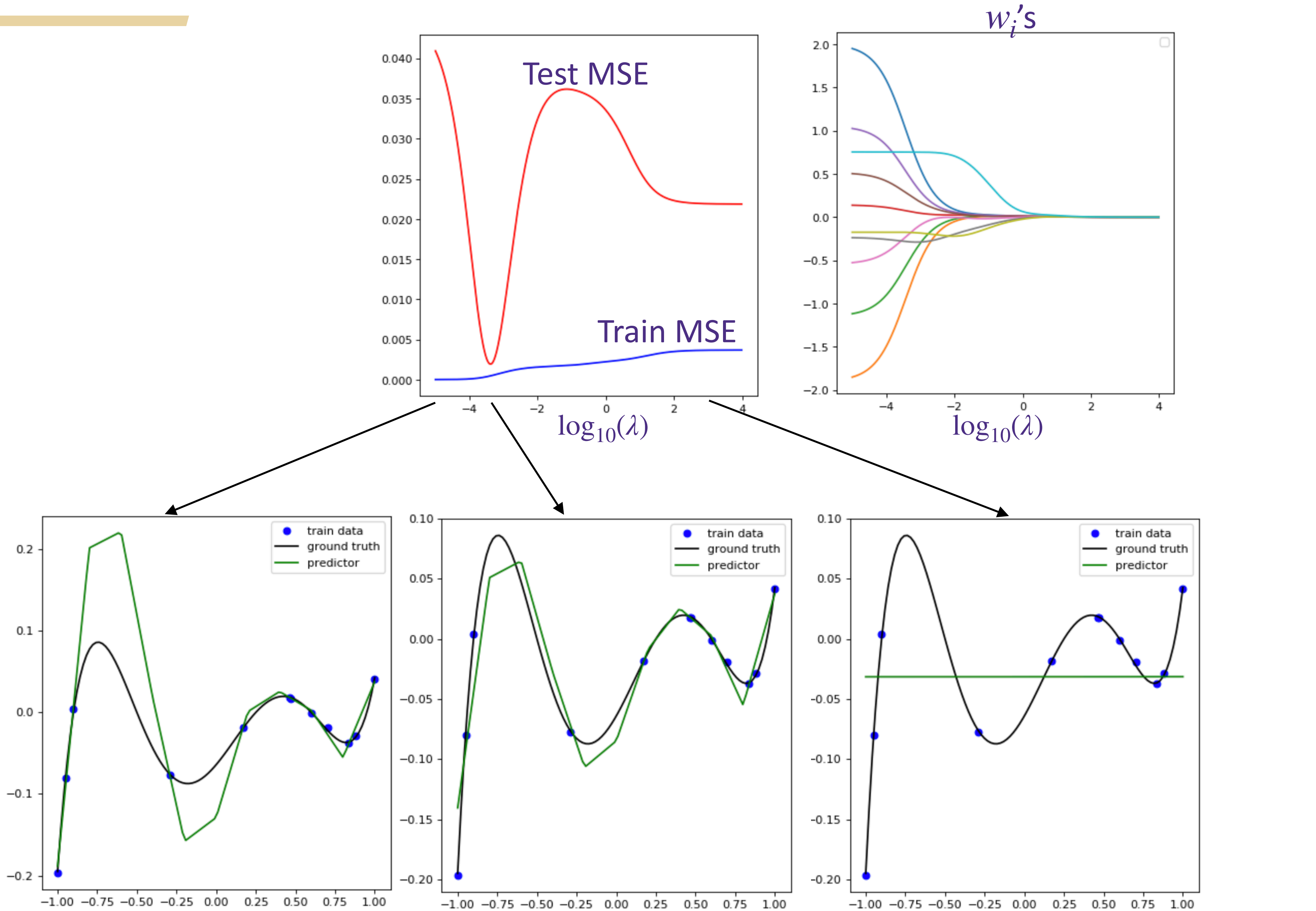
Example: piecewise linear fit (ridge regression)



$\lambda = 1$ $\lambda = 0.005$ $\lambda = 0.000001$

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

Can avoid overfitting even $w \in \mathbb{R}^{10}$ and n=11 samples



Questions?

