

# Cross-Validation

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Test error : an unbiased estimate of TRUE ERROR

BUT ONLY IF YOU DON'T TOUCH TEST DATA AT ALL in training

So, use your training data to “simulate” test data/error in model selection

# How... How... How???????

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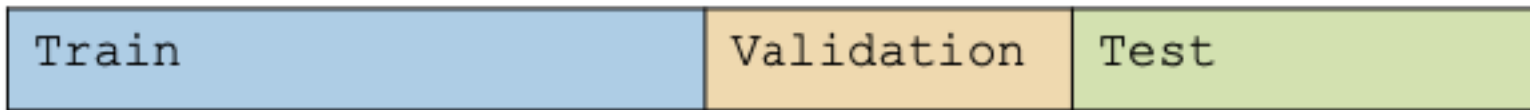
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- > We could use the test data, but...
  - Never ever ever ever ever ever ever ever ever ever ever ever ever ever ever ever ever ever ever train, or even look at the performance on the test data if you're making any decisions based on that performance.

# Validation Set

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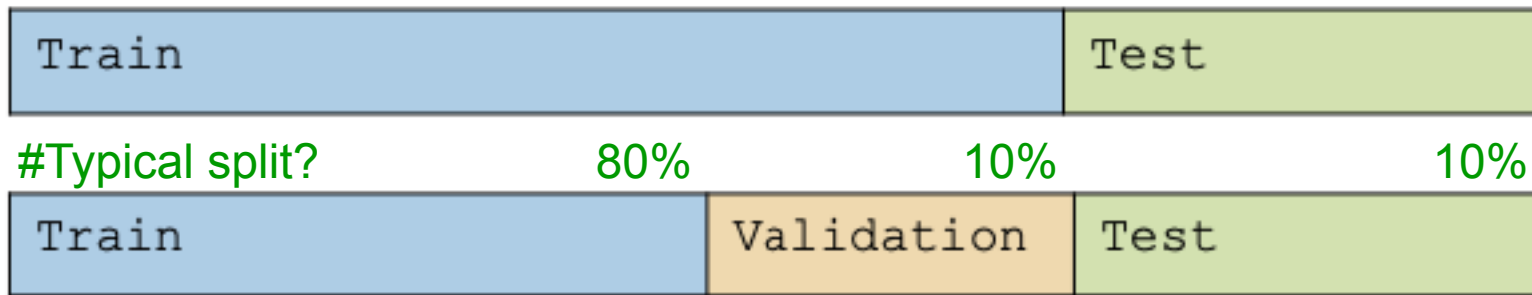
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- > Each set has its own role
  - > **Train:** Used to train a model of each model complexity
  - > **Validation:** Used as a hold-out to evaluate each model. Generally choose model complexity with lowest validation error.
  - > **Test:** Once the model is chosen, can get an estimate of future error by test. This would be what you report. **Only do this once!**

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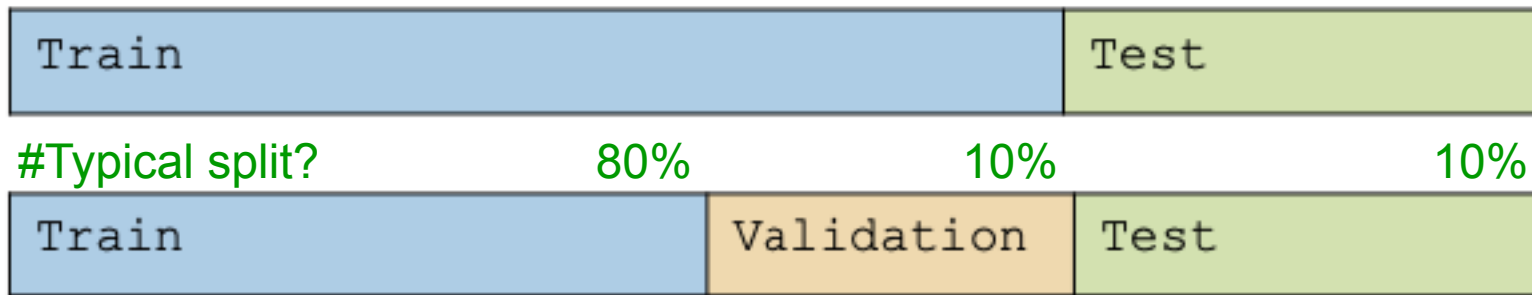
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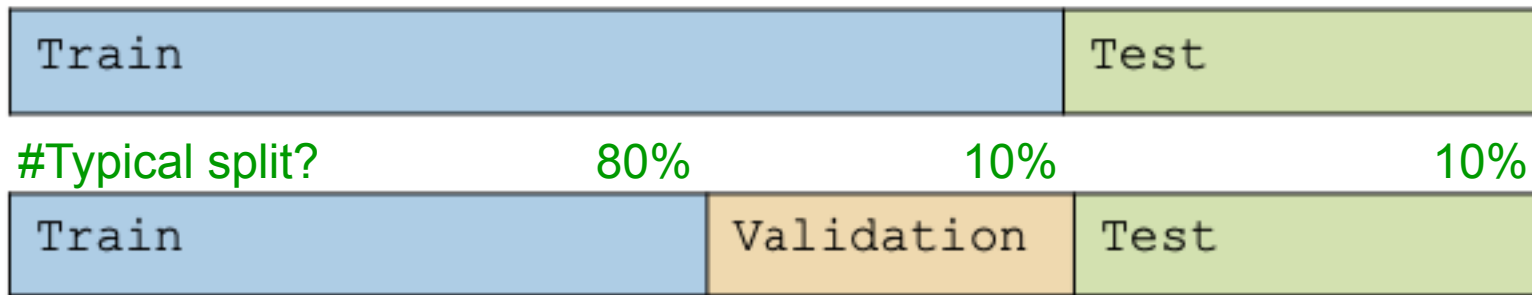
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  - > **Train:** Used to train a model of each model complexity
  - > **Validation:** Used as a hold-out to evaluate each model. Generally choose model complexity with lowest validation error. # Choose *hyperparameters*, like polynomial degree  $p$
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# (LOO) Leave-one-out cross validation

---

- > **Consider a validation set with 1 example:**
  - **D** – training data
  - **$D \setminus j$**  – training data with  $j$  th data point  $(x_j, y_j)$  moved to validation set
- > **Learn model  $f_{D \setminus j}$  with  $D \setminus j$  dataset**
- > **Estimate true error as squared error on predicting  $y_j$ :**
  - **Unbiased estimate of error<sub>true</sub>( $f_{D \setminus j}$ )!**

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- > Estimate true error as squared error on predicting  $y_j$ :
  - Unbiased estimate of  $\text{error}_{\text{true}}(f_{D \setminus j})$ !
- > **LOO cross validation:** Average over all data points  $j$ :
  - For each data point you leave out, learn a new model  $f_{D \setminus j}$
  - Estimate error as:

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

# LOO cross validation is (almost) unbiased estimate!

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- > When computing LOOCV error, we only use  $N-1$  data points
  - So it's not quite an 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! Why not use LOO error for model selection!
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# You just fit  $n$  models!!

# Computational cost of LOO

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- > 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

–  $D_1, \dots, D_k$

> For each  $i$

– Learn model  $f_{D \setminus D_i}$  using data point not in  $D_i$

– Estimate error of  $f_{D \setminus D_i}$  on validation set  $D_i$ :

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

| 1     | 2     | 3          | 4     | 5     |
|-------|-------|------------|-------|-------|
| Train | Train | Validation | Train | Train |

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

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

> **k-fold cross validation properties:**

- Much faster to compute than LOO
- More (pessimistically) biased – using much less data, only  $n(k-1)/k$
- Usually,  $k = 10$

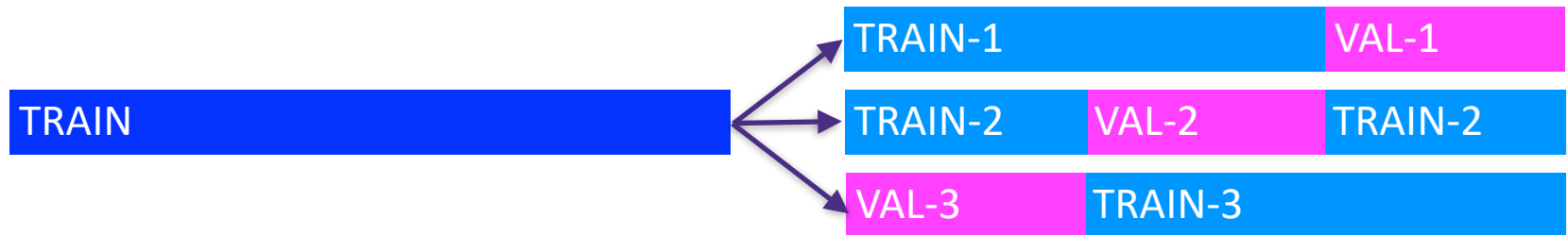
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# Recap

- > 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 degree



- > 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 1

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- > You wish to predict the stock price of zoom.us given historical stock price data
- > You use all daily stock price up to Jan 1, 2020 as **TRAIN** and Jan 2, 2020 - April 13, 2020 as **TEST**
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    - Nope! Future data is o.o.d. (out of distribution) from the training data
  - Why is “wrong” in square quotes?
    - You might still want to do this. It's economically valuable, if you could.

# 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 entire dataset:

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 break data into train and test dataset.
- > We train linear regression on these selected features on the training set. We compute the test error and report it
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  - Top 50 features might be redundant with each other.

# Recap

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## > Learning is...

- Collect some data
  - > E.g., potato delivery features and delivery time
- 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 **on TRAIN**
- Choose an optimization procedure
  - > E.g., set derivative to zero to obtain estimator, **cross-validation on VAL to pick num. features**
- > Justifying the accuracy of the estimate
  - > E.g., report **TEST error**

# Bias-Variance Tradeoff

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# Optimal Prediction

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

Find function  $\eta$  that minimizes

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

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

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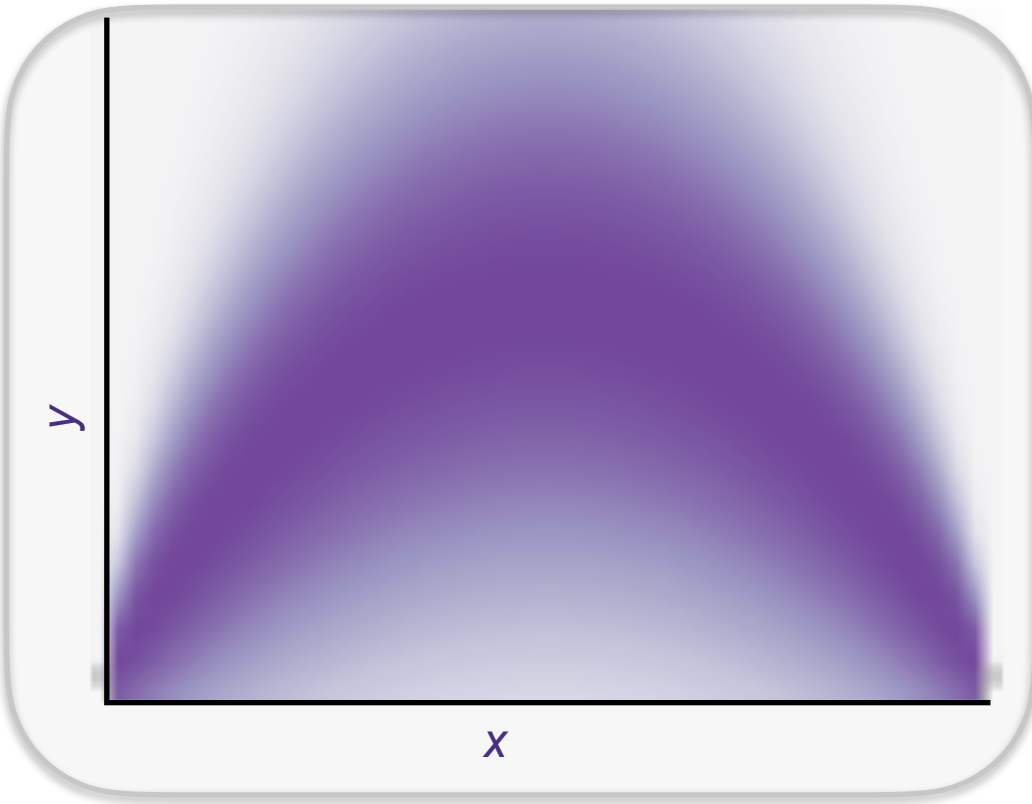
$$\begin{aligned} 0 &= \frac{d}{dc_x} \mathbb{E}_{Y|X}[(Y - c_x)^2 | X = x] \\ &= \mathbb{E}_{Y|X} \left[ \frac{d}{dc_x} (Y - c_x)^2 | X = x \right] \\ &= \mathbb{E}_{Y|X}[-2(Y - c_x) | X = x] = -2\mathbb{E}_{Y|X}[Y | X = x] + 2c_x \end{aligned}$$

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

# Statistical Learning

$$\mathbb{E}_{XY}[(Y - \eta(X))^2]$$

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

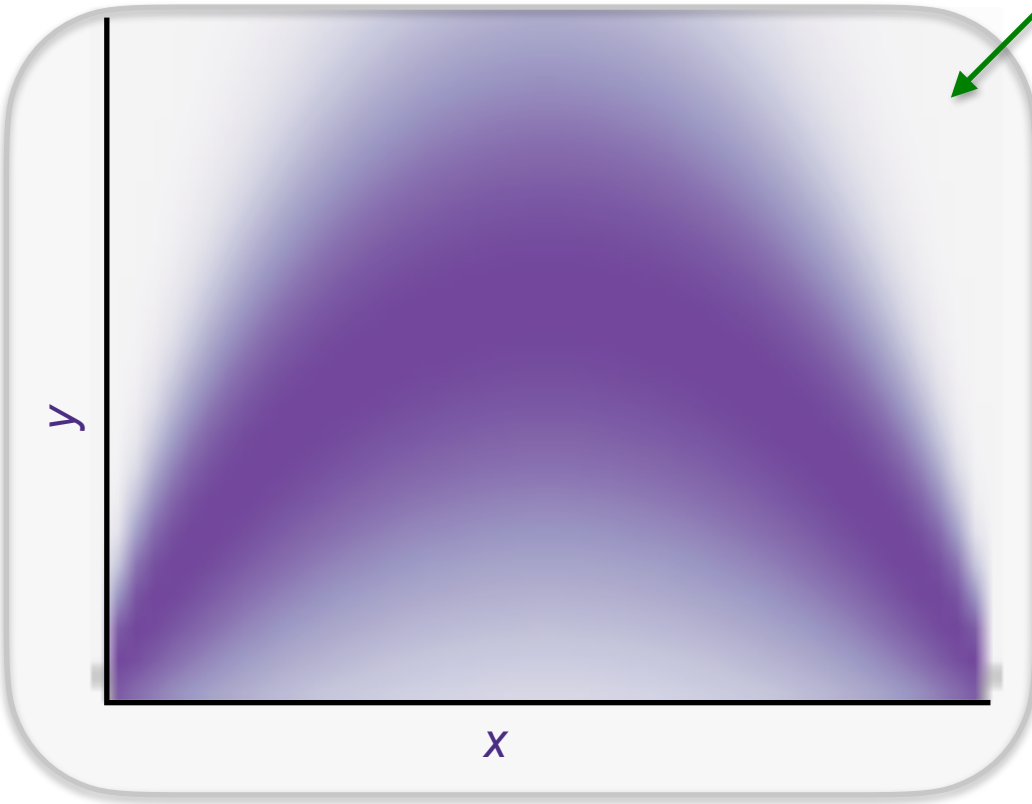


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# Low density



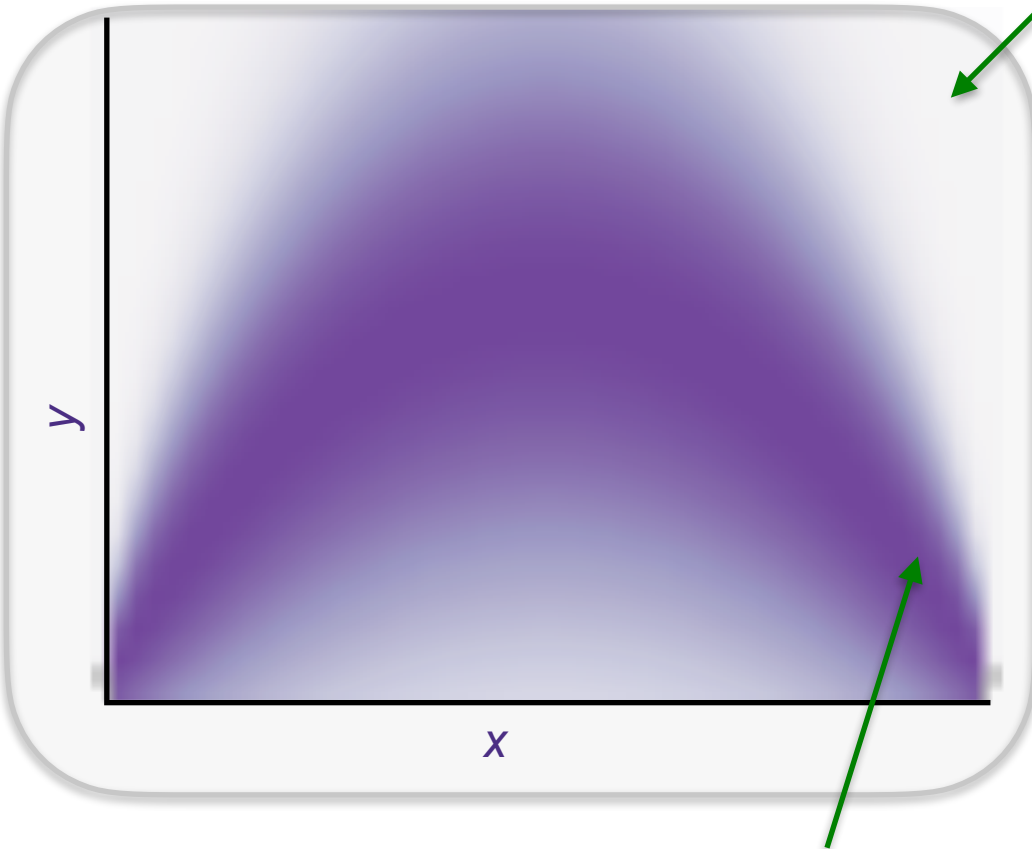
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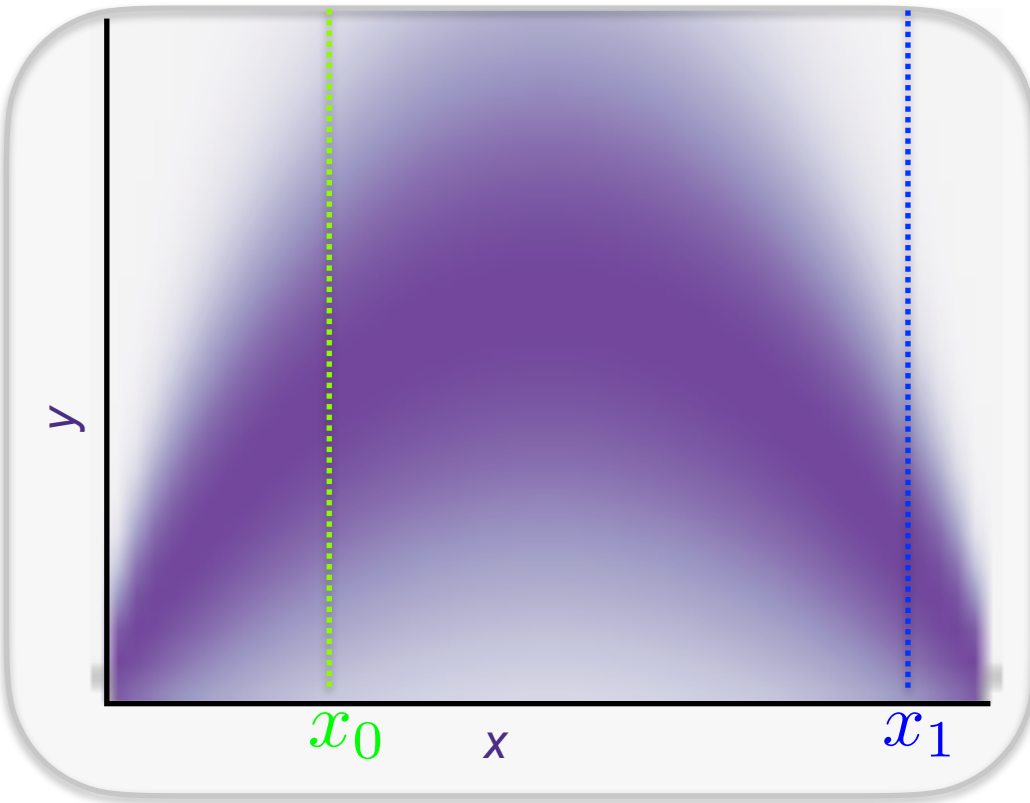
# High density



