What you need to know…

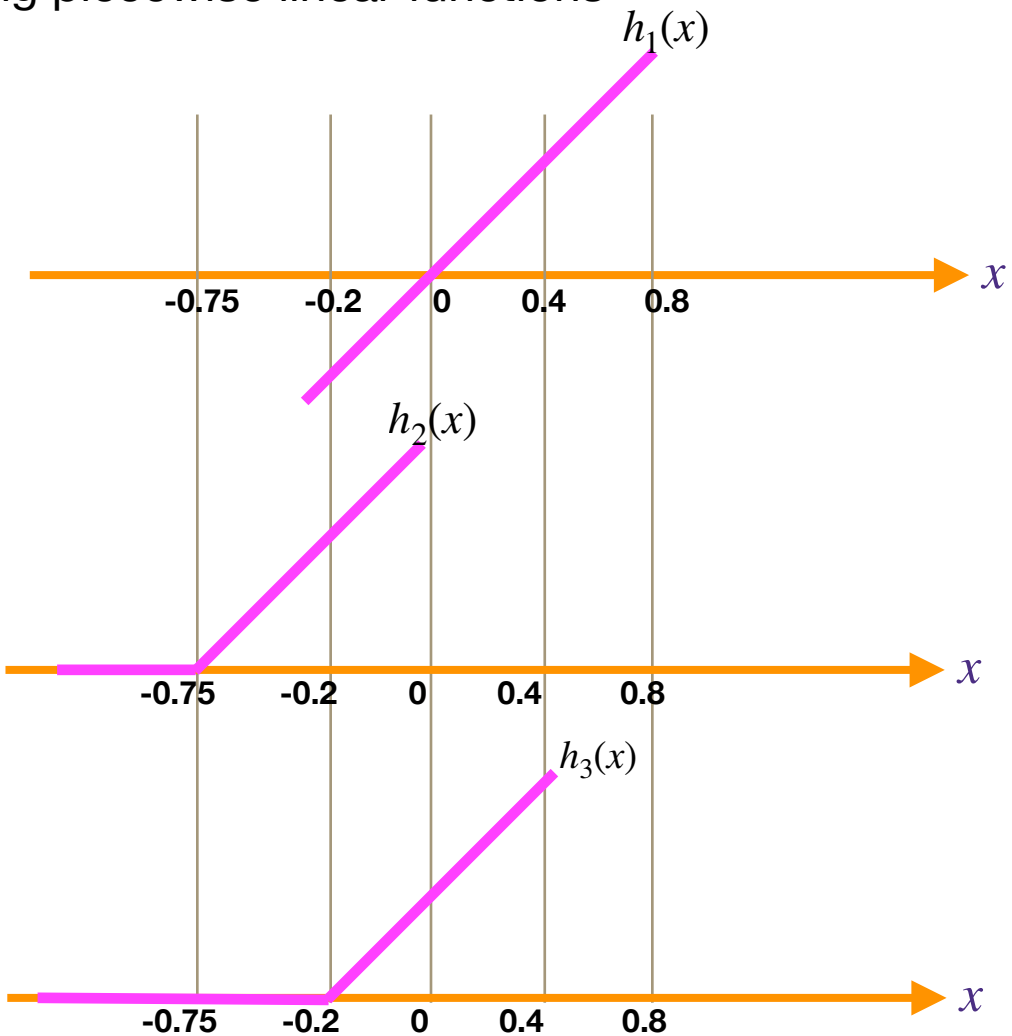
- Regularization
  - Penalizes complex models towards preferred, simpler models
- Ridge regression
  - L_2 penalized least-squares regression
  - Regularization parameter trades off model complexity with training error
  - Never regularize the offset!