Logistics

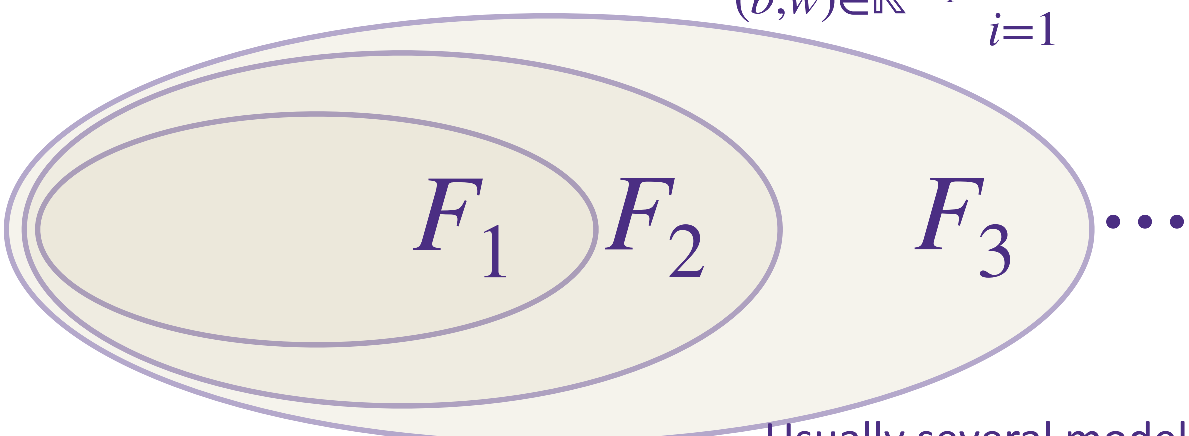
- Question from a student: can we get access to the recording from the past offerings of CSE44
  - For FERPA reasons, we are not able to release them.
- We put other public video lectures in the course website that covers a free online textbook
- Office hours are there to help you not just with homework for more generally.

Lecture 8: Model selection using Cross-validation

Parameter and hyper-parameter

- A **model class** is set of functions, each function is indexed by its **parameters** representing the function
  - e.g., a model class $F_p = \{\text{all degree-}p \text{ polynomials in } \mathbb{R}\}$ each function in that class is represented (or indexed) by parameter $(b, w) \in \mathbb{R}^{p+1}$, which can be also written more explicitly as
- $F_p = \{f_{b,w} : \mathbb{R} \to \mathbb{R} \,|\, f_{b,w}(x) = b + w_1 x + \cdots + w_p x^p, \text{ for some} (b, w) \in \mathbb{R}^{1+p}\}$
  - **Parameter** is what is optimized when training a model

    e.g., $(\widehat{b}_p, \widehat{w}_p) = \arg \min_{(b,w)\in\mathbb{R}^{1+p}} \sum_{i=1}^{n} \left(y_i - (h(x_i)^T w + b) \right)^2$