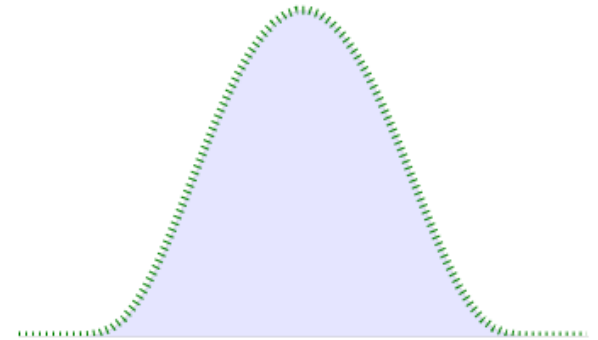
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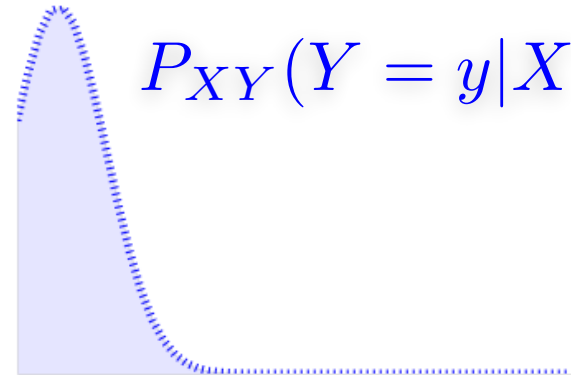
$$P_{XY}(X = x, Y = y)$$



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



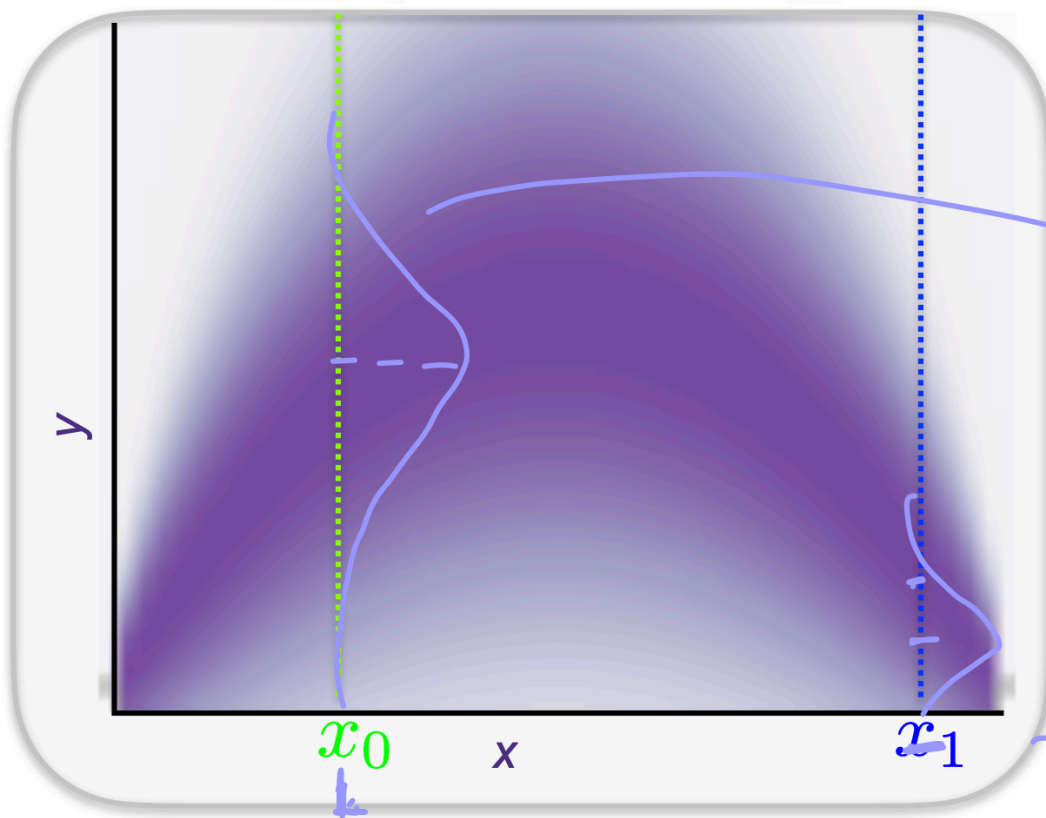
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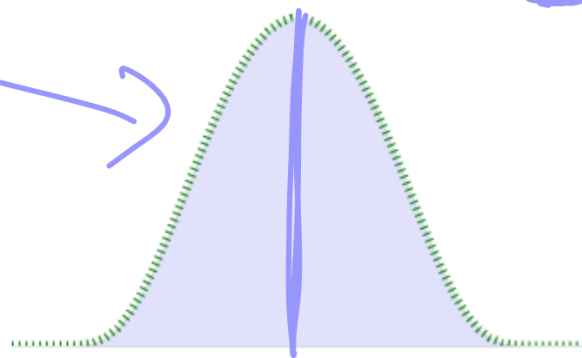
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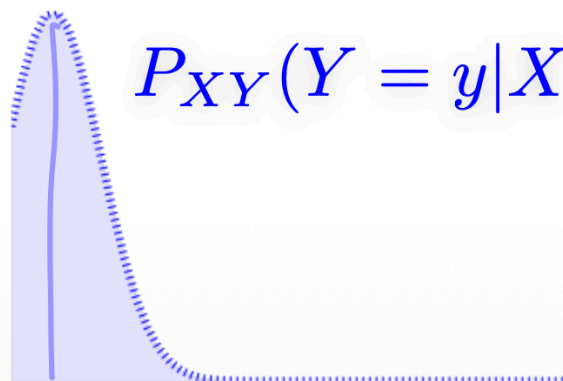
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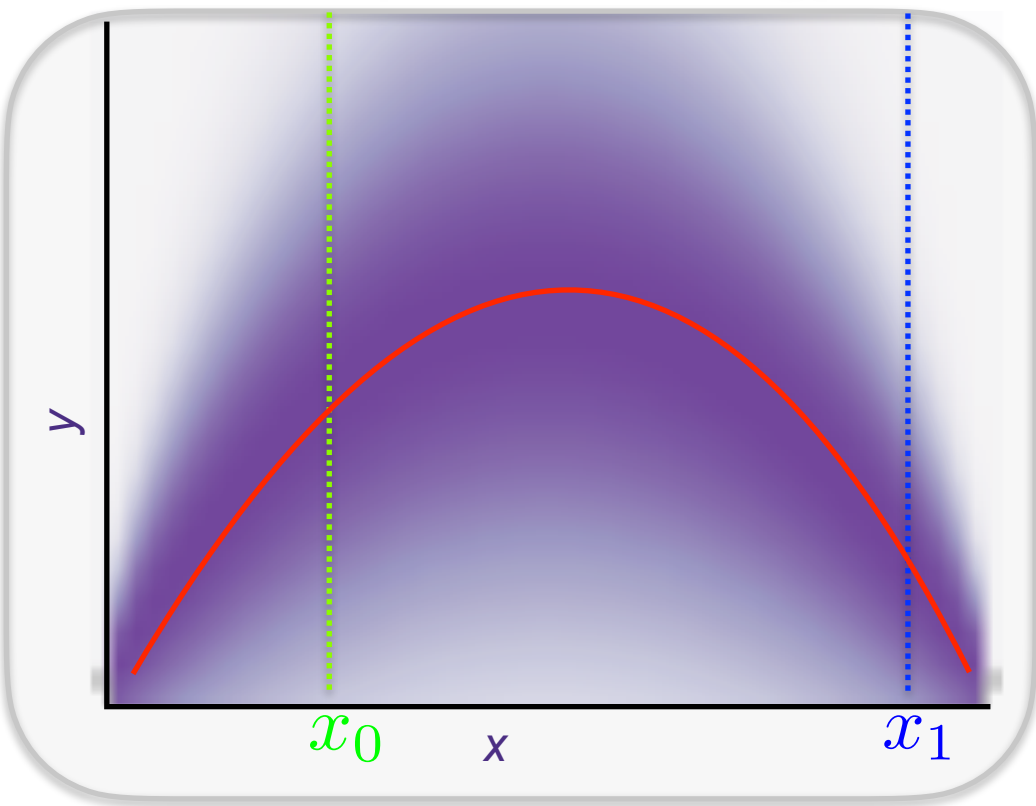
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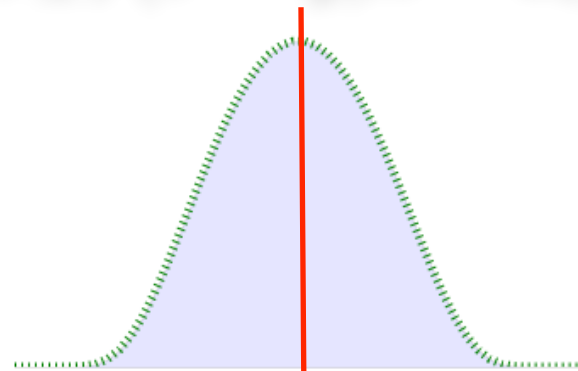
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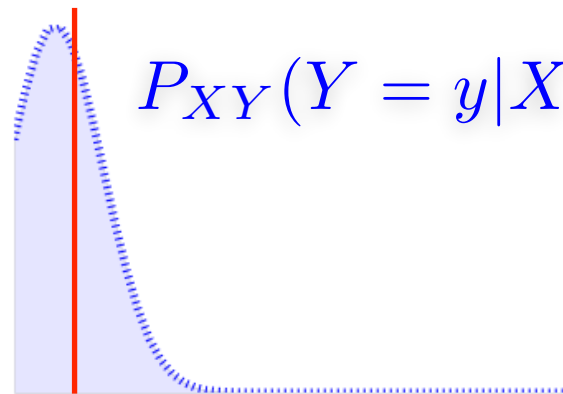
Ideally, we want to find:

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

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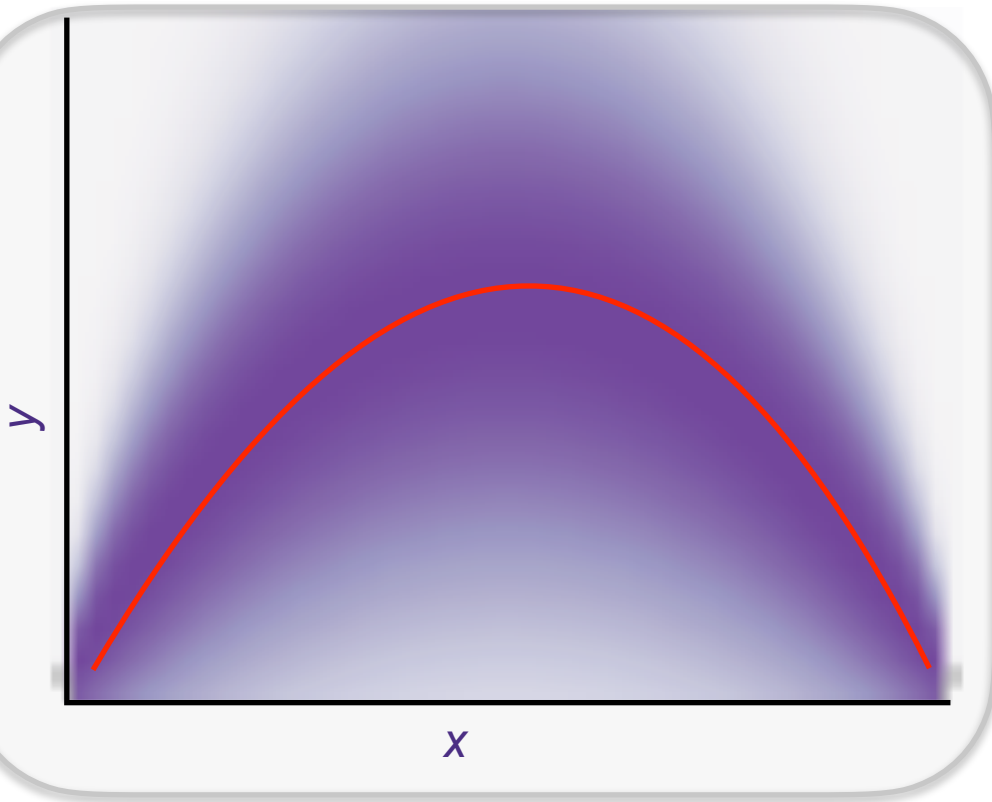


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Ideally, we want to find:

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

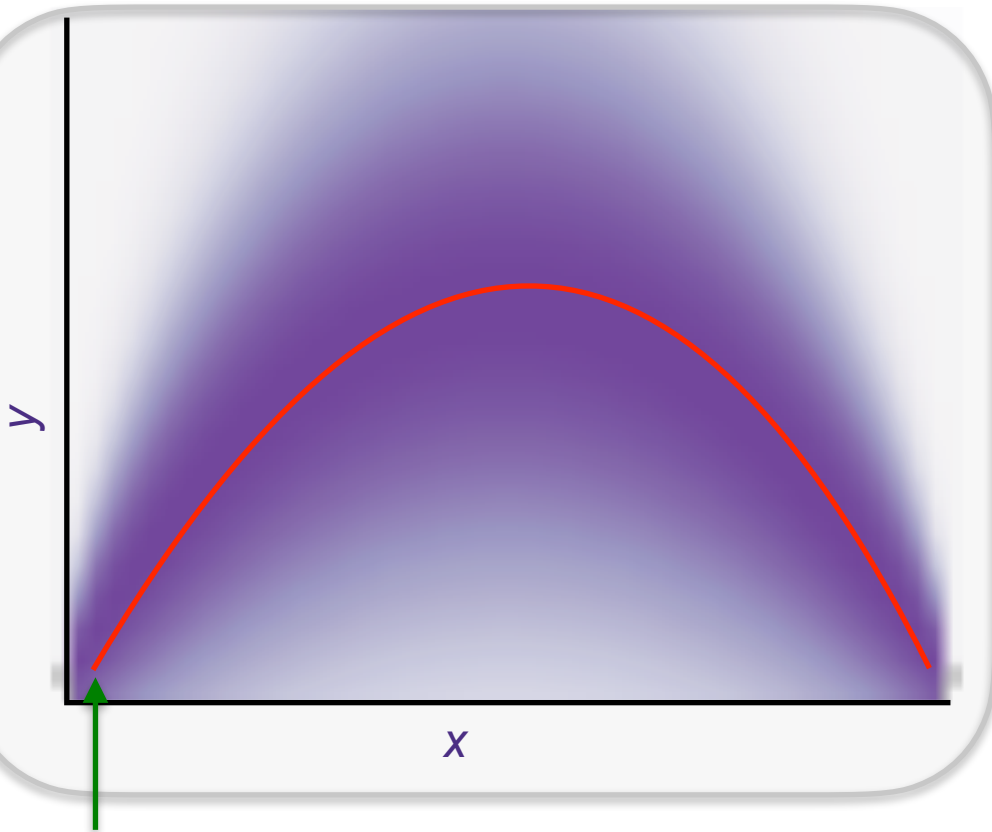


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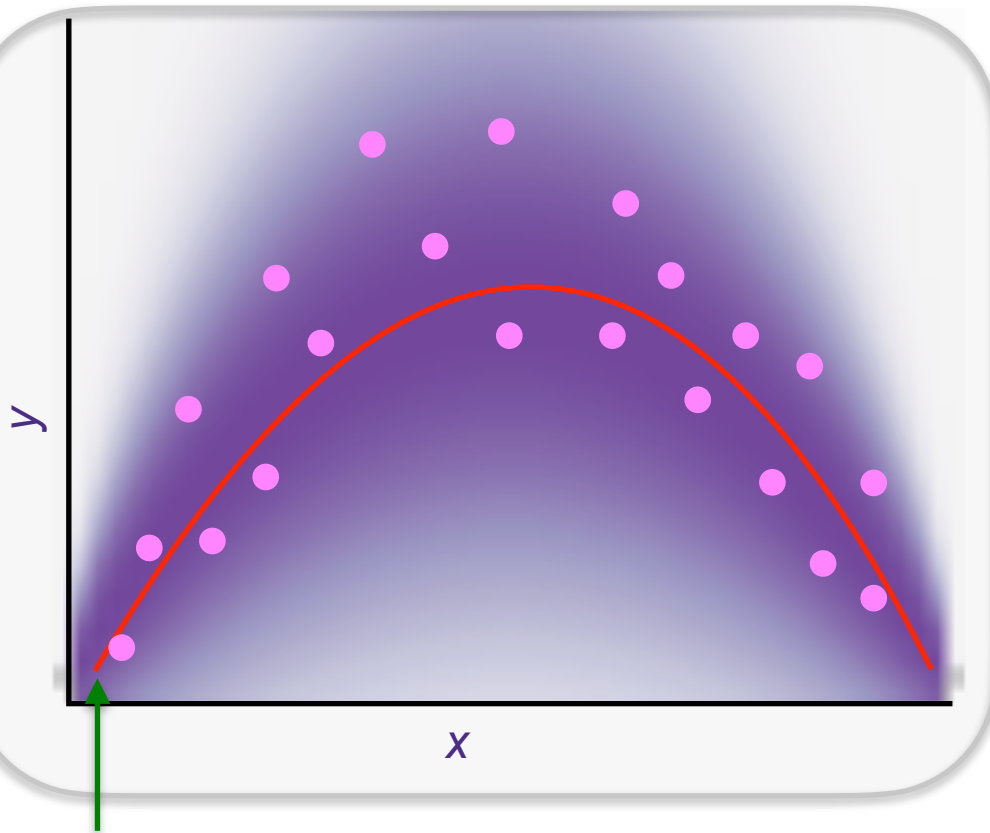
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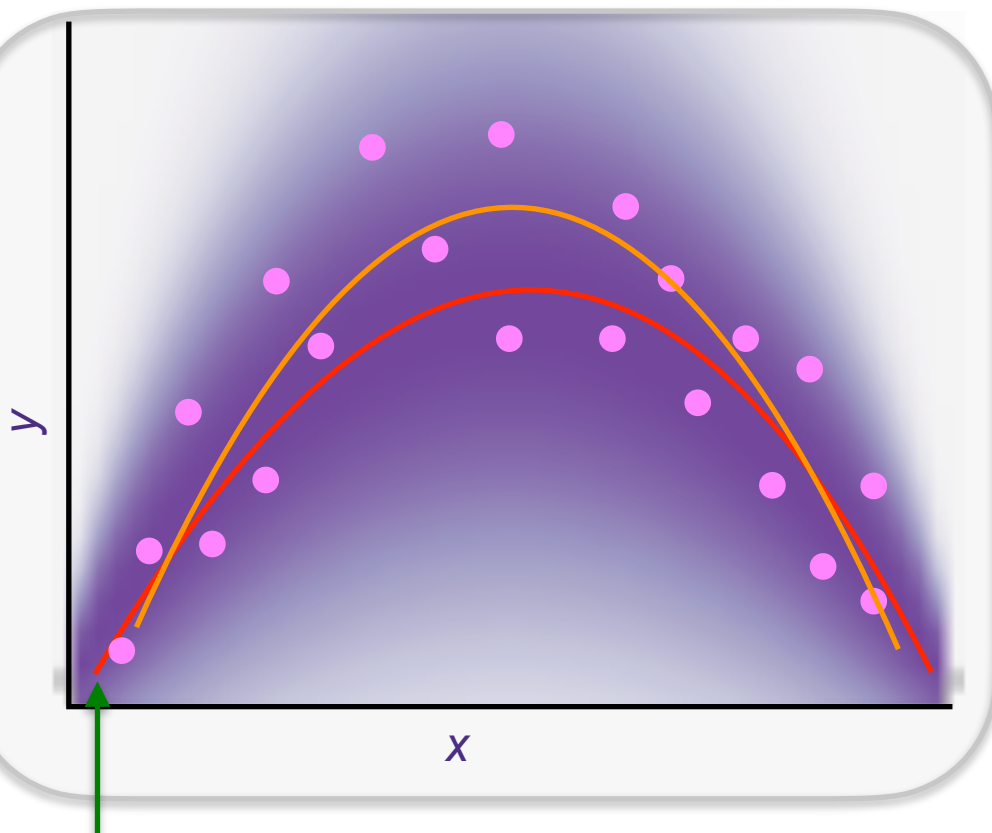
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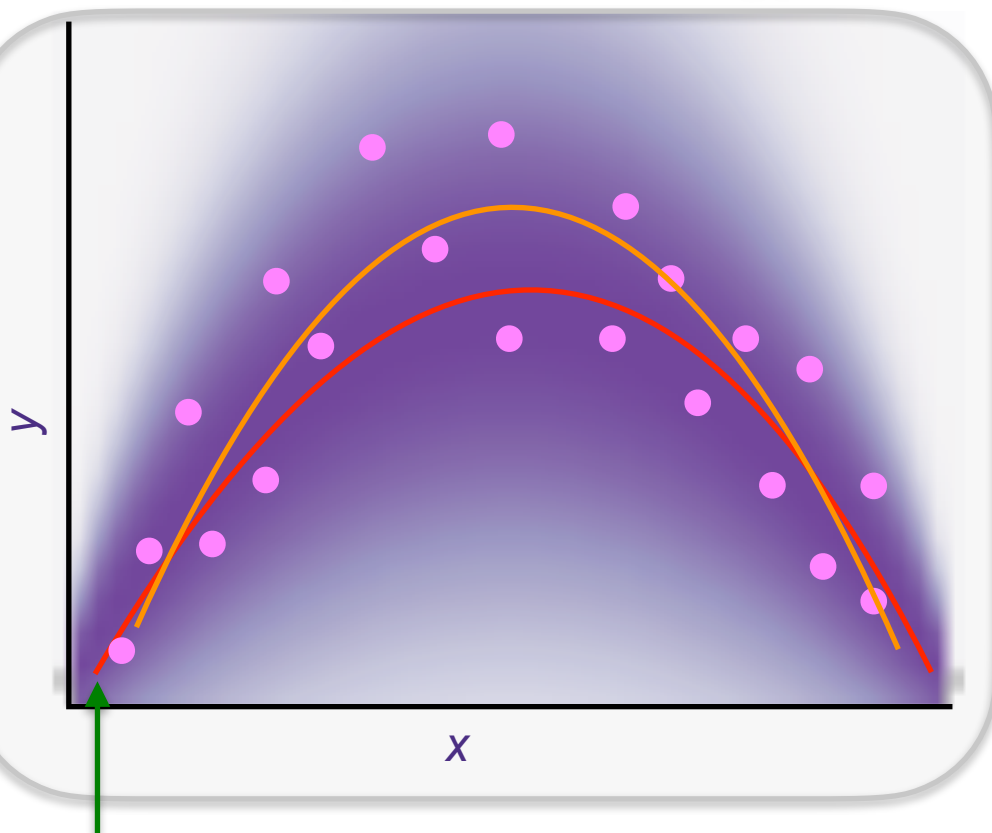
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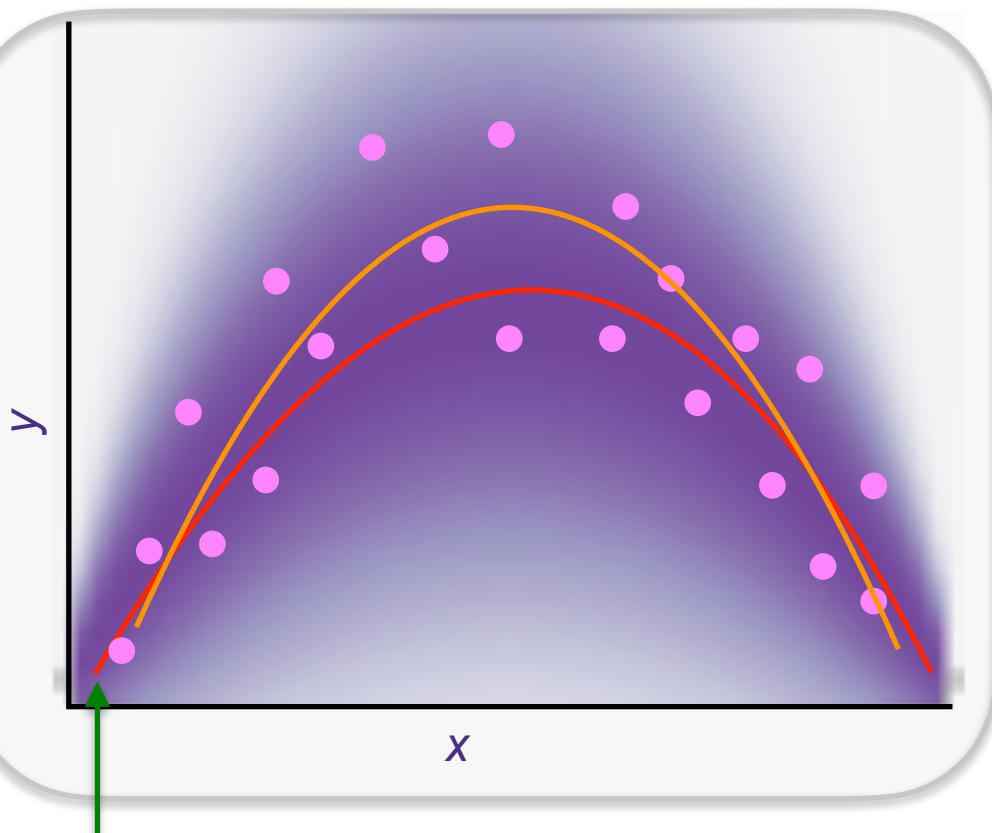
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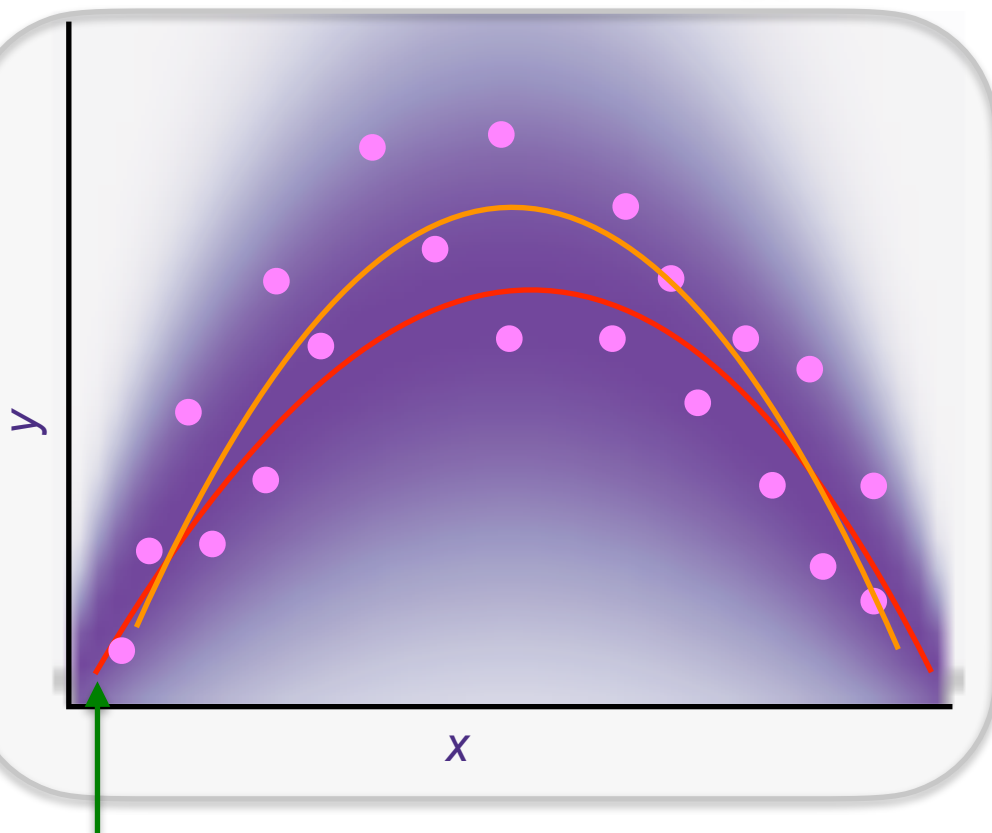
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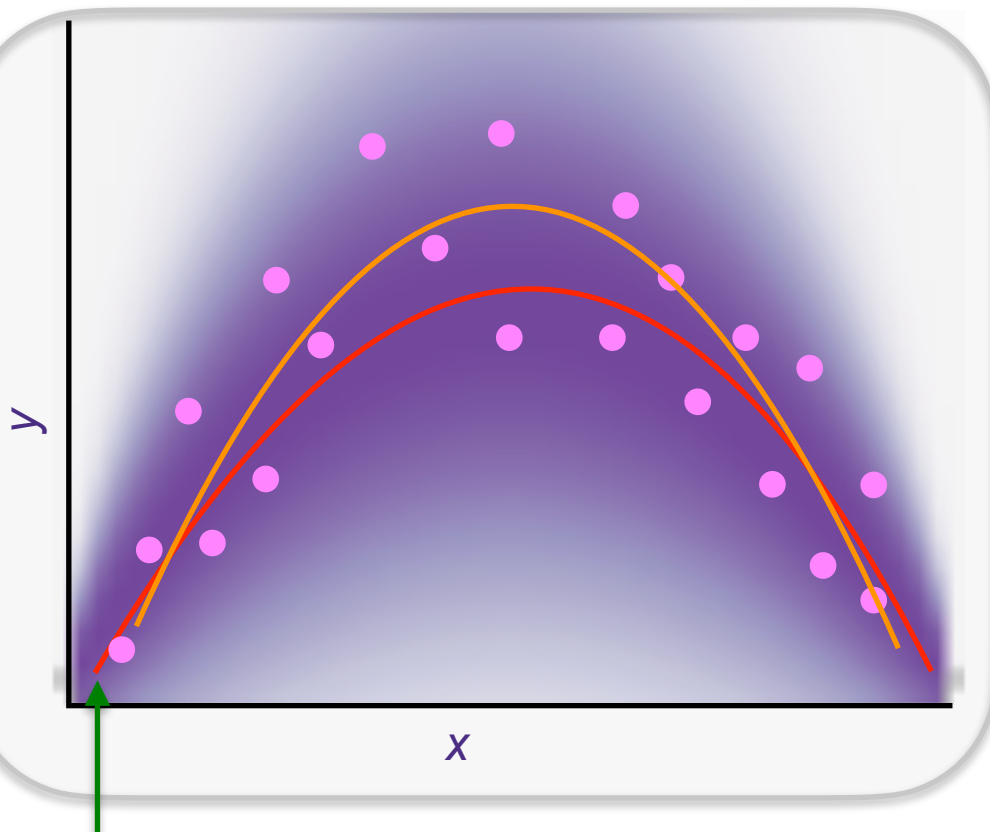
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wrong model class  $\mathcal{F}$

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---

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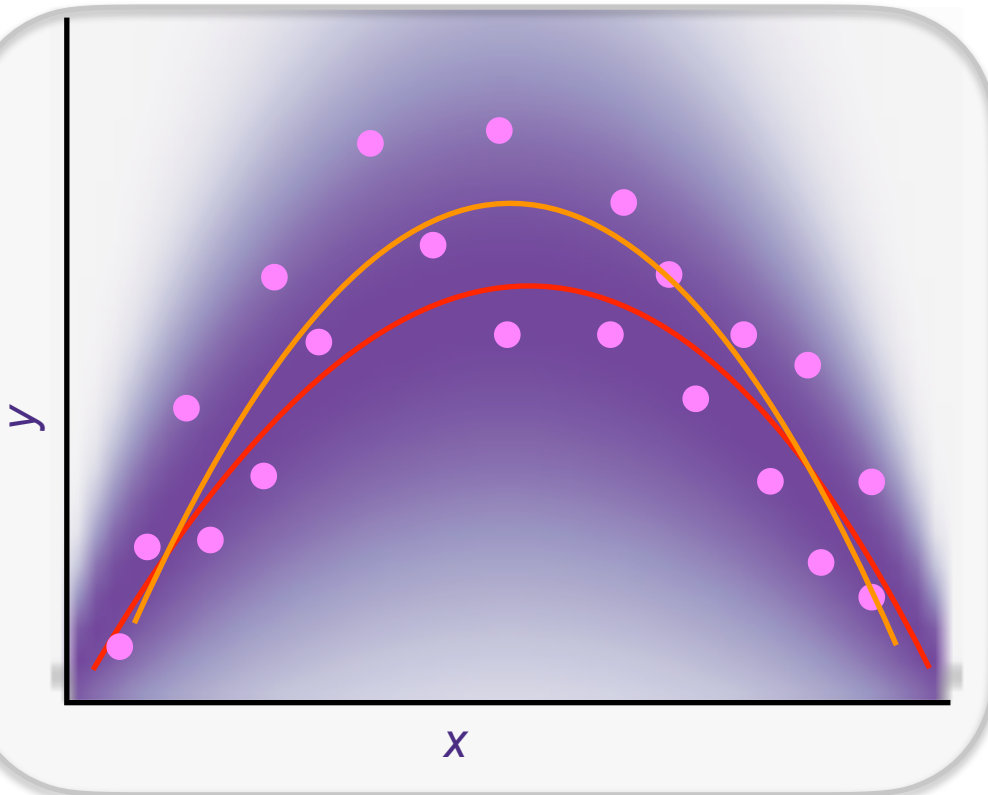
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Minimizing ERE  $\rightarrow$  minimizing squared error loss in general  
(*in expectation....*)

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We care about future predictions:  $\mathbb{E}_{XY}[(Y - \hat{f}(X))^2]$

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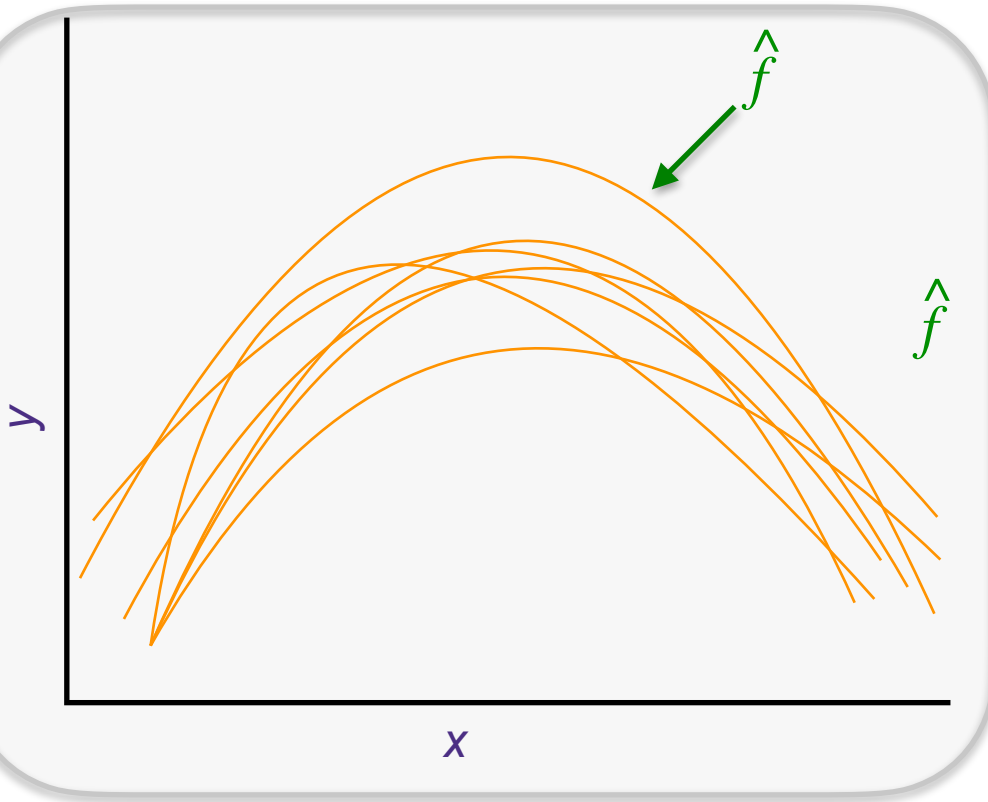
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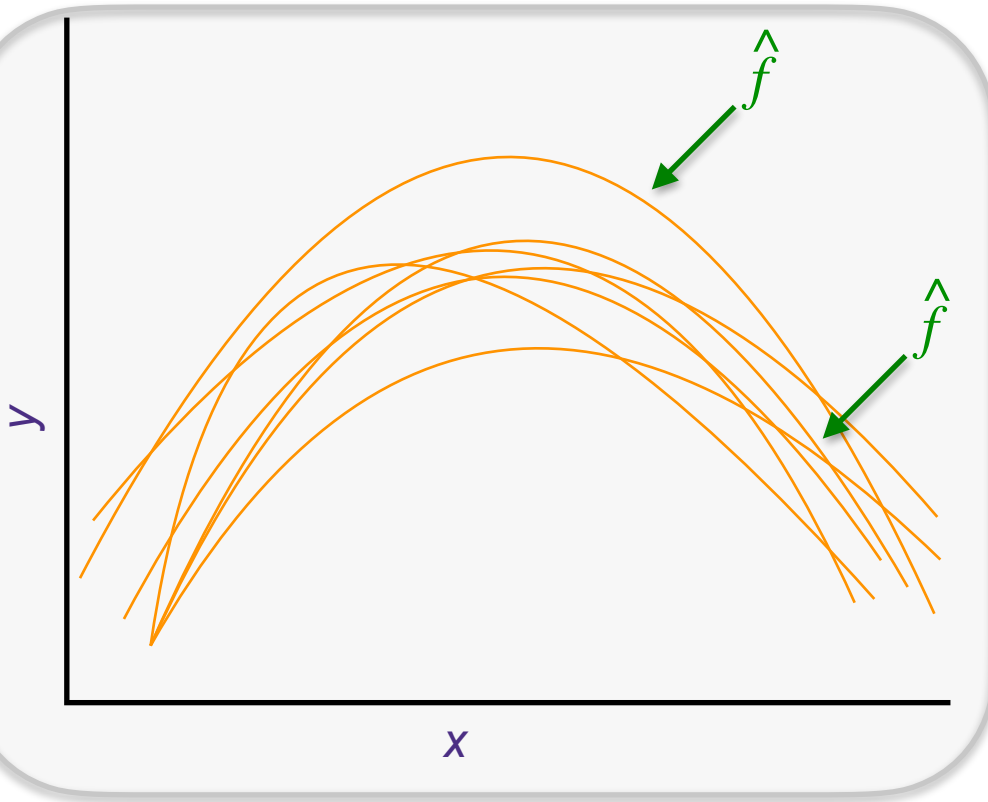
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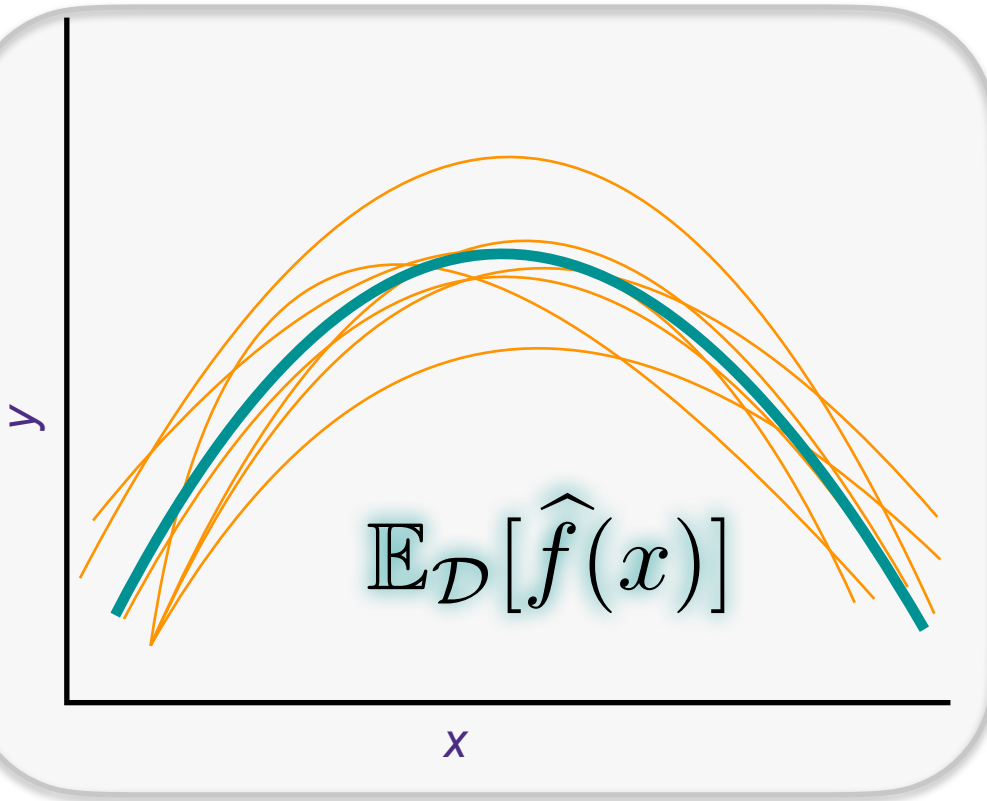
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# Bias-Variance Tradeoff