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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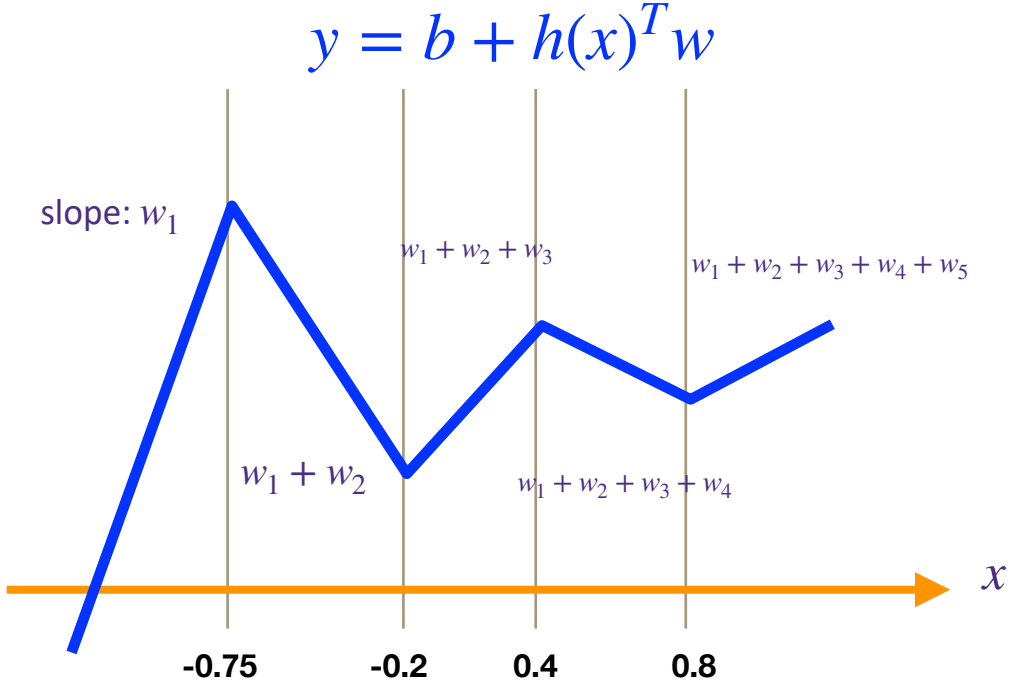