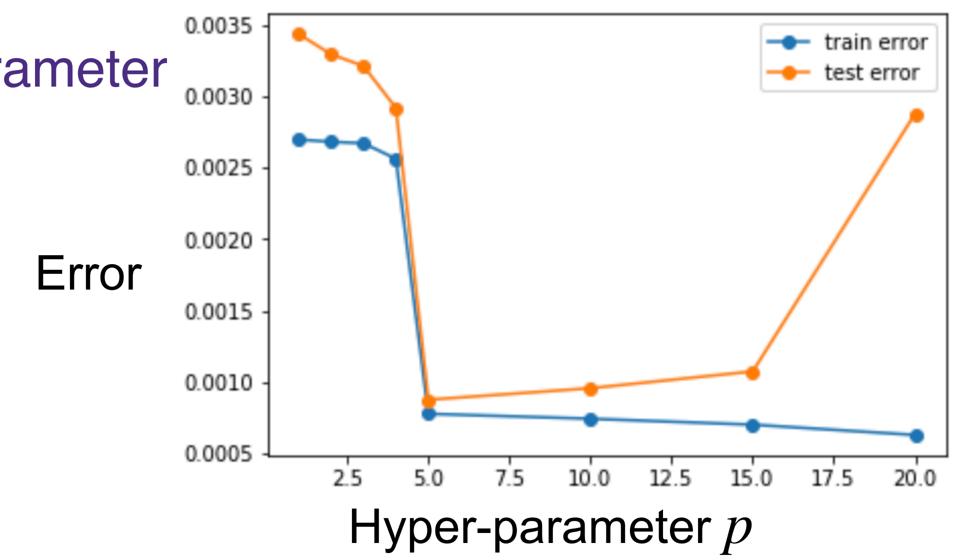


Usually several model classes form
a nested hierarchy of classes with increasing complexities

Parameter and hyper-parameter

- **A family of model classes** is a set of model classes, each class indexed by its **hyper-parameter** representing a model class
  - e.g., a family $\mathscr{F} = \{F_p \,|\, p \in \{1,2,\ldots\}\}$ is a set of model classes with hyper-parameter $p \in \{1,2,\ldots\}$, where F_p is a class of degree-p polynomials
  - Hyper-parameter is usually fixed during training

    e.g., $\hat{f}_p = \arg\min_{f \in F_p} \sum_{i=1}^{n} \left(y_i - f(x_i) \right)^2$
  - And we run multiple training for multiple choices of the hyper-parameter

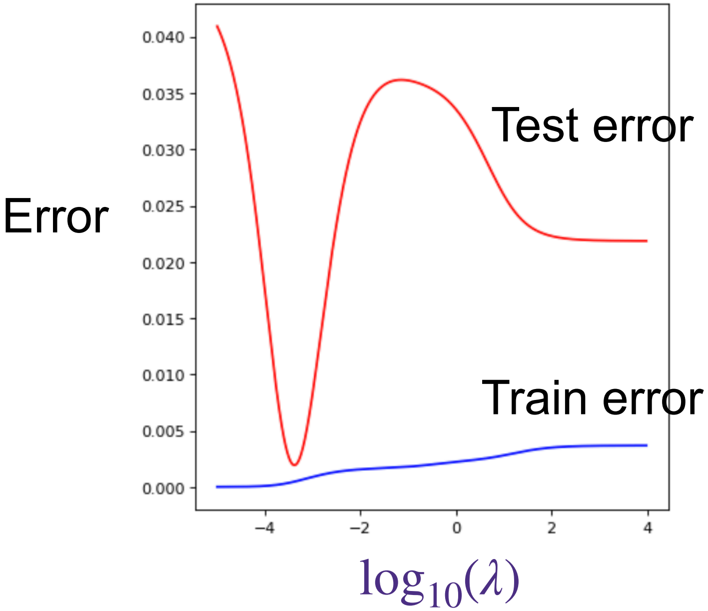


Hyper-parameter for ridge regression

- Hyper parameter does not have to represent a model class
- It can represent the algorithm being used also
- **hyper-parameter** λ for ridge regression
  - e.g., a linear model class $F_1 = \{f(x) = b + x^T w \,|\, (b, w) \in \mathbb{R}^{d+1}\}$ trained by minimizing a regularized loss