---

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

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

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**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

# Bias-Variance Tradeoff

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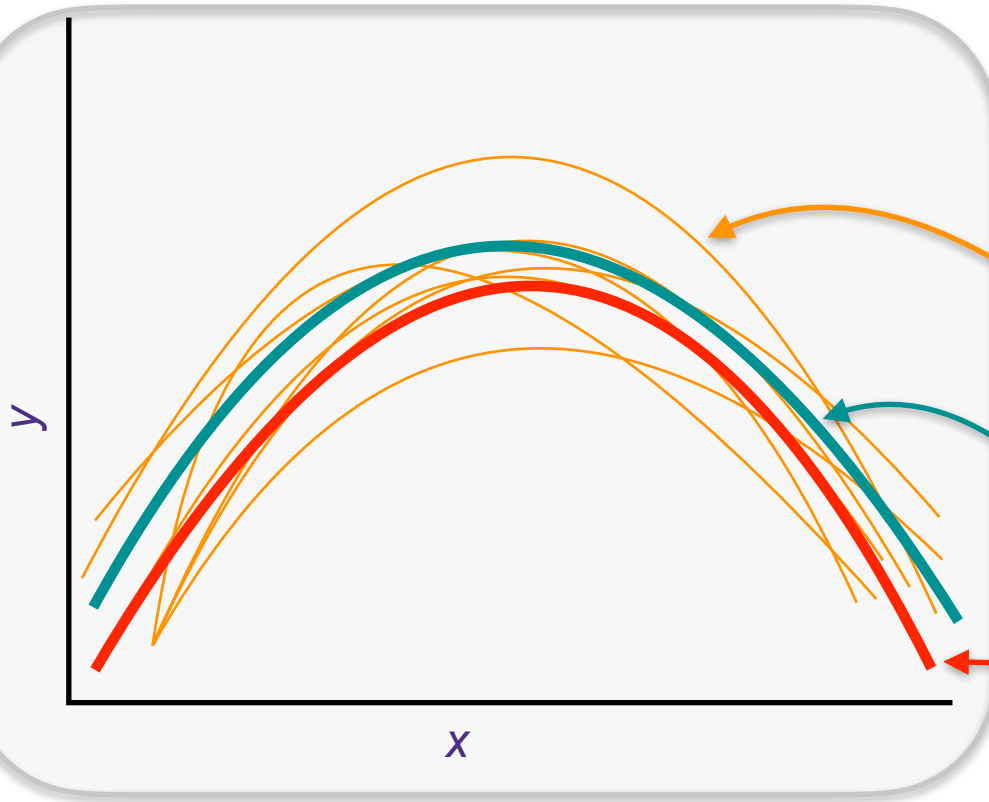
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# Statistical Learning

$$\underbrace{\mathbb{E}_{\mathcal{D}}[(\eta(x) - \hat{f}_{\mathcal{D}}(x))^2]}_{\text{learning error}} = \underbrace{(\eta(x) - \mathbb{E}_{\mathcal{D}}[\hat{f}_{\mathcal{D}}(x)])^2}_{\text{biased squared}} + \underbrace{\mathbb{E}_{\mathcal{D}}[(\mathbb{E}_{\mathcal{D}}[\hat{f}_{\mathcal{D}}(x)] - \hat{f}_{\mathcal{D}}(x))^2]}_{\text{variance}}$$



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

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

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

# Bias-Variance Tradeoff

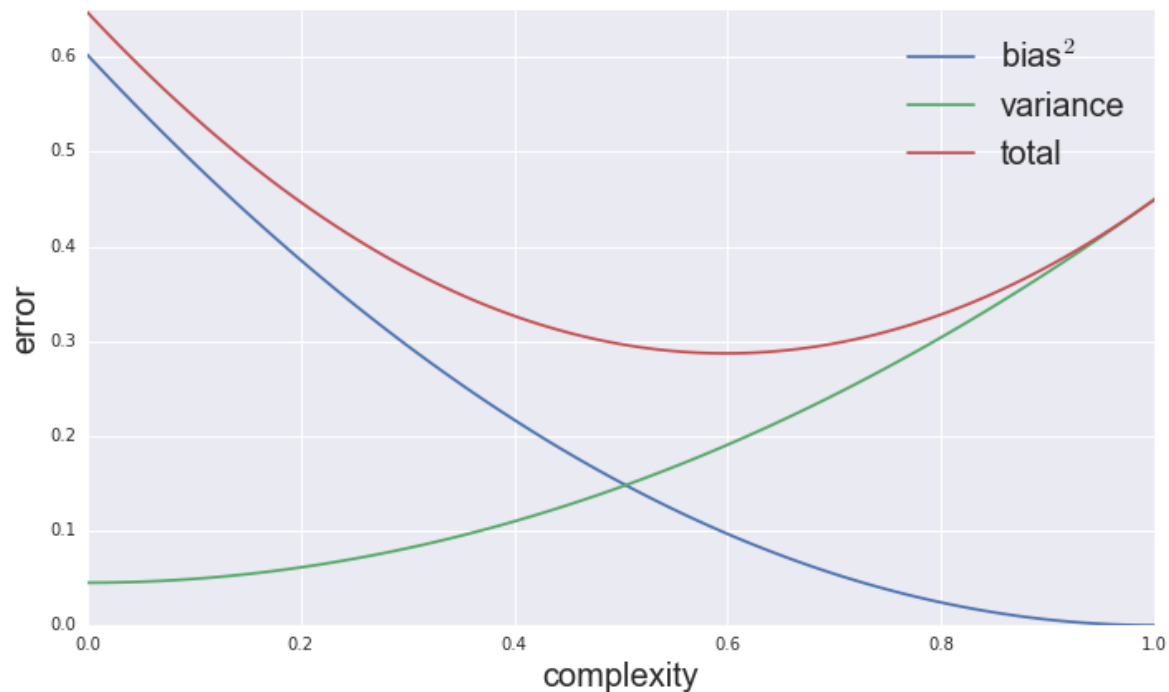
$$\mathbb{E}_{Y|X}[\mathbb{E}_{\mathcal{D}}[(Y - \hat{f}_{\mathcal{D}}(x))^2] | X = x] = \underbrace{\mathbb{E}_{Y|X}[(Y - \eta(x))^2 | X = x]}_{\text{irreducible error}}$$

**irreducible error**

$$+ \underbrace{(\eta(x) - \mathbb{E}_{\mathcal{D}}[\hat{f}_{\mathcal{D}}(x)])^2}_{\text{biased squared}} + \underbrace{\mathbb{E}_{\mathcal{D}}[(\mathbb{E}_{\mathcal{D}}[\hat{f}_{\mathcal{D}}(x)] - \hat{f}_{\mathcal{D}}(x))^2]}_{\text{variance}}$$

**biased squared**

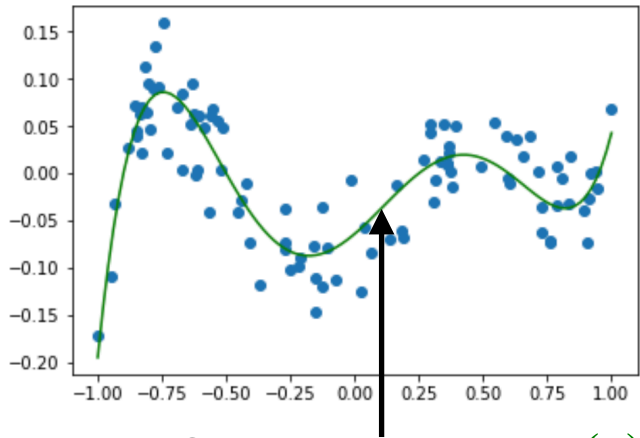
**variance**



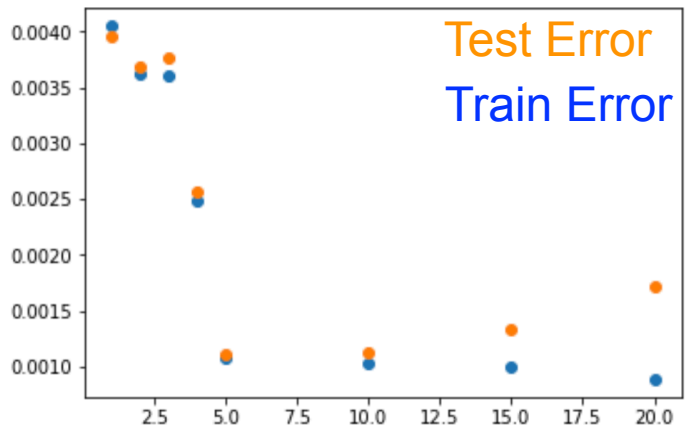
# Overfitting

---

# Test error vs. model complexity

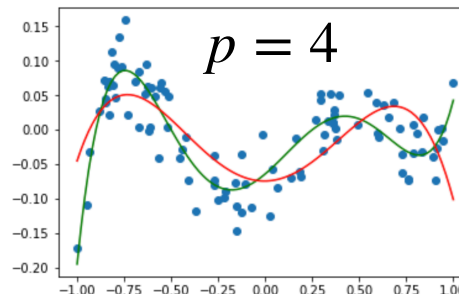
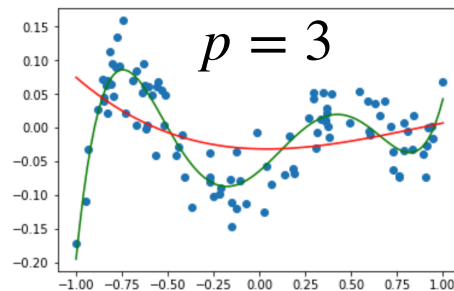
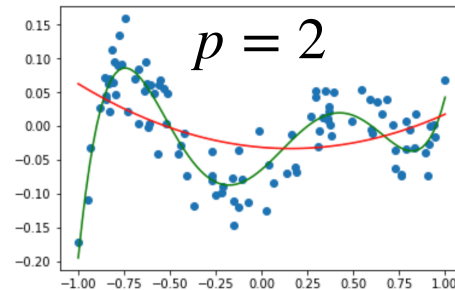
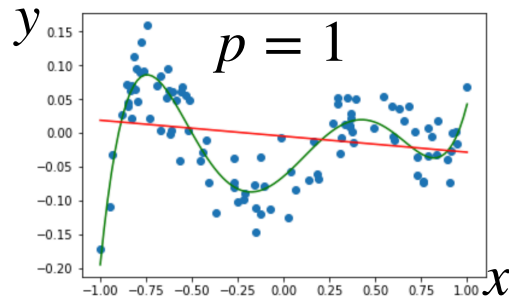


Error

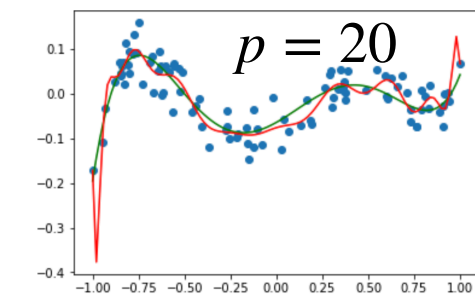
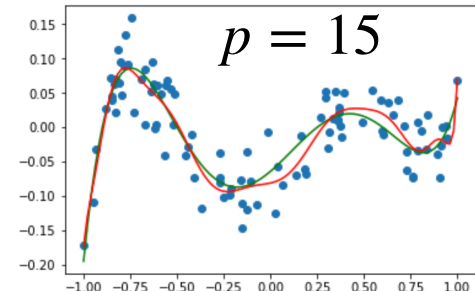
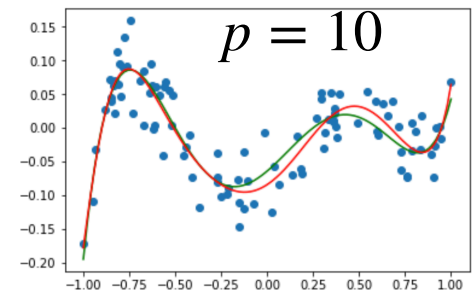
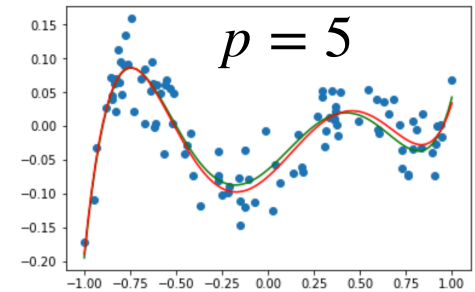


degree  $p$  of the polynomial regression

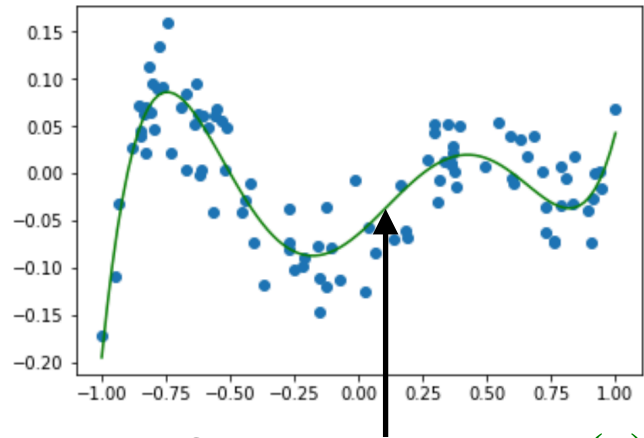
**Simple model:**  
Model complexity is below the complexity of  $\eta(x)$



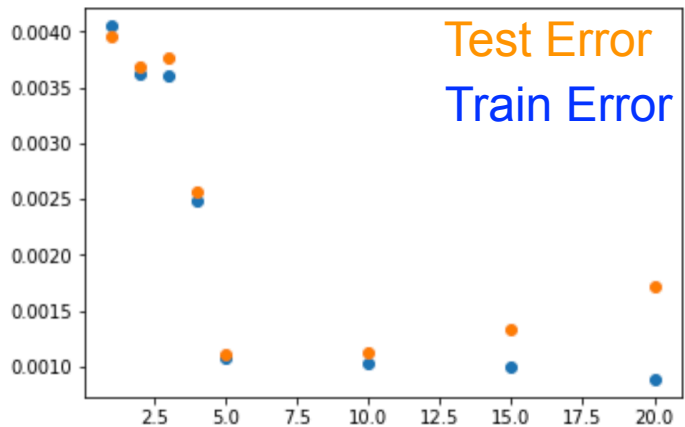
**Complex model:**  
Fits noise in train data, diverging from  $\eta(x)$



# Test error vs. model complexity

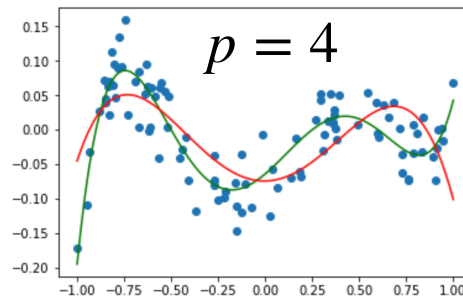
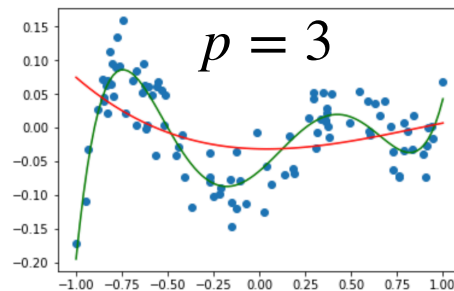
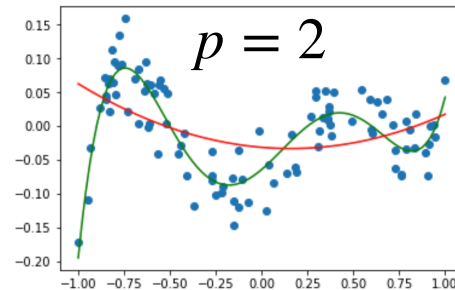
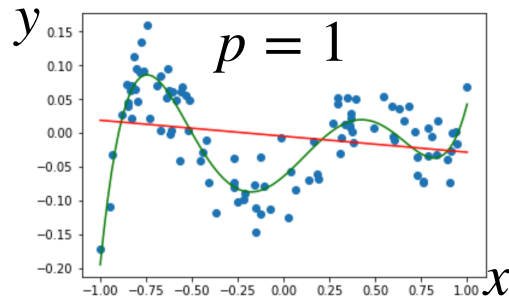