the weights capture the change in the slopes

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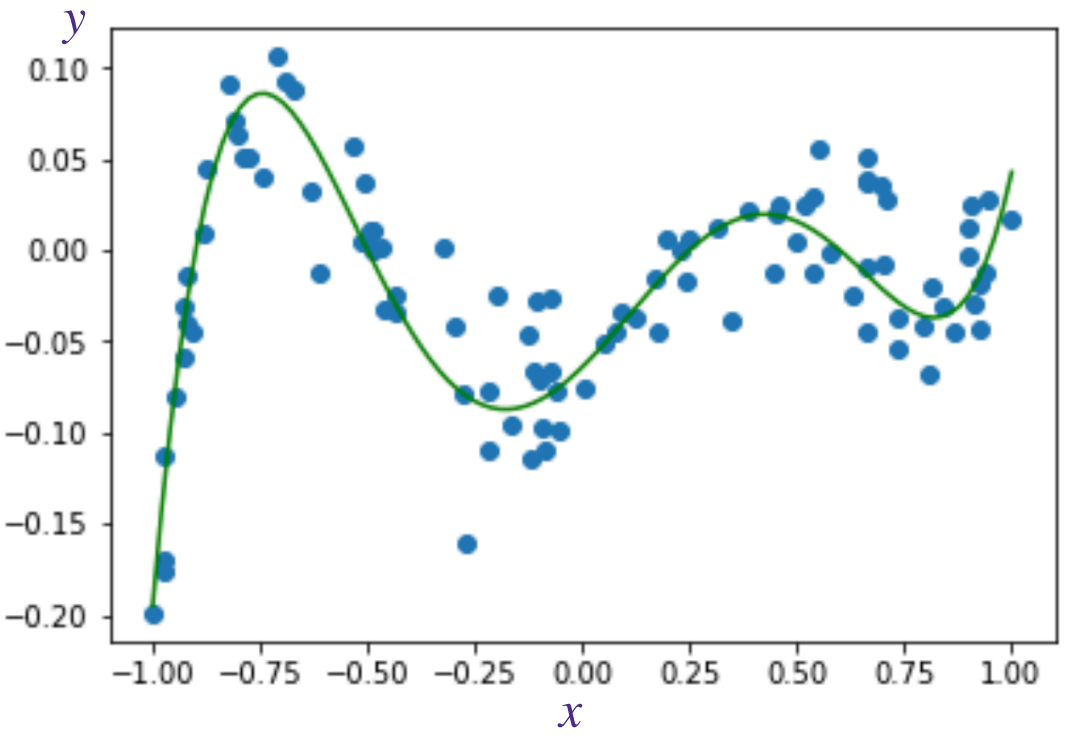
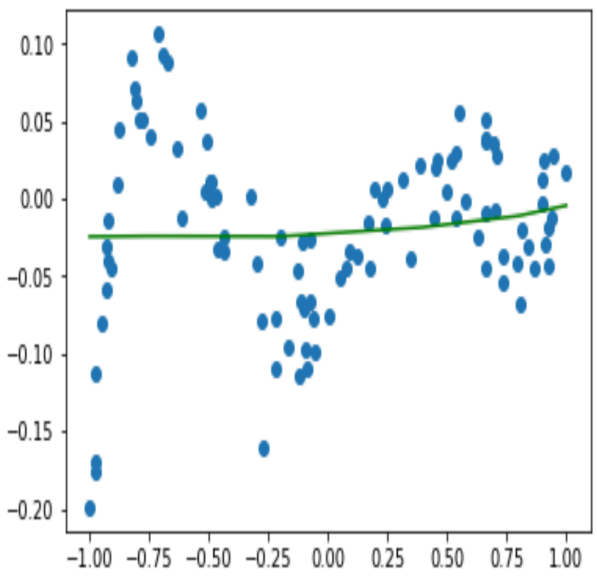
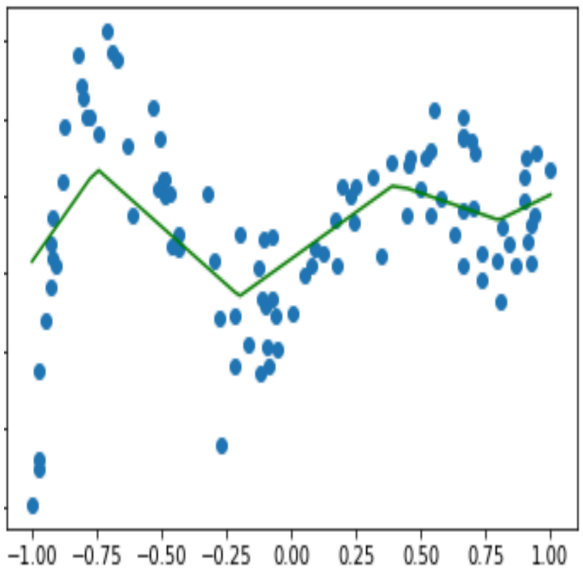


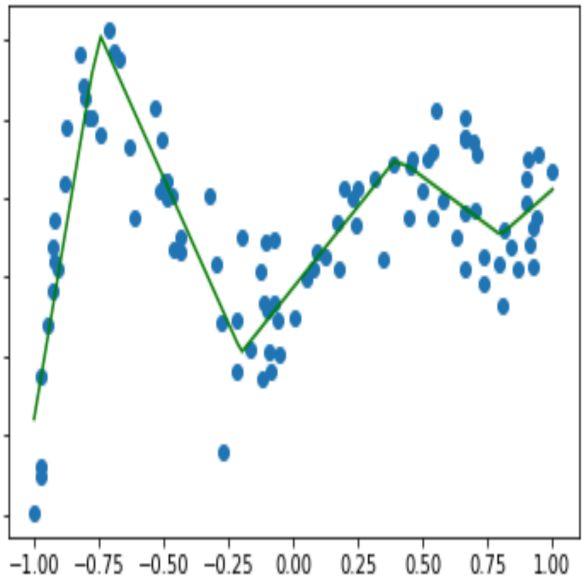
Example: piecewise linear fit (ridge regression)