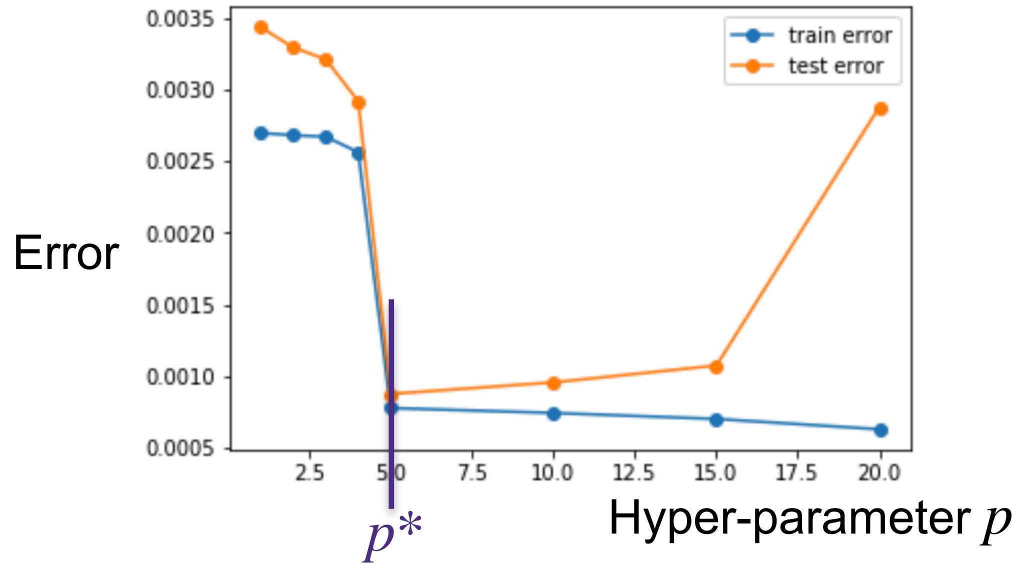
$$(\hat{b}_\lambda, \hat{w}_\lambda) = \arg \min_{(b,w)\in\mathbb{R}^{d+1}} \sum_{i=1}^{n} (y_i - (b + x_i^T w))^2 \; + \; \lambda \|w\|_2^2$$

  - λ is a hyper-parameter, because it is fixed during training
  - And we run multiple training for multiple choices of the hyper-parameter



Model selection

- **Model selection** asks the following question: among all the models we got for different hyper-parameters, how do we choose the "best" one to deploy?
- Wrong approach 1:
  - Randomly split the dataset into Train Set and Test Set with 80/20 split
  - Train models for various hyper-parameters and report the Train Error and Test Error
  - Deploy the model $\widehat{w}_{p*}$ achieving minimum Test Error
  - Report its Test Error as an approximation of the True Error
- Issue:



Why using test error for model selection gives under estimation of the true error

- Consider a simple experiment where we have two coins
  - $x_i \sim \text{Bern}(p)$ and $y_i \sim \text{Bern}(q)$ such that

$$x_i = \begin{cases} 1 & \text{with probability } p \\ 0 & \text{with probability } 1-p \end{cases} \qquad y_i = \begin{cases} 1 & \text{with probability } q \\ 0 & \text{with probability } 1-q \end{cases}$$

- I want to find out $\min\{p, q\}$ given n samples from each
- Using test set to both select the model and report the test error is same as
  - Computing the empirical averages $\hat{p} = \frac{1}{n}\sum_{i=1}^{n} x_i$ and $\hat{q} = \frac{1}{n}\sum_{i=1}^{n} y_i$ and reporting the smaller one, i.e., $\min\{\hat{p}, \hat{q}\}$
  - We can show that this reported value is strictly smaller than what we wanted in expectation: $\mathbb{E}[\min\{\hat{p}, \hat{q}\}] < \min\{p, q\}$
  - For example, if $n = 1$, then $\mathbb{E}[\min\{\hat{p}, \hat{q}\}] = \mathbb{E}[\min\{x_1, y_1\}] =$