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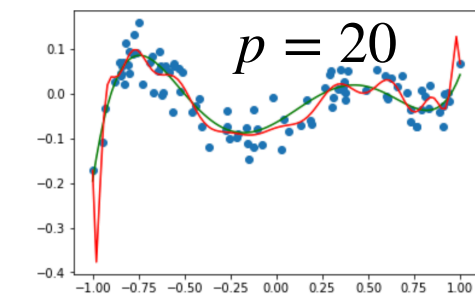
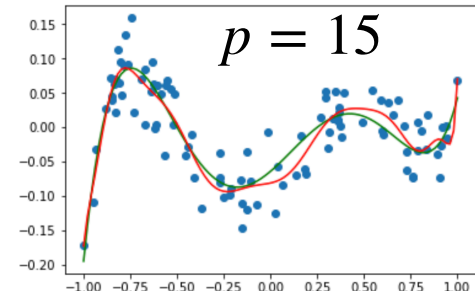
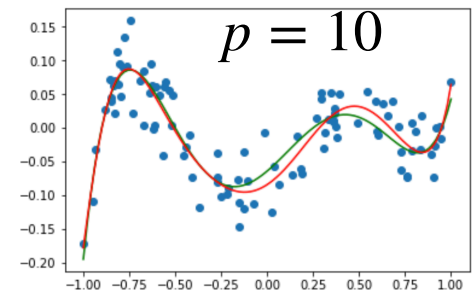
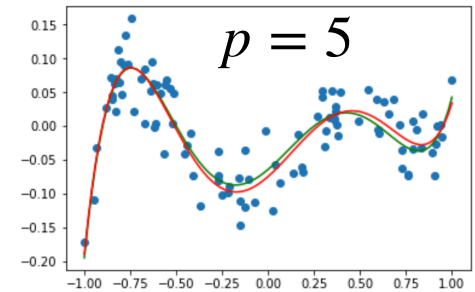


degree  $p$  of the polynomial regression

**Simple model:** # bias  
Model complexity is below the complexity of  $\eta(x)$

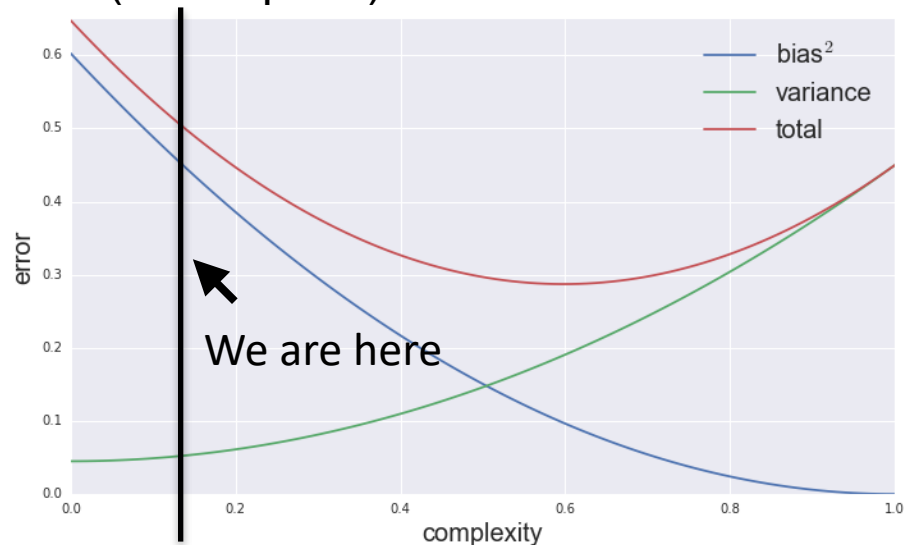


**Complex model:**  
Fits noise in train data, diverging from  $\eta(x)$



# Recap: Bias-variance tradeoff with simple model

(Conceptual) bias variance tradeoff

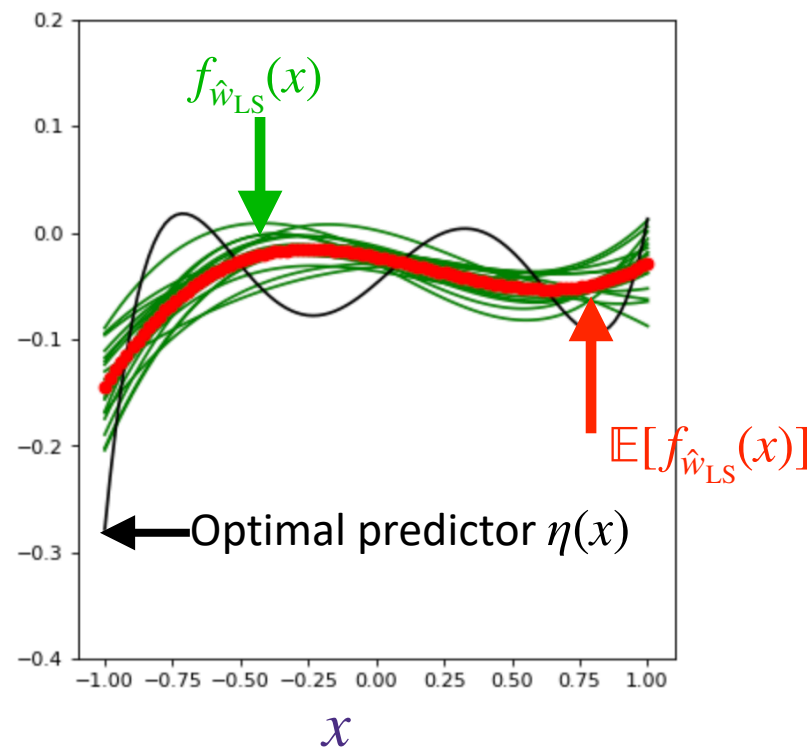


- When model **complexity is low** (lower than the optimal predictor  $\eta(x)$ )

- Bias<sup>2</sup> of our predictor,  
$$\left( \eta(x) - \mathbb{E}_{\mathcal{D}}[\hat{f}_{\mathcal{D}}(x)] \right)^2$$

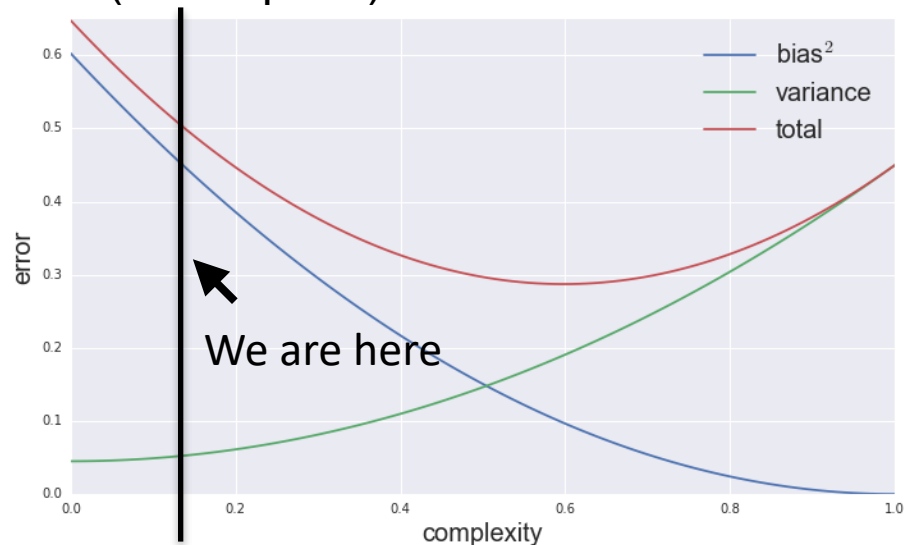
- Variance of our predictor,  
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With degree-3 polynomials, we underfit



# Recap: Bias-variance tradeoff with simple model

(Conceptual) bias variance tradeoff



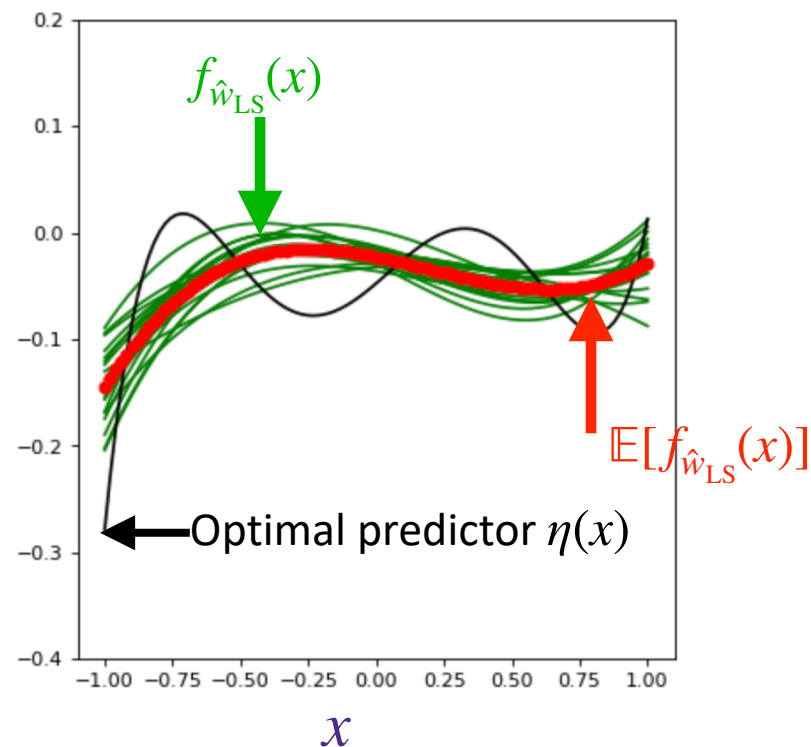
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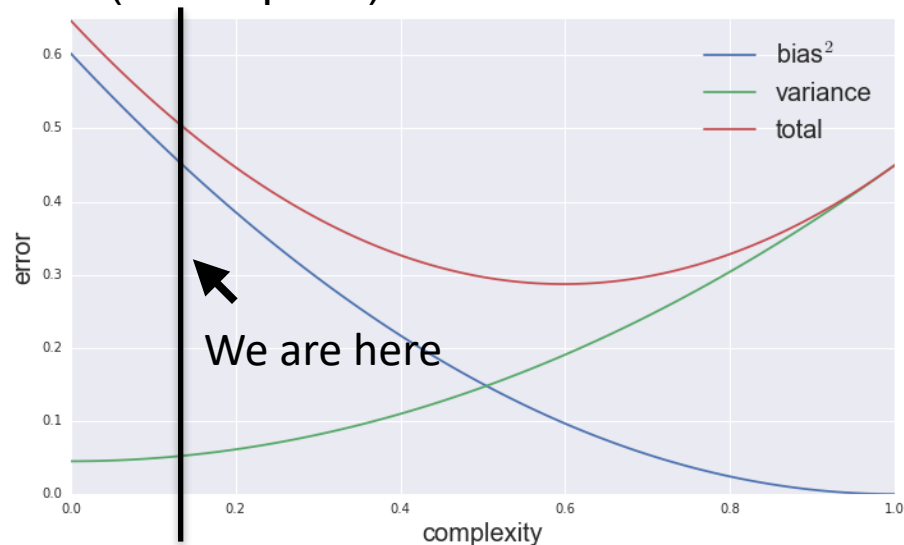
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(Conceptual) bias variance tradeoff



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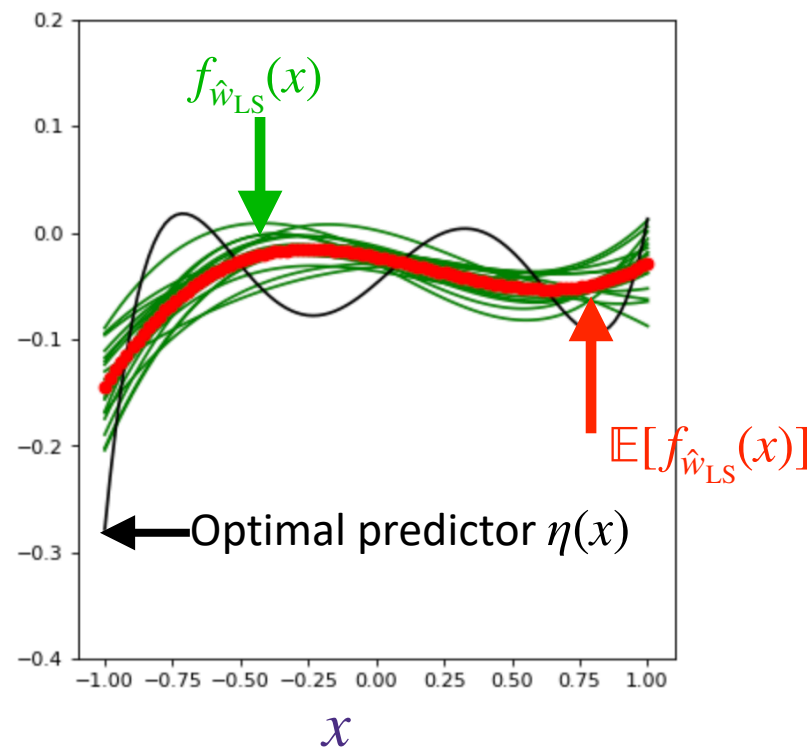
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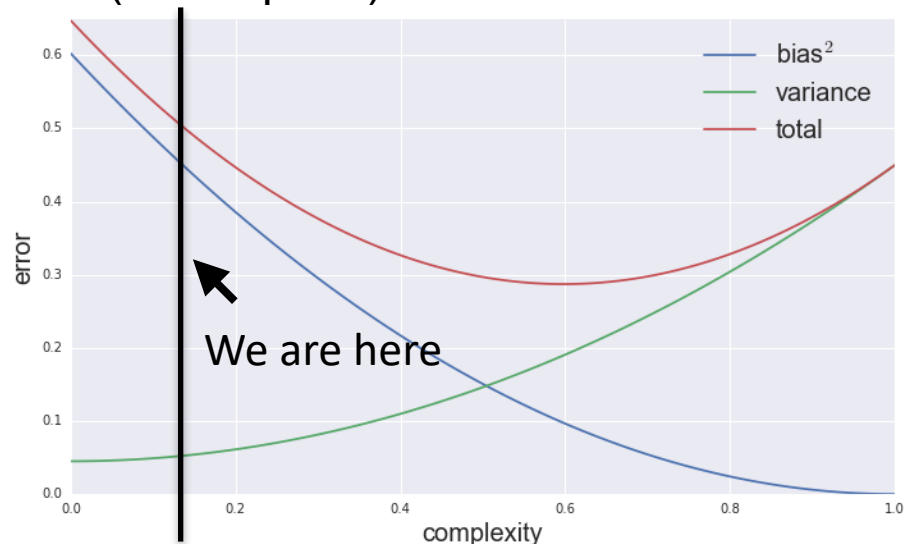
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# Recap: Bias-variance tradeoff with simple model

(Conceptual) bias variance tradeoff



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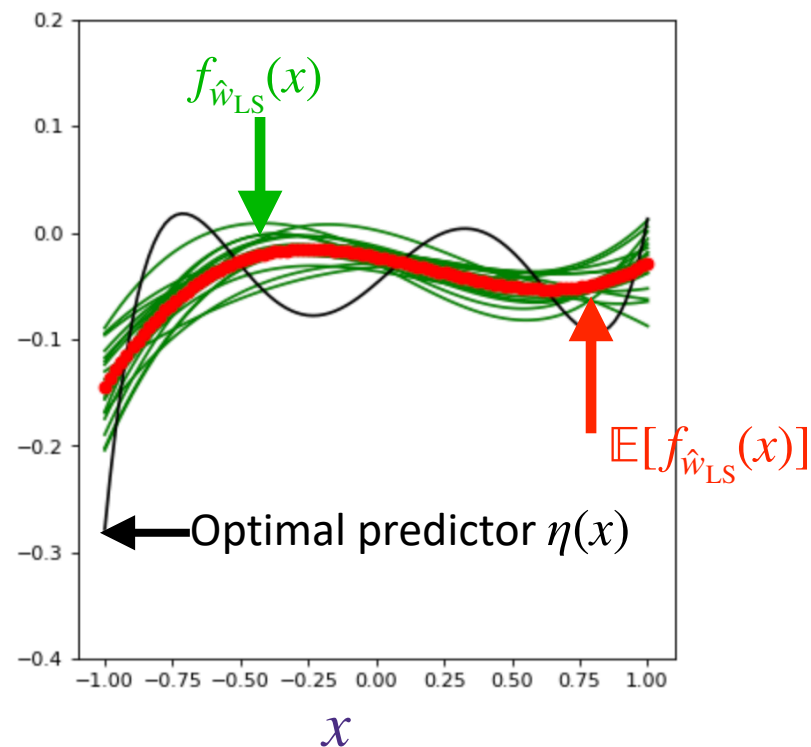
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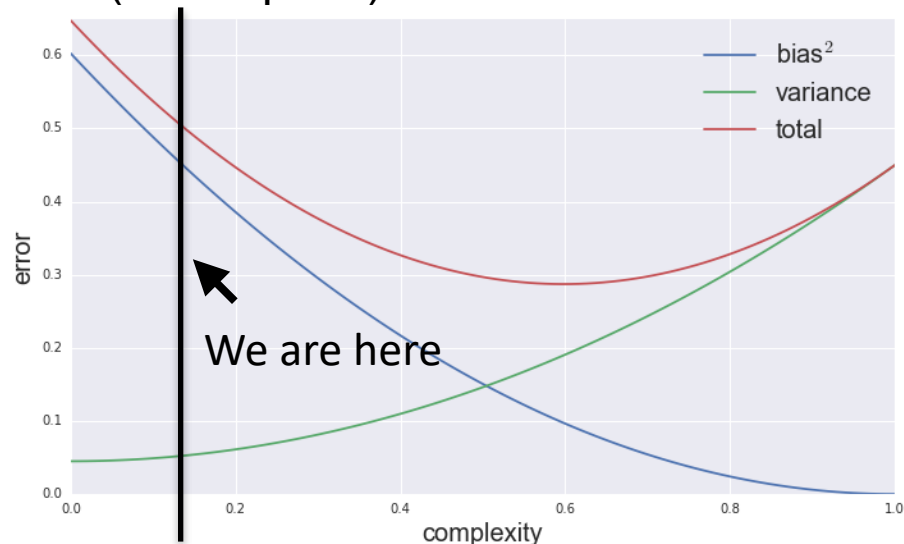
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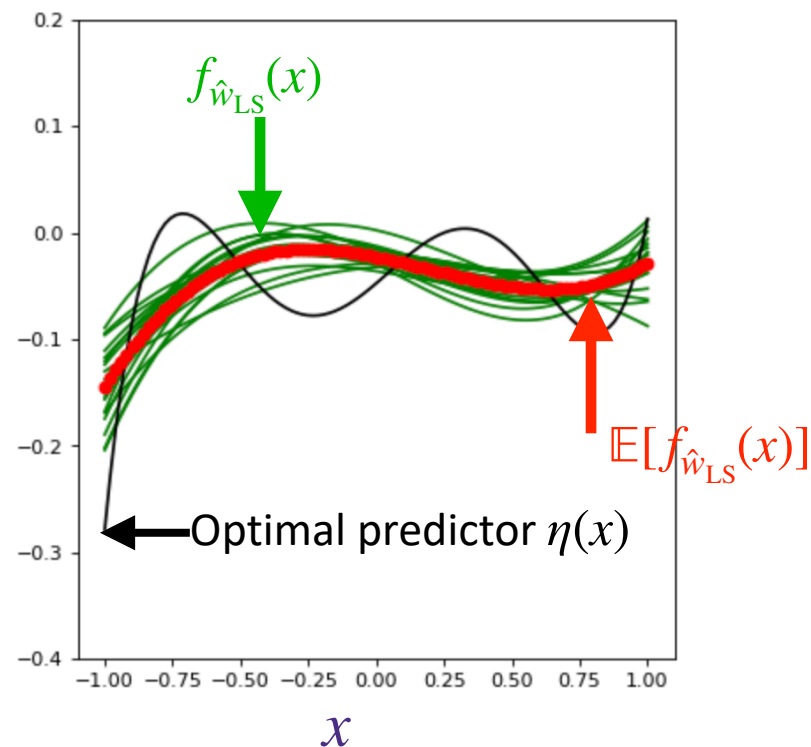
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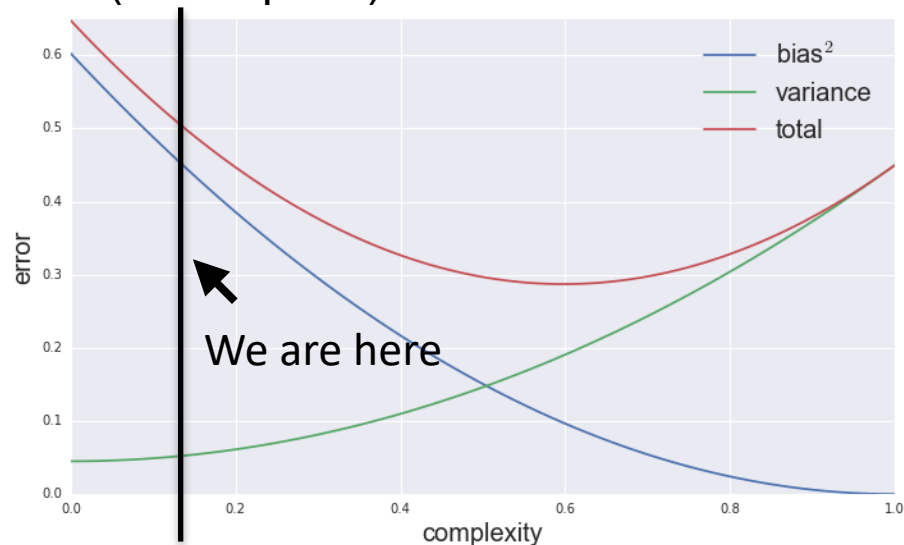
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(Conceptual) bias variance tradeoff