$\lambda = 1$



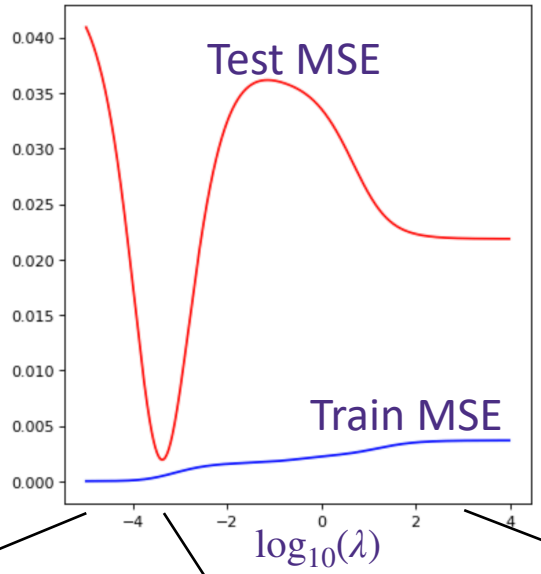
$\lambda = 0.005$

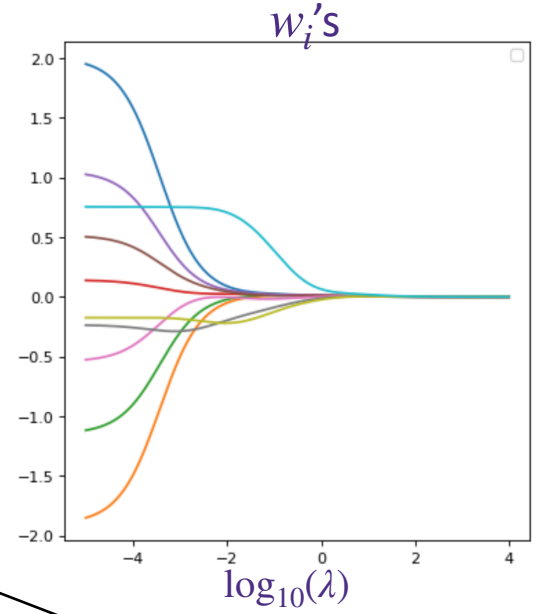


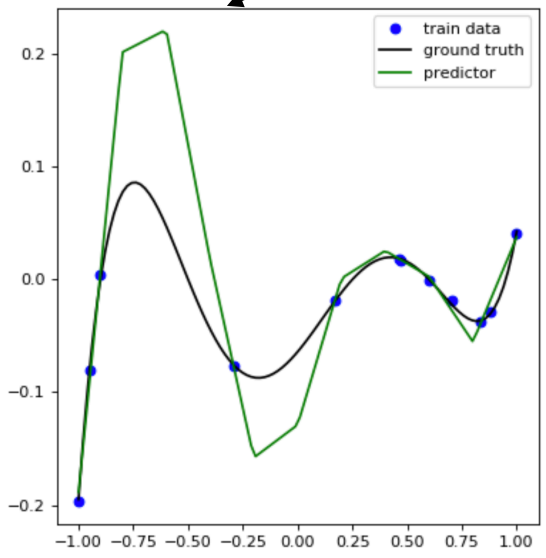
$\lambda = 0.000001$

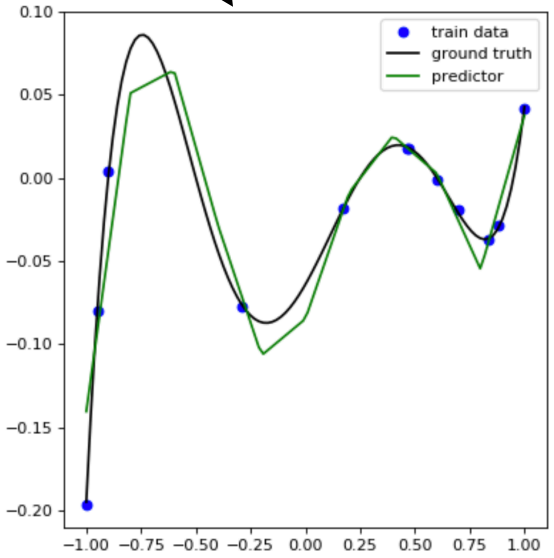
We do not observe overfitting, as d=5 and n=100