To avoid underestimating test error

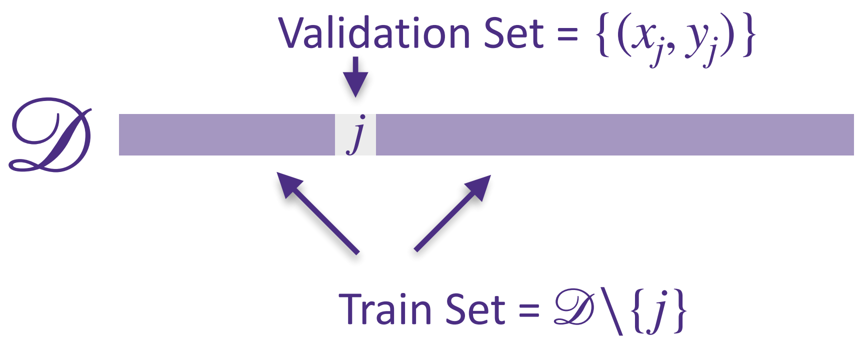
- Never use the **test set** for
  - training any model, or
  - tuning hyper-parameter = model selection
- **Test set** should only be used once to report test error (as an approximation of the true error) in the end
- Idea:
  - use part of training data (called **Validation Set**) to estimated the error and for model selection
  - For example:

    - **Train set**: train (multiple) models for different hyper-parameters
    - **Validation set**: compute validation error, to be used in model selection
    - **Test set**: use it once in the end to report test error for the selected model

(LOO) Leave-one-out cross validation

- Consider a validation set with 1 example:
  - $\mathscr{D}$: dataset
  - $\mathscr{D} \backslash \{j\}$: train set with j-th data point (x_j, y_j) moved to validation set
- Learn model $f_{\mathscr{D}\backslash\{j\}}$ with $\mathscr{D} \backslash \{j\}$ dataset: $f_{\mathscr{D}\backslash\{j\}} = \arg\min_f \sum_{i \in \mathscr{D}\backslash\{j\}} (y_i - f(x_i))^2$

> Notation:
> $A \backslash B = A \cap B^C$ denotes setminus



- **Validation error**: $\text{error}_j \triangleq (y_j - f_{\mathscr{D}\backslash\{j\}}(x_j))^2$
  - It is an unbiased estimate of the error

$$\text{error}_{\text{true}}(f_{\mathscr{D}\backslash\{j\}}) \triangleq \mathbb{E}_{(x,y)\sim P_{x,y}}[(y - f_{\mathscr{D}\backslash\{j\}}(x))^2]$$

  - but, variance of error_j is too large. Why?
  - Any ideas?

(LOO) Leave-one-out cross validation

- To reduce the variance of the validation error, use instead
- **LOO cross validation**: Average over all possible single sample validation set $\{j\}$ for $j \in \{1,\ldots,n\}$:
  - Train n times:
    for each data point you leave out, learn a new classifier $f_{\mathscr{D}\setminus\{j\}}$
  - **Validation error** is now averaged over all different splits:

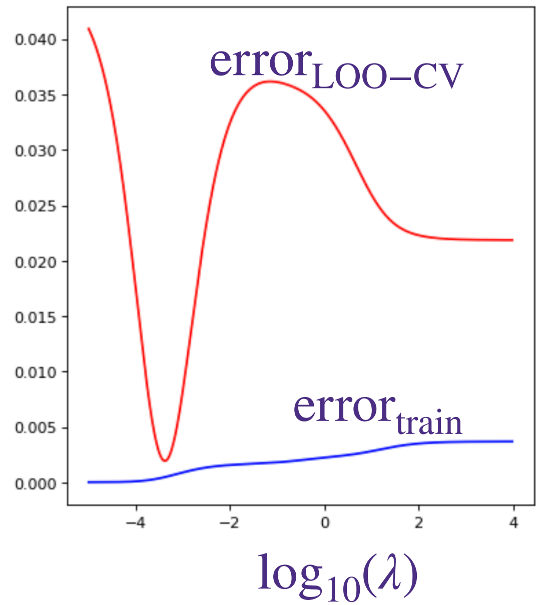
$$\text{error}_{\text{LOO-CV}} = \frac{1}{n}\sum_{j=1}^{n}\text{error}_j = \frac{1}{n}\sum_{j=1}^{n}(y_j - f_{\mathscr{D}\setminus\{j\}}(x_j))^2$$

LOO cross validation is (almost) unbiased estimate!