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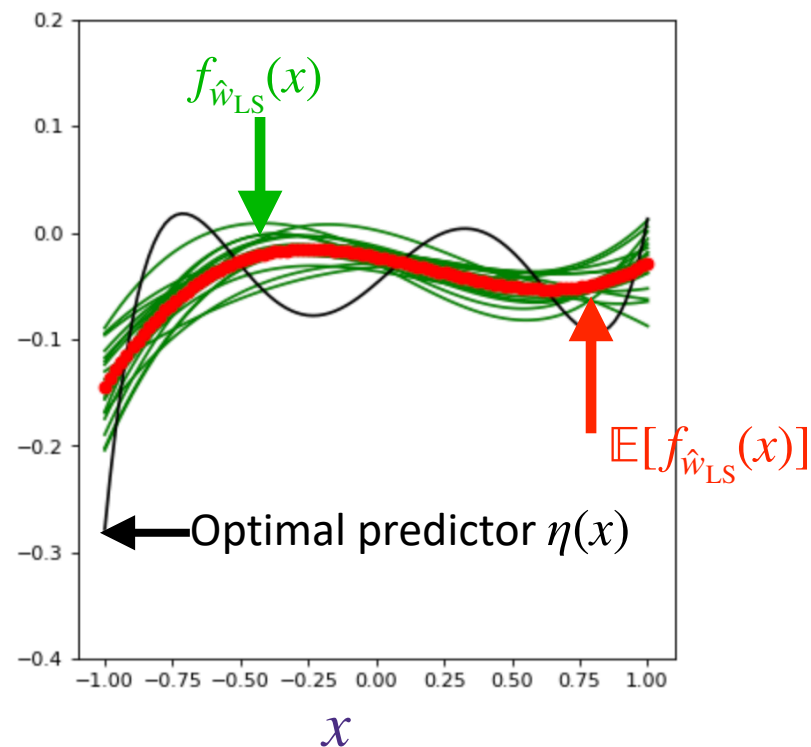
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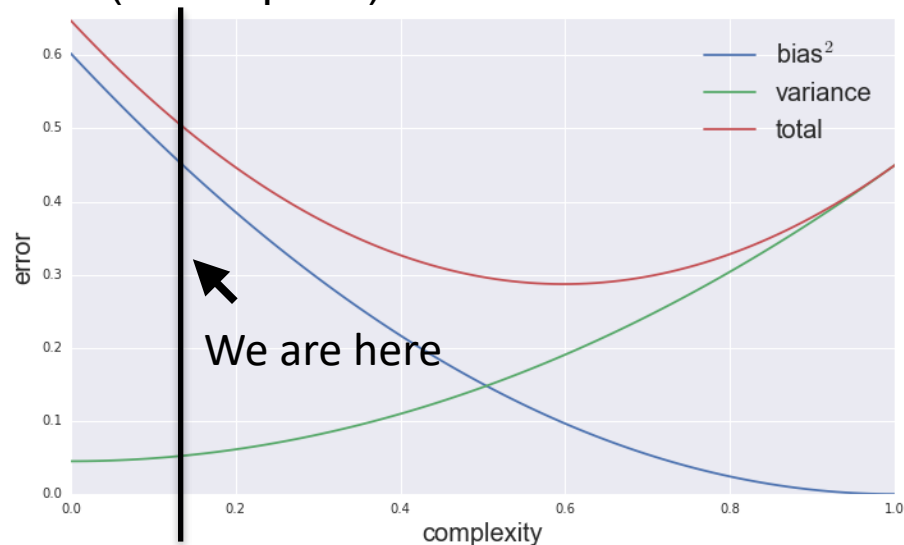
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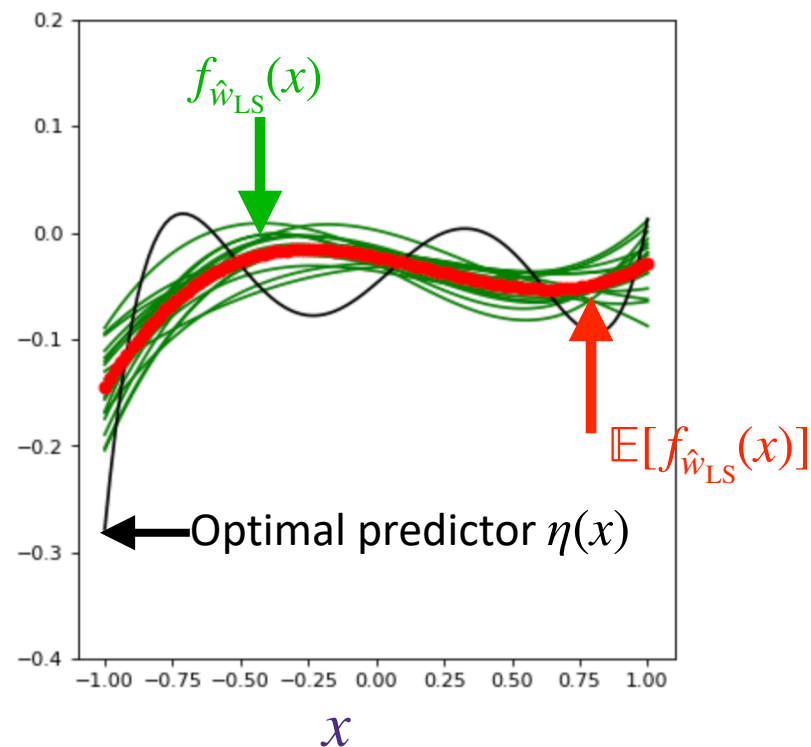
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# Large

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

# Small

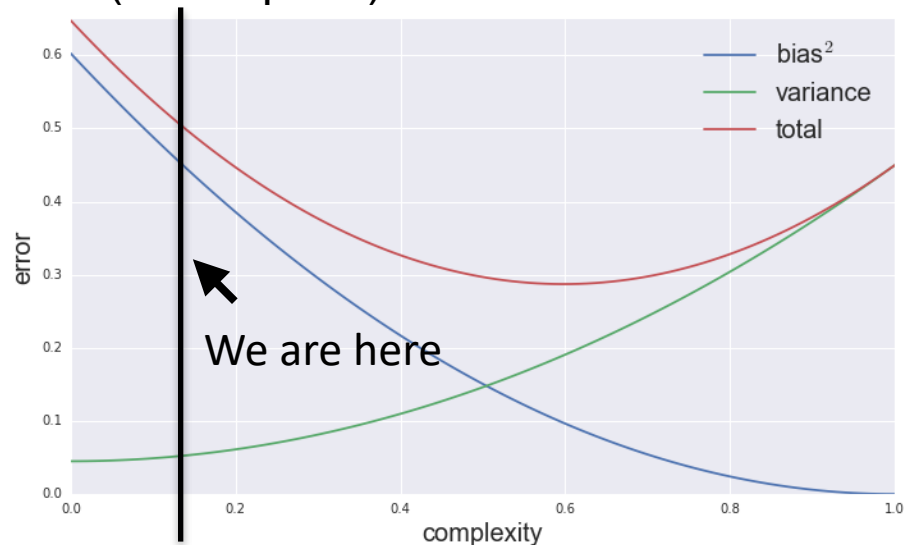
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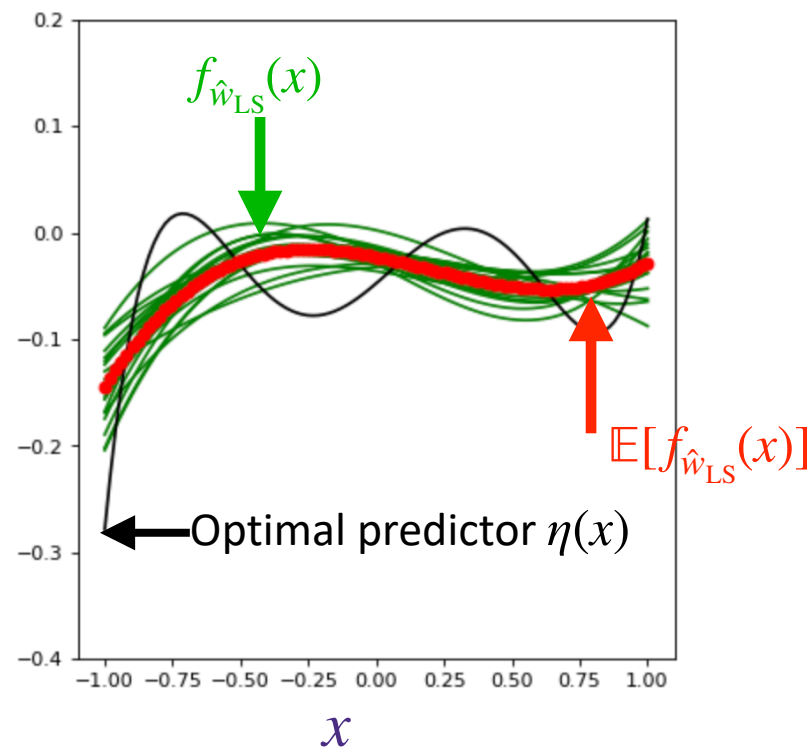
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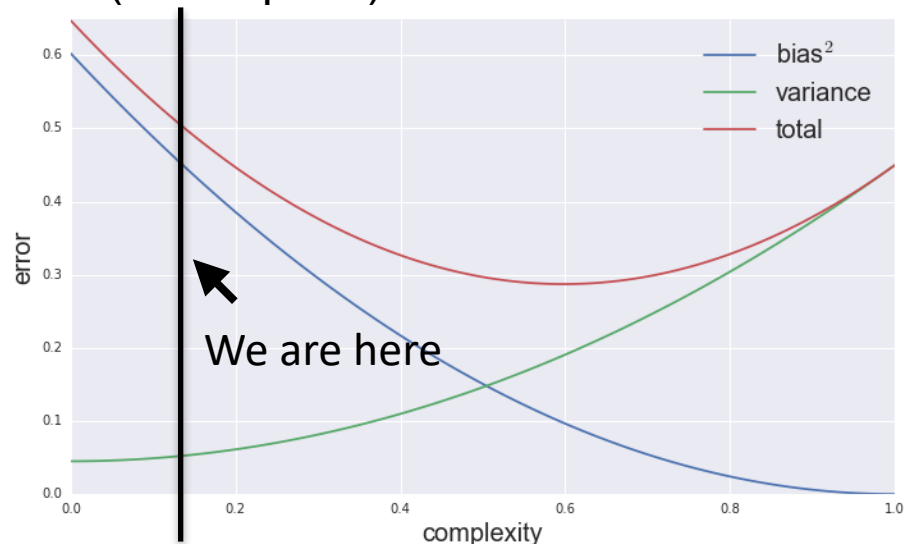
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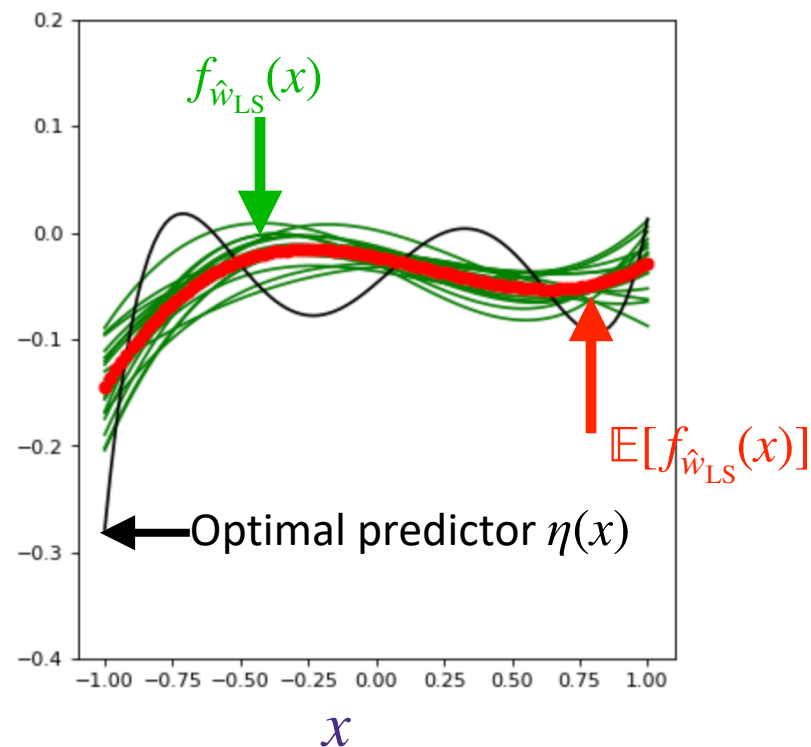
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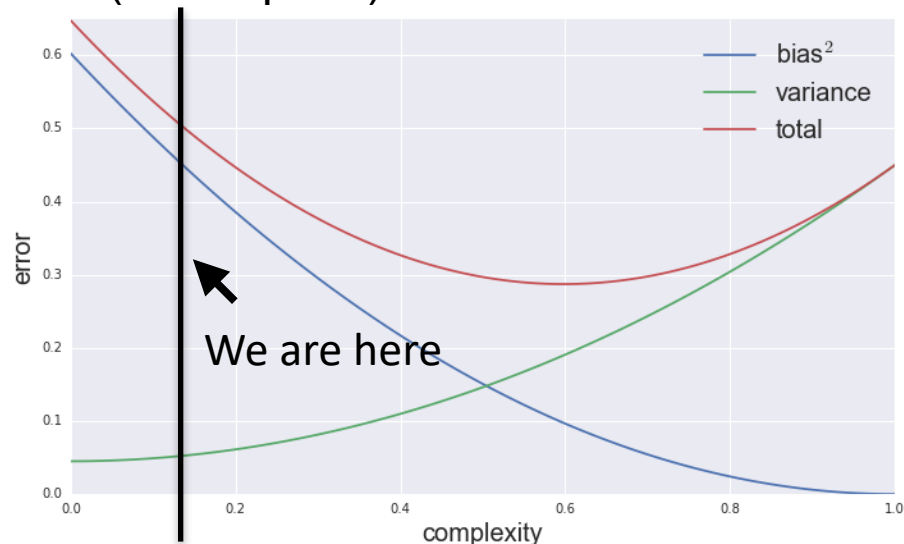
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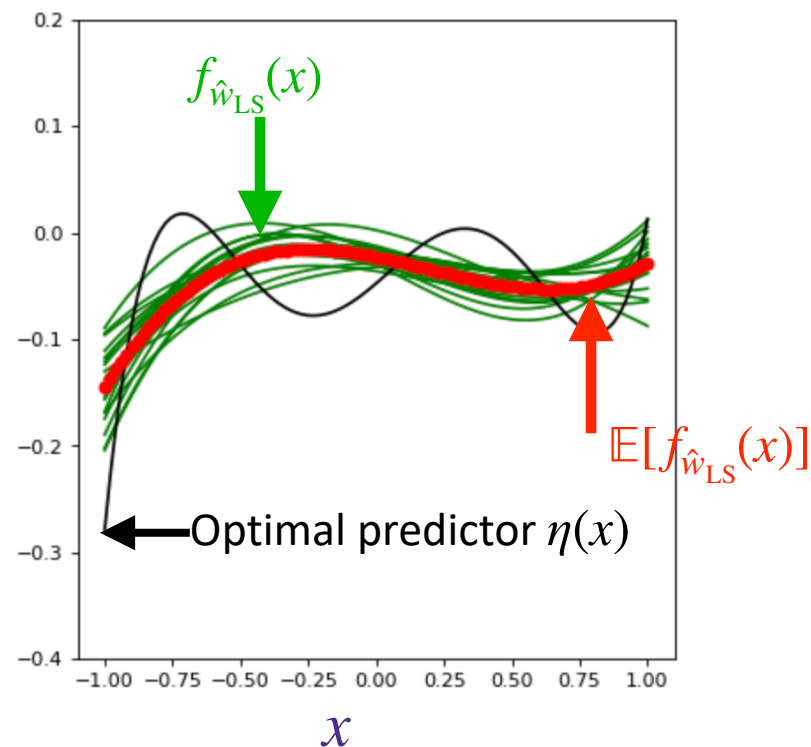
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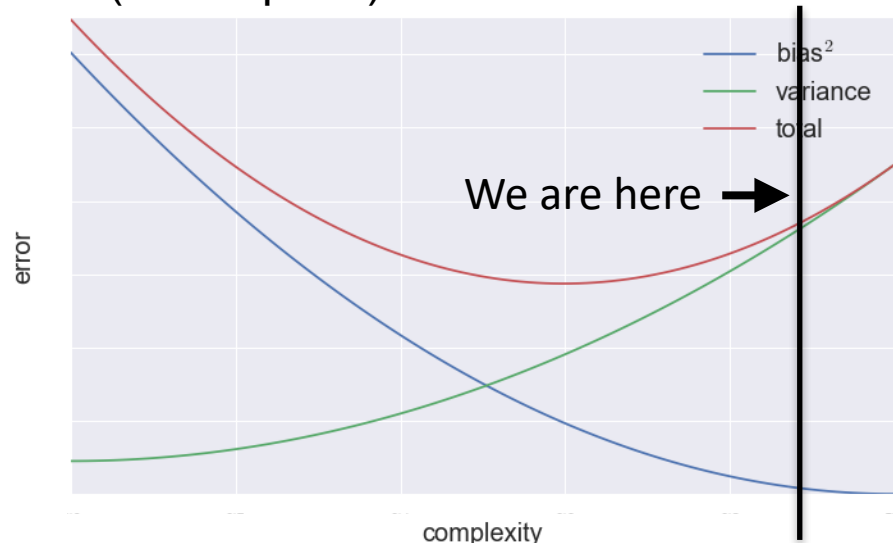
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- If we have more samples (larger  $n$ ), then
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    - What happens to overall test error?
- # Stays high because bias was dominating our error term

# Recap: Bias-variance tradeoff with complex model

(Conceptual) bias variance tradeoff

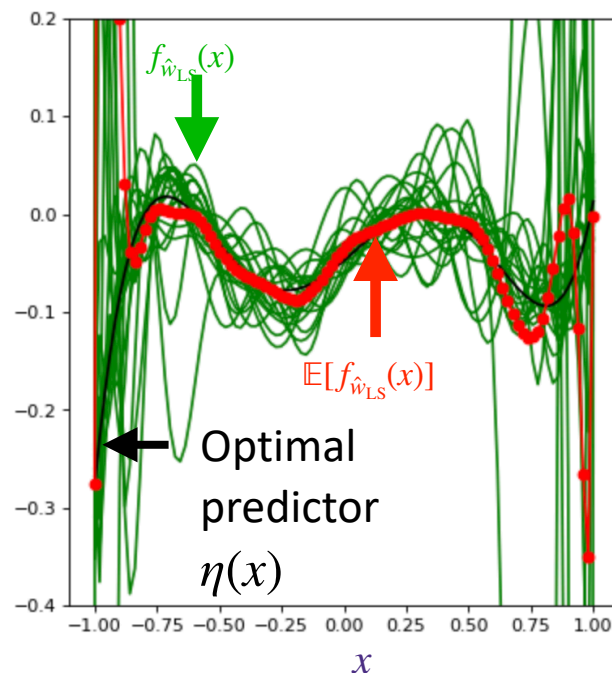


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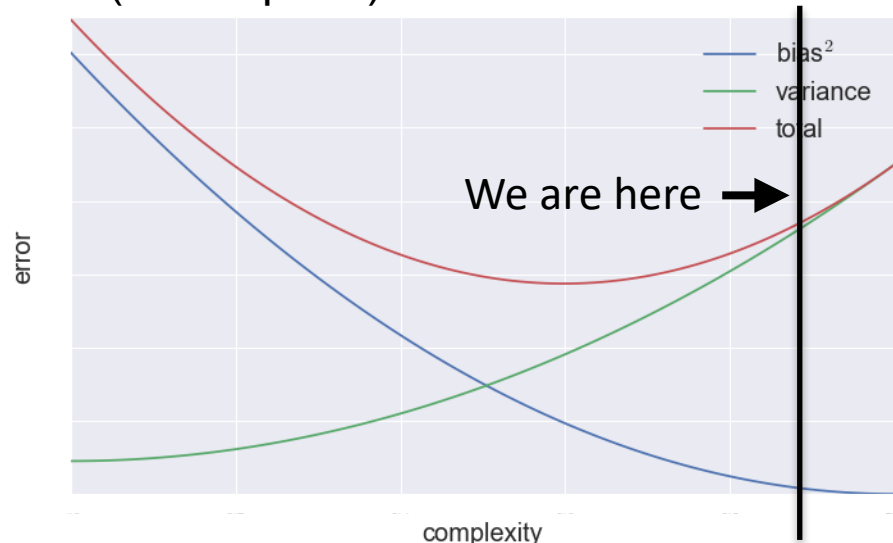
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With degree-20 polynomials, we overfit