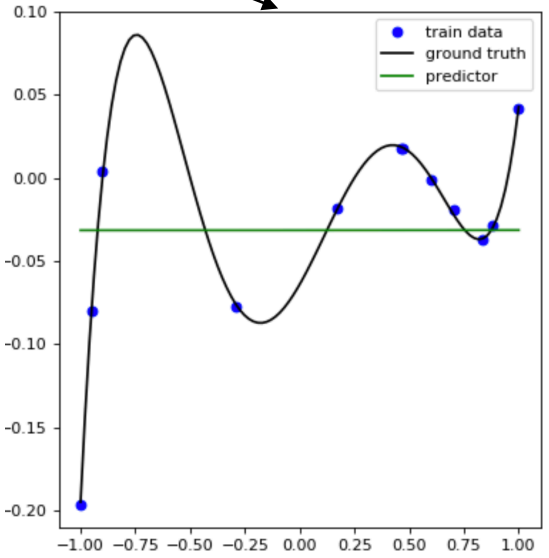
Piecewise linear with $w \in \mathbb{R}^{10}$ and n=11 samples









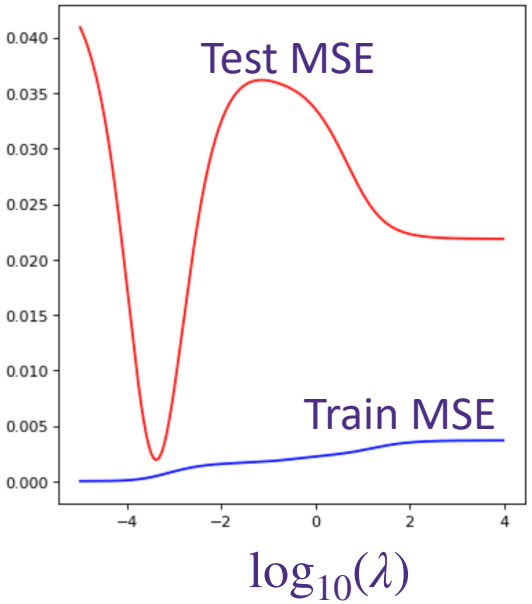


Model selection using Cross-validation

How… How… How???????

- Ridge regression:
  How do we pick the regularization constant λ…
- Polynomial features:
  How do we pick the number of basis functions…

- We could use the test data, but…



How… How… How????????

- Ridge regression:
  How do we pick the regularization constant λ…
- Polynomial features:
  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 **train on the test data**
  - Use test data only for reporting the test error
    (once in the end)

(LOO) Leave-one-out cross validation

- Consider a validation set with 1 example:
  - $\mathscr{D}$: training data
  - $\mathscr{D} \setminus j$: training data with j-th data point (x_j, y_j) moved to validation set
- Learn model $f_{\mathscr{D} \setminus j}$ with $\mathscr{D} \setminus j$ dataset
- The squared error on predicting y_j: $(y_j - f_{\mathscr{D} \setminus j}(x_j))^2$

  is an unbiased estimate of the **true error**

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

  but, variance of $(y_j - f_{\mathscr{D} \setminus j}(x_j))^2$ is too large

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  but variance of $(y_j - f_{\mathscr{D} \setminus j}(x_j))^2$ is too large, so instead