- When computing LOO-CV error, we only use $n-1$ data points to train
  - So it's not an estimate of true error of learning with n data points

    true error = $\mathbb{E}_{X,Y}[\,(Y - f_{\mathcal{D}}(X))^2\,]$
  - Usually (slightly) pessimistic – learning with less data typically gives worse answer.
  - Leads to a (slight) over estimation of the error compared to true error

- LOO-CV is almost unbiased! Use LOO-CV error for model selection!!!
  - **E.g., picking λ**



Computational cost of LOO

- Suppose you have 100,000 data points
- say, you implemented a fast version of your learning algorithm
  - Learns in only 1 second
- Computing LOO will take about 1 day
- In general, LOO takes n times longer than training one model
- Any ideas?

Use *k*-fold cross validation

- Randomly divide data into *k* equal parts
  - $D_1, \ldots, D_k$
- For each *i*
  - Learn model $f_{\mathscr{D}\backslash\mathscr{D}_i}$ using data point not in $\mathscr{D}_i$
  - Estimate error of $f_{\mathscr{D}\backslash\mathscr{D}_i}$ on validation set $\mathscr{D}_i$:

$$\text{error}_{\mathcal{D}_i} = \frac{1}{|\mathcal{D}_i|} \sum_{(x_j, y_j) \in \mathcal{D}_i} (y_j - f_{\mathcal{D}\backslash\mathcal{D}_i}(x_j))^2$$

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

$$\text{error}_{k-\text{fold}} = \frac{1}{k} \sum_{i=1}^{k} \text{error}_{\mathscr{D}_i}$$

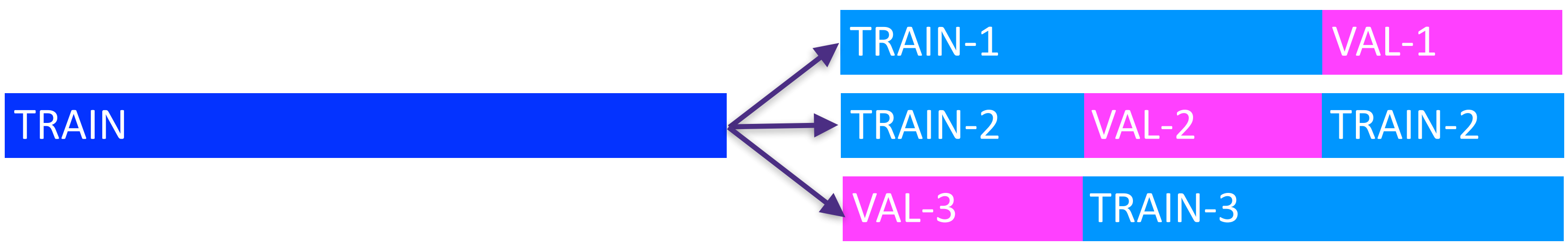
- k-fold cross validation properties:
  - Much faster to compute than LOO-CV as $k \ll n$
  - More (pessimistically) biased – using much less data, only $n - \frac{n}{k}$
  - Usually, k = 10

$\mathscr{D} =$	$\mathscr{D}_1$	$\mathscr{D}_2$	$\mathscr{D}_3$	$\mathscr{D}_4$	$\mathscr{D}_5$
$f_{\mathscr{D}\backslash\mathscr{D}_3}$	Train	Train	Validation	Train	Train

Recap

> Given a dataset, begin by splitting into

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



> Model assessment: Use TEST to assess the accuracy of the model you output

- Never train or choose parameters based on the test data

Example 1

- You wish to predict the stock price of zoom.us given historical stock price data y_i's (for each i-th day) and the historical news articles x_i's
- You use all daily stock price up to Jan 1, 2020 as TRAIN and Jan 2, 2020 - April 13, 2020 as TEST
- What's wrong with this procedure?
-

Example 2

- 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 with the training set 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 select TEST set and split the remaining dataset into TRAIN, and VAL (multiple splits are needed if doing cross validation)
    - E.g., 80%, 10%, and 10%, respectively
  - Choose a hypothesis class or model
    - E.g., linear with non-linear features (also called 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

Questions?