# Recap: Bias-variance tradeoff with complex model

(Conceptual) bias variance tradeoff



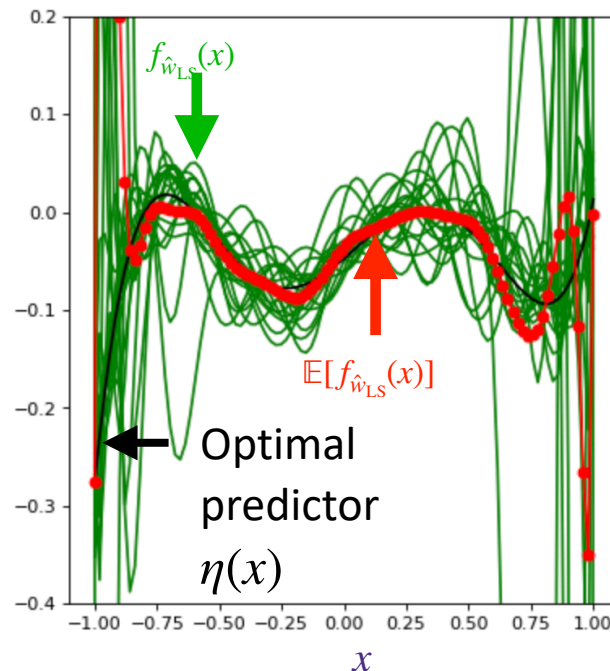
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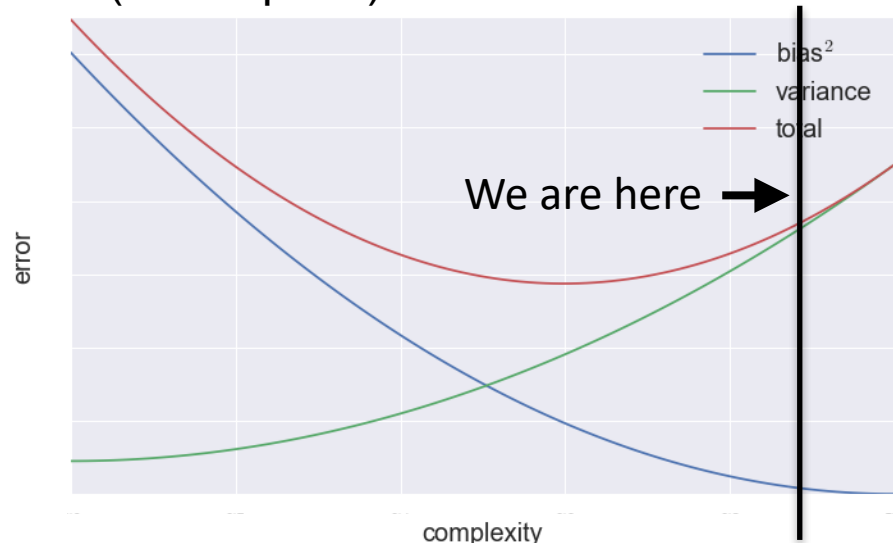
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(Conceptual) bias variance tradeoff



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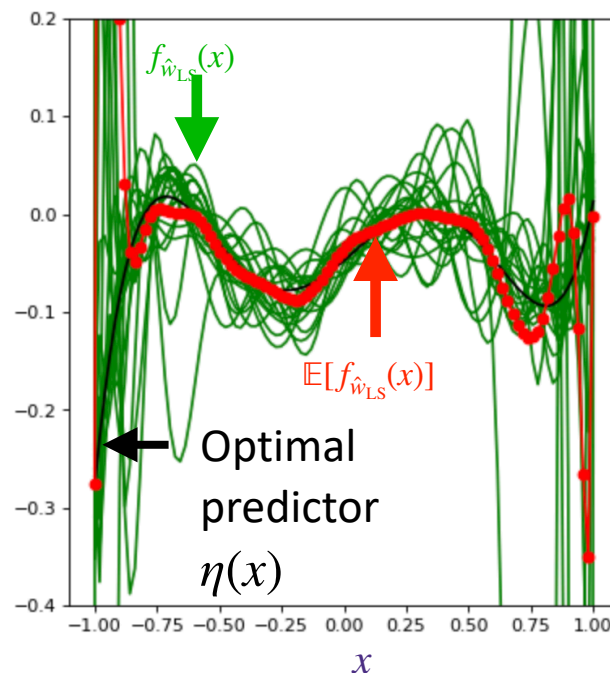
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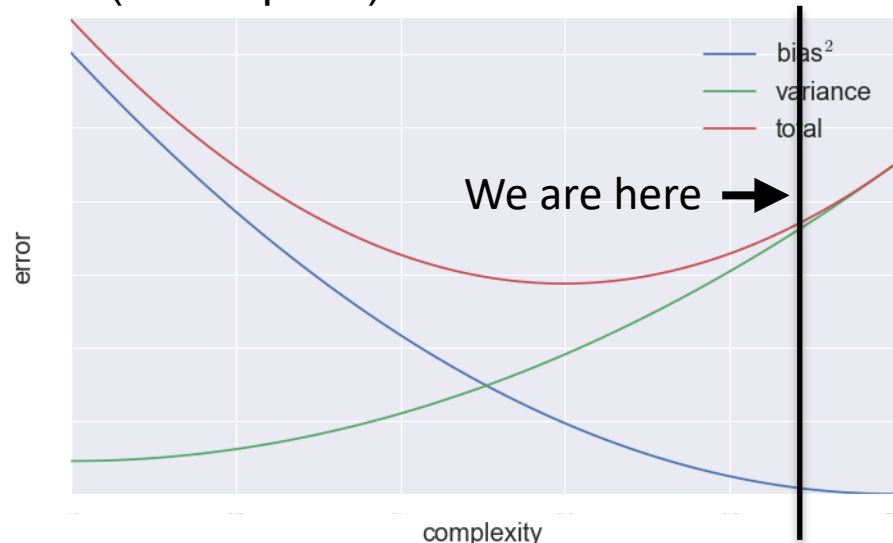
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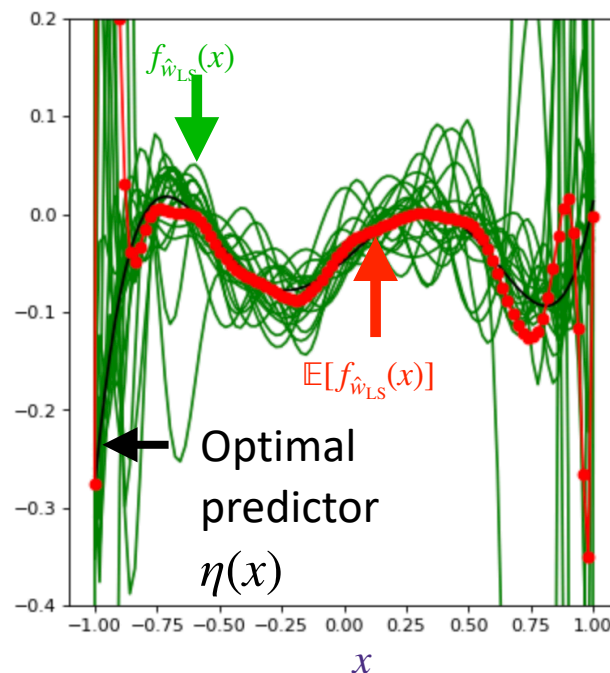
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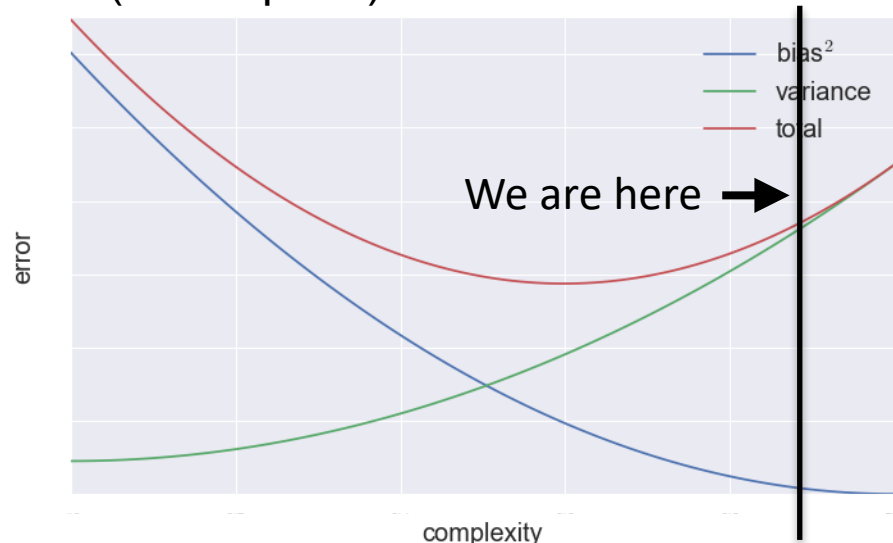
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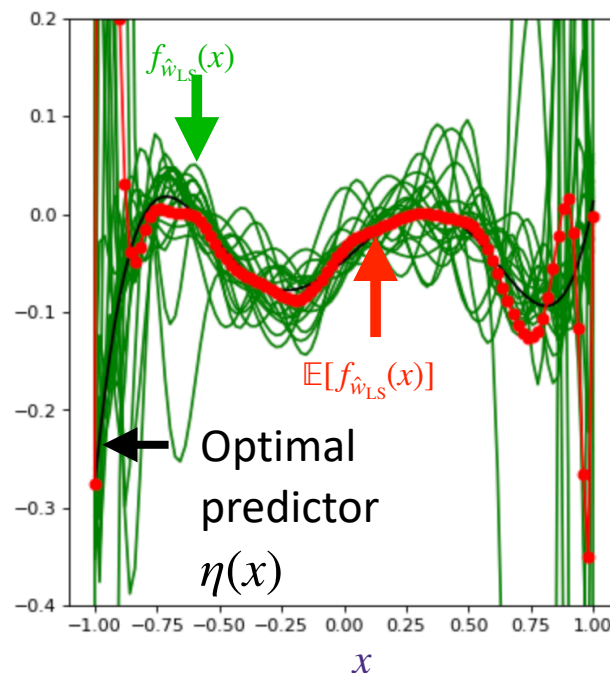
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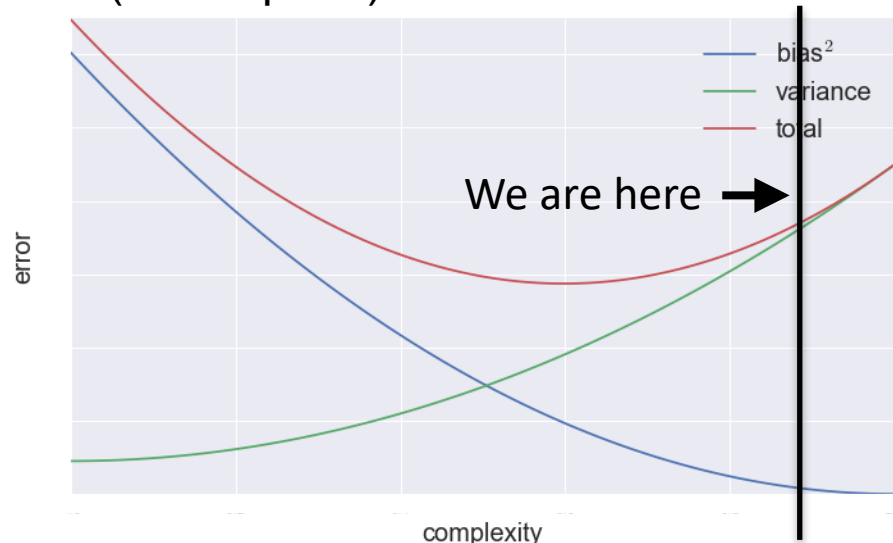
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(Conceptual) bias variance tradeoff