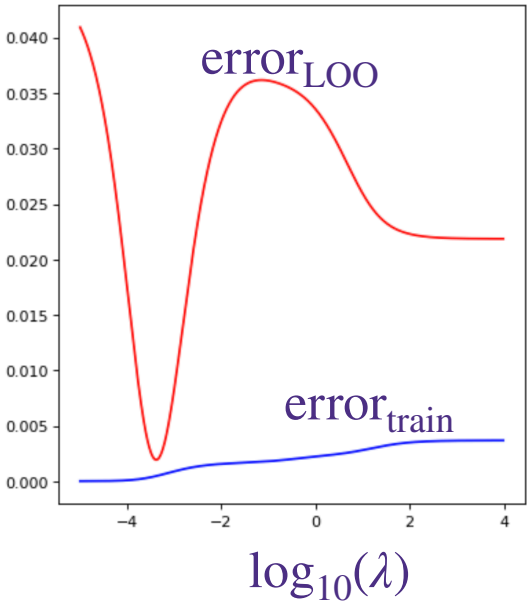
- **LOO cross validation**: Average over all data points *j*:
  - Train n times:
    for each data point you leave out, learn a new classifier $f_{\mathscr{D} \setminus j}$
  - **Estimate the true error** as:

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

LOO cross validation is (almost) unbiased estimate!

- When computing LOOCV error, we only use $n-1$ data points to train
  - So it's not estimate of true error of learning with n data points
  - Usually pessimistic – learning with less data typically gives worse answer. (Leads to an over estimation of the error)

- 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
- say, you implemented a fast 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 model $f_{\mathcal{D}\setminus\mathcal{D}_i}$ using data point not in $\mathcal{D}_i$
  - Estimate error of $f_{\mathcal{D}\setminus\mathcal{D}_i}$ on validation set $\mathcal{D}_i$:

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

$\mathcal{D} =$

$\mathcal{D}_1$	$\mathcal{D}_2$	$\mathcal{D}_3$	$\mathcal{D}_4$	$\mathcal{D}_5$
Train	Train	Validation	Train	Train

$f_{\mathcal{D}\setminus\mathcal{D}_3}$

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

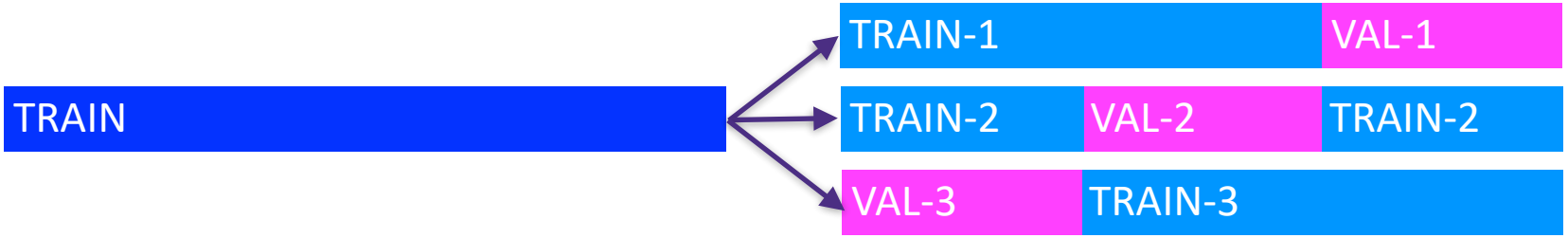
$$\text{error}_{k-\text{fold}} = \frac{1}{k}\sum_{i=1}^{k} \text{error}_{\mathcal{D}_i}$$

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

Model selection using cross validation

- **For** $\lambda \in \{0.001, 0.01, 0.1, 1, 10\}$
  - **For** $j \in \{1, \ldots, k\}$
    - $$\hat{w}_{\lambda,\text{Train}-j} \leftarrow \arg\min_{w} \sum_{i \in \text{Train}-j} (y_i - w^T x_i)^2 + \lambda \|w\|_2^2$$
- $$\hat{\lambda} \leftarrow \arg\min_{\lambda} \frac{1}{k} \sum_{j=1}^{k} \sum_{i \in \text{Val}-j} (y_i - \hat{w}_{\lambda,\text{Train}-j}^T x_i)^2$$

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 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

Questions?