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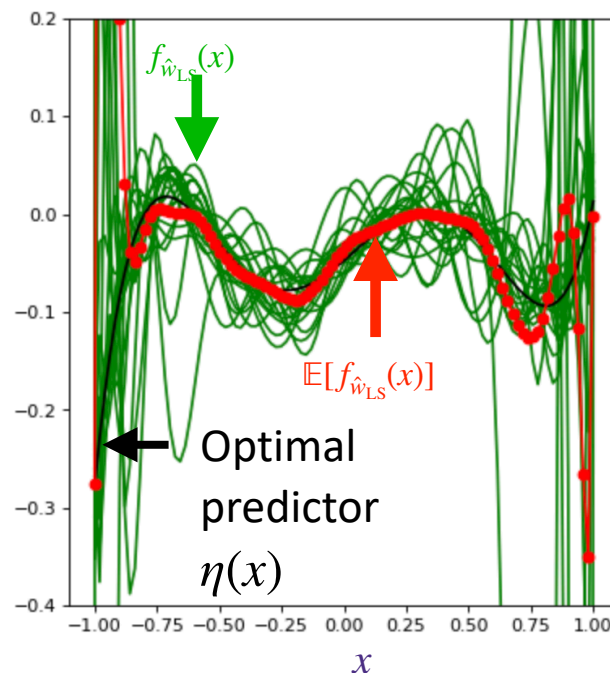
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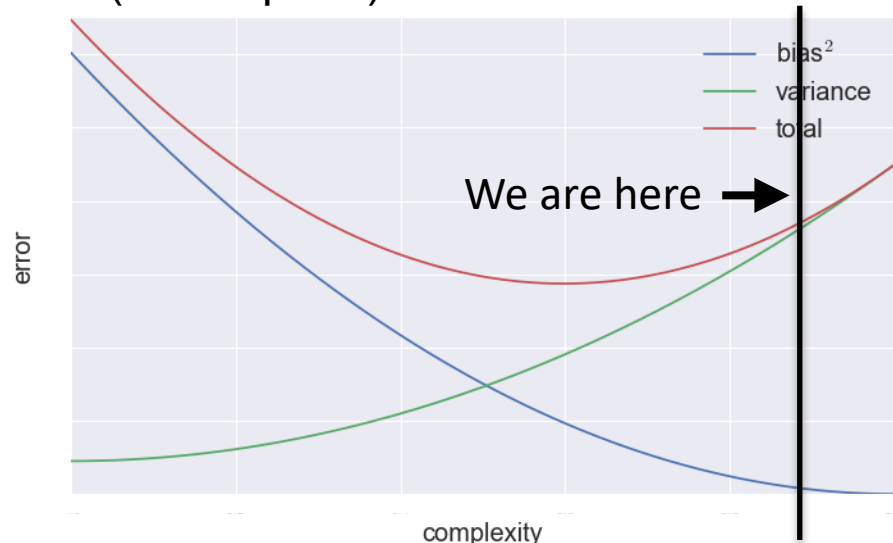
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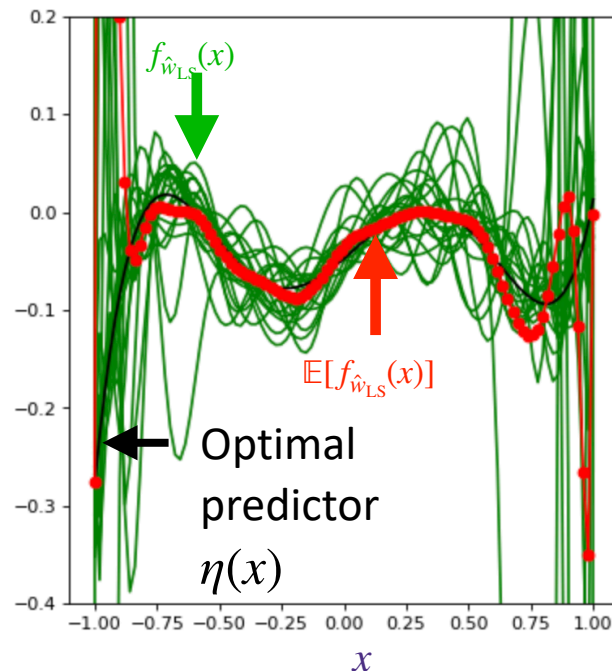
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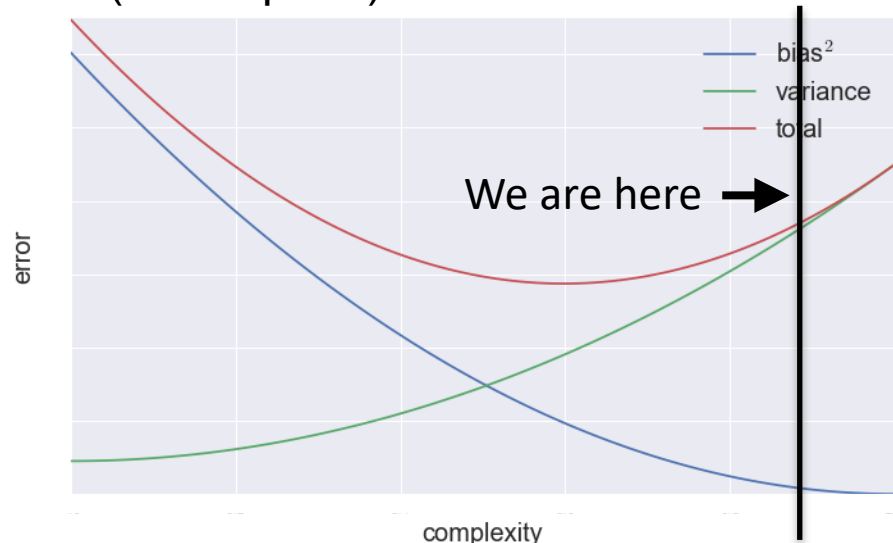
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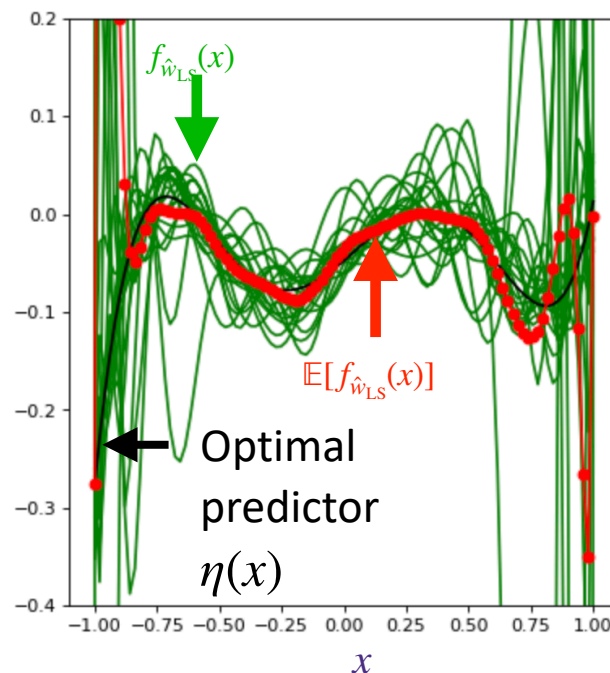
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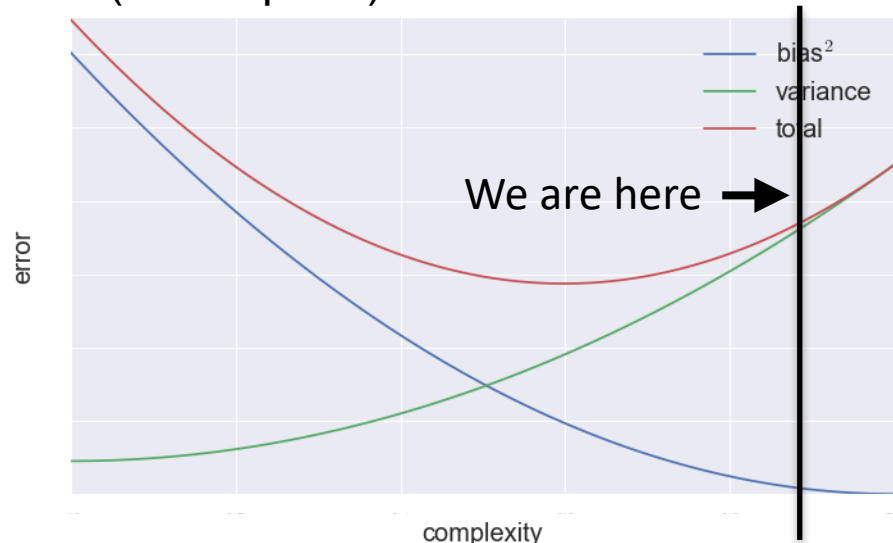
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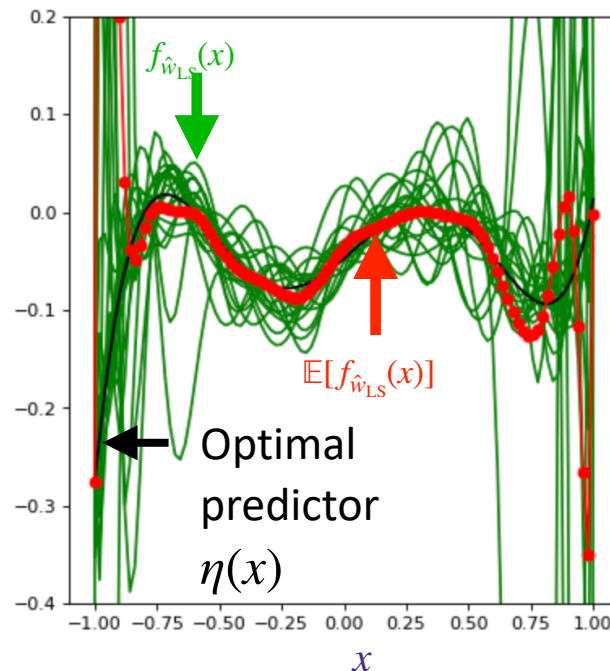
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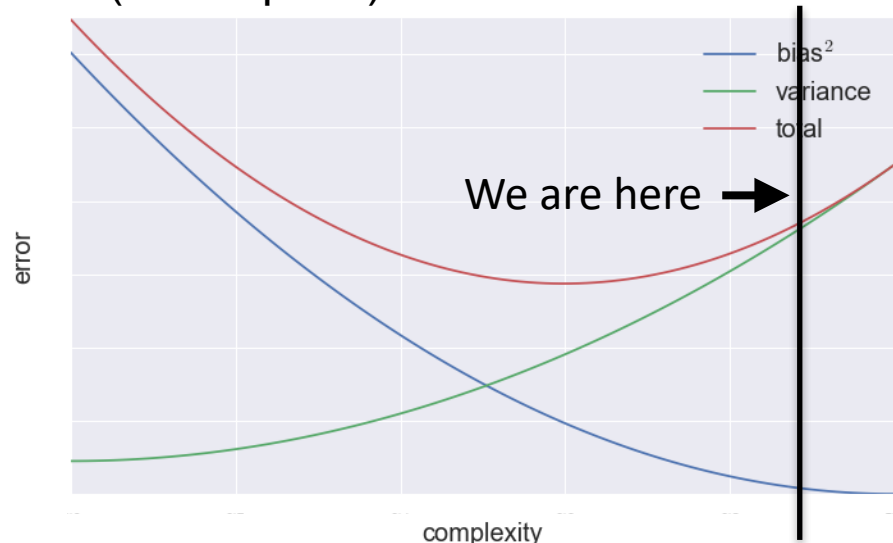
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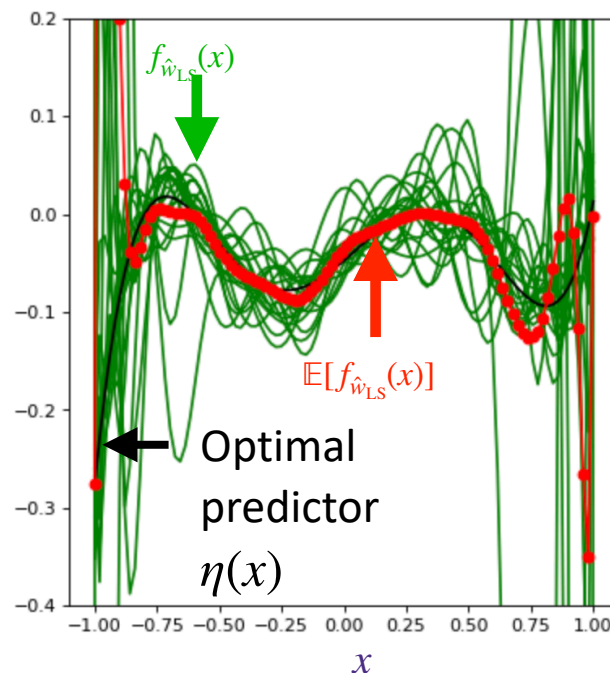
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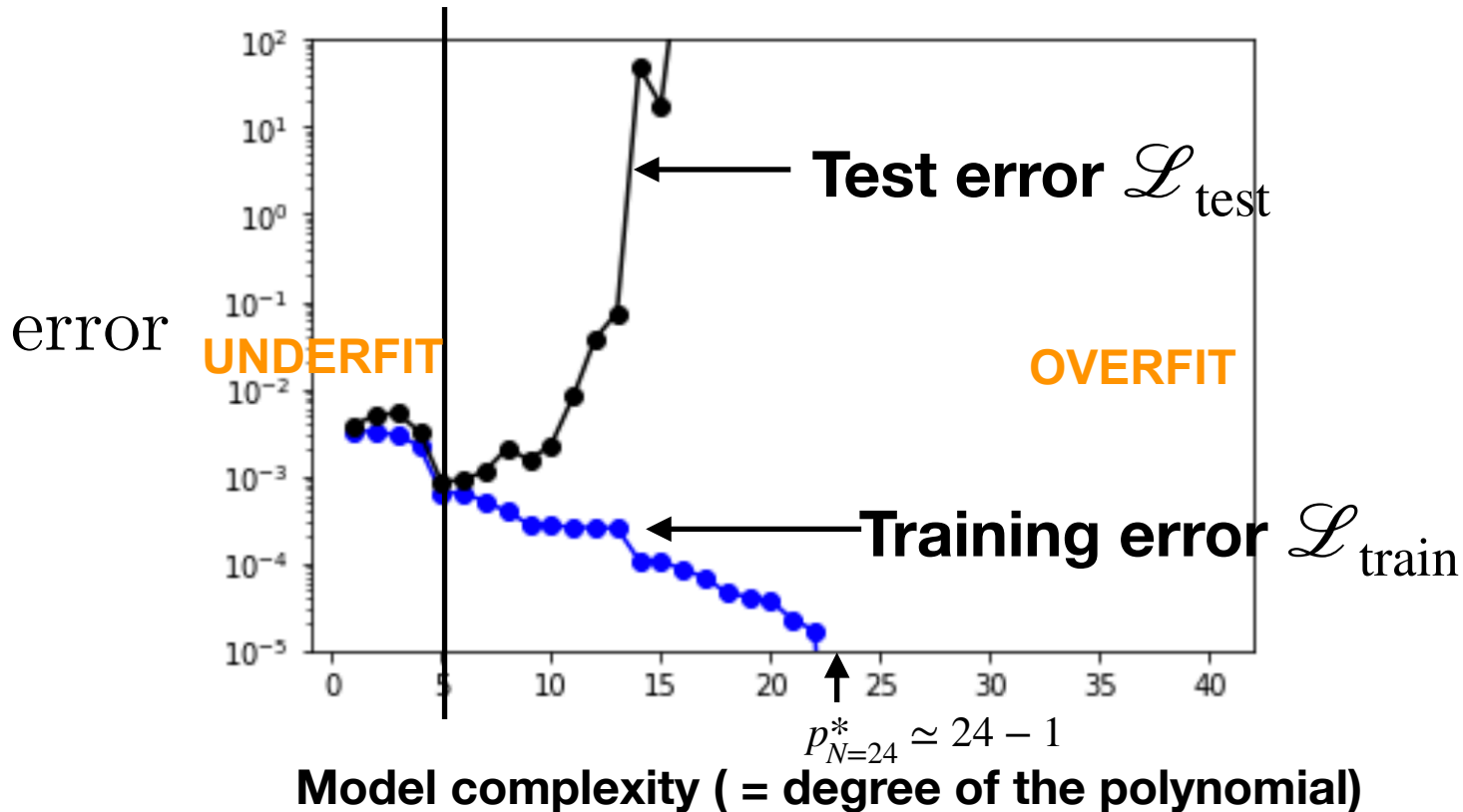


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# decreases

# Optimal model complexity depends on dataset size

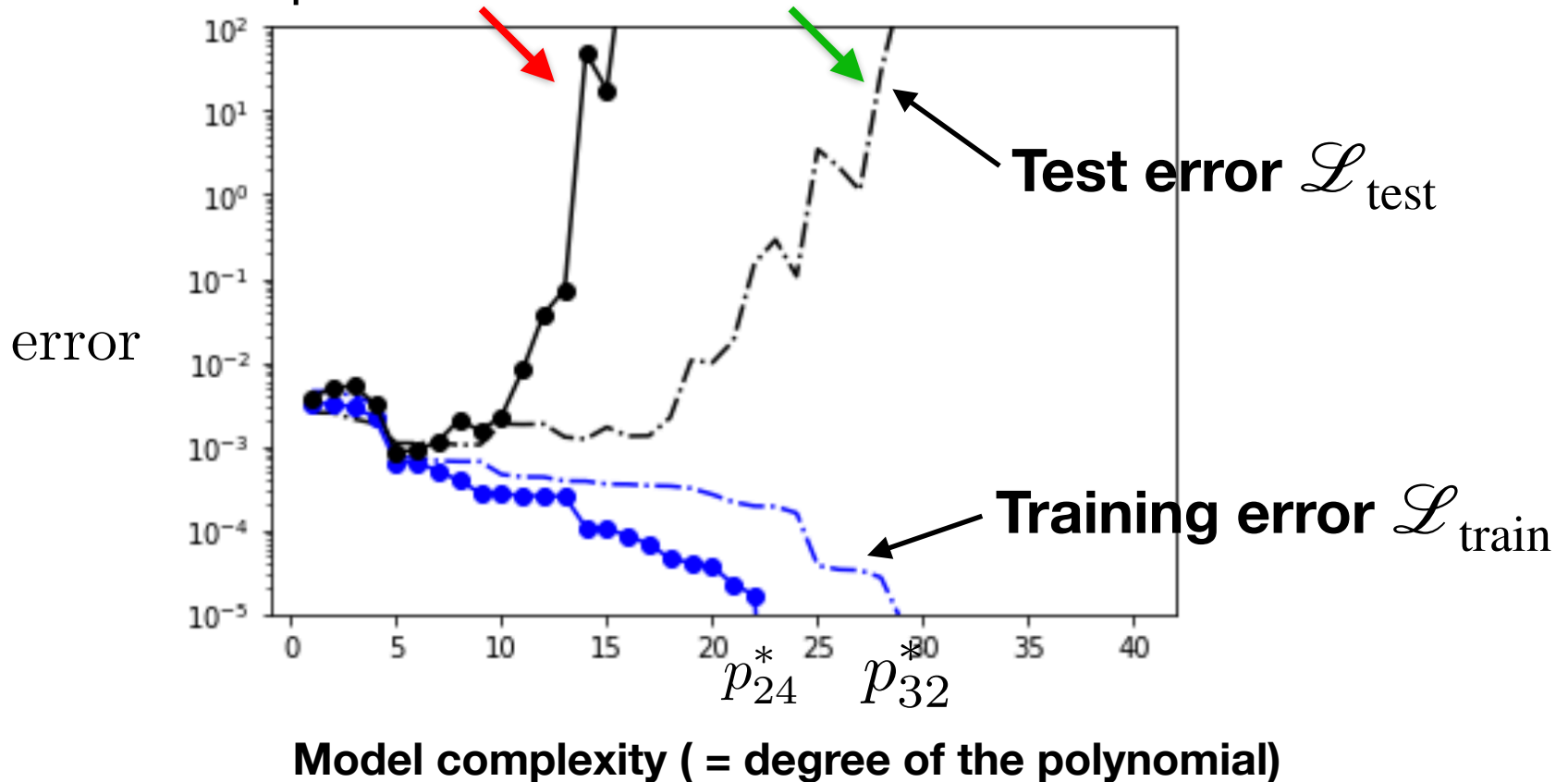
- Assume  $N=30$



- Given sample size  $N$  there is a threshold,  $p_N^*$ , where training error is zero
- Training error is **always** monotonically non-increasing
- Test error has a trend of going down and then up, but fluctuates

# Variance decreases with more data, letting you fit more complex models

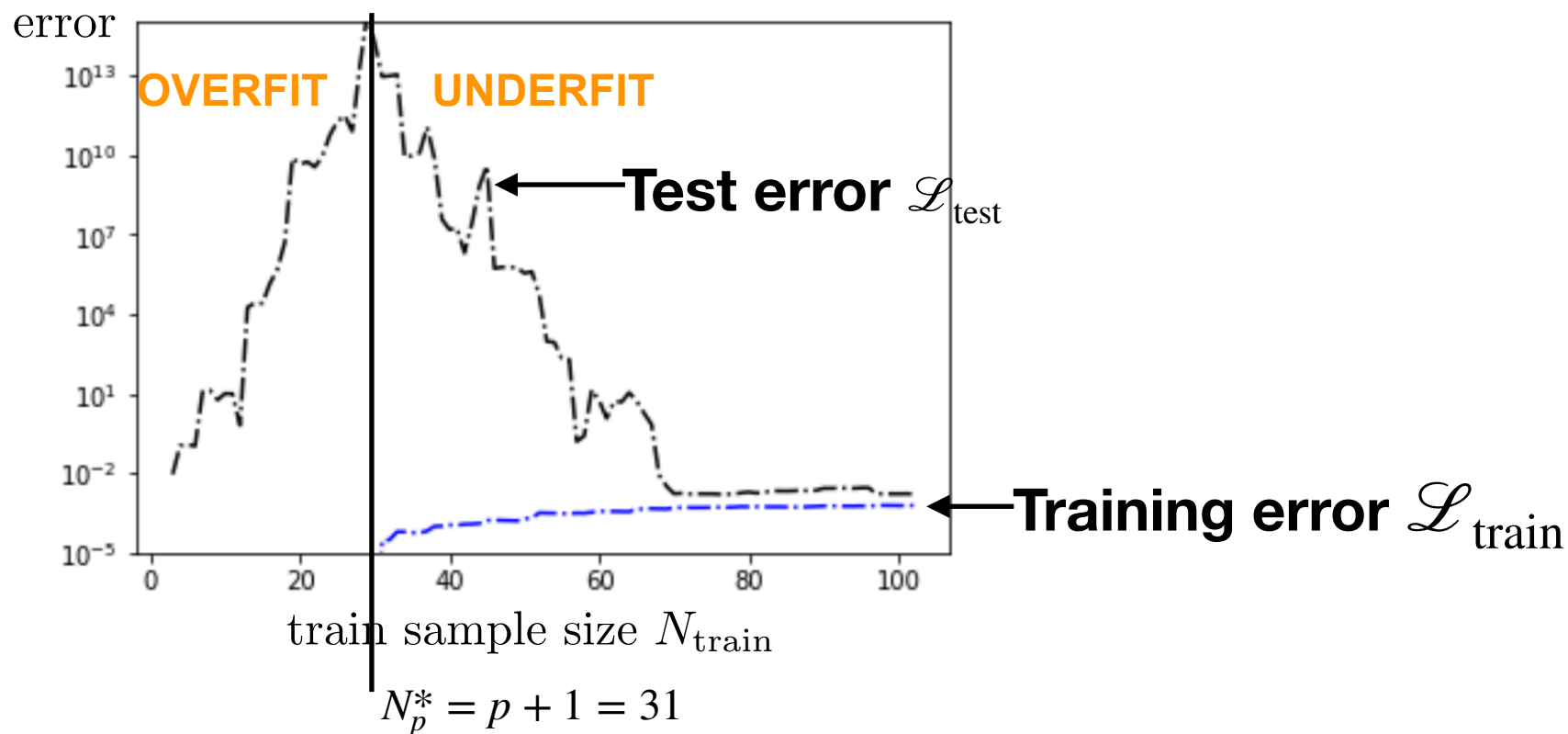
- Now compare  **$N=30$**  case to  **$N=40$**



- The threshold,  $p_N^*$ , moves right as dataset size increases**
- Training error tends to increase, because more points need to fit
- Test error tends to decrease, because Variance decreases

# Variance decreases with more data, letting you fit more complex models

- Choose model complexity  $p=30$ , vary dataset size  $n$



- There is a threshold,  $N_p^*$ , below which training error is zero (extreme overfit)
- Above the threshold, test error tends to decrease
- Training error tends to increase (harder to fit so much data with simple model)

# Ridge Regression

---

# Regularization in Linear Regression

---

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

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

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

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What if  $x_i \in \mathbb{R}^d$  and  $d > n$ ?

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

Implies optimal solution is *not unique* 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”



**Regularization imposes “simpler” solutions by a “complexity” penalty**

# Sensitivity increases overfitting

- 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  $x_j$
- 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)

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


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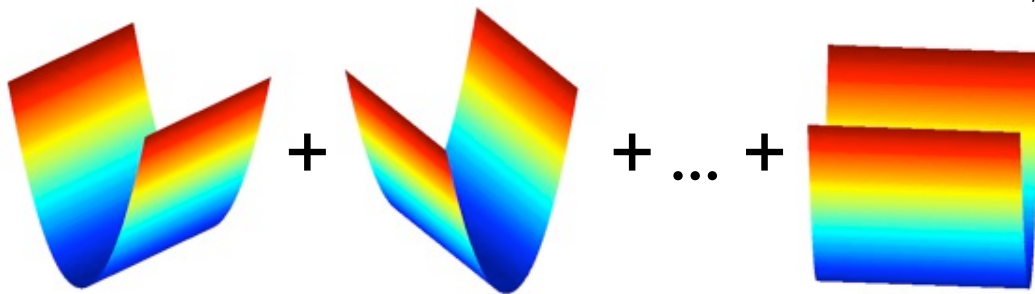

# Regularize to make weights smaller / less sensitive. Multiple ways to do that. We'll start with L2 norm

# Ridge Regression

# if  $d > n$

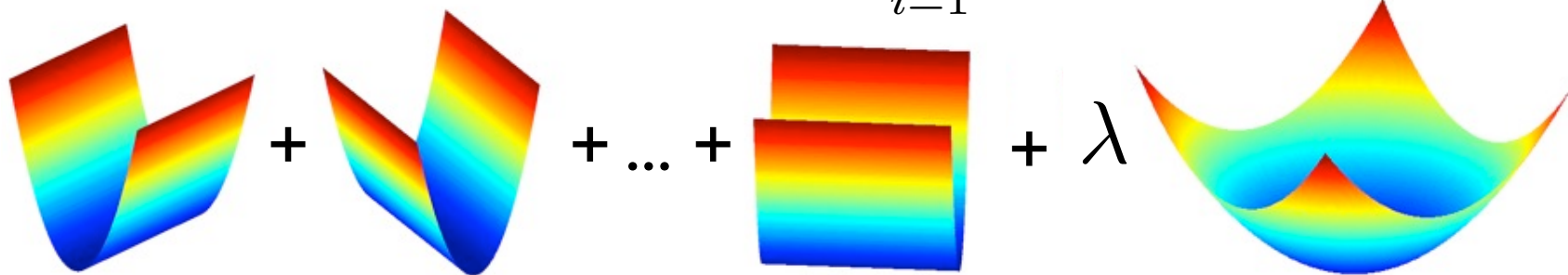
- Old Least squares objective:

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- Ridge Regression objective:

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# Minimizing the Ridge Regression Objective

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

# More identities

| Scalar derivative                | Vector derivative                                                       |
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# From previous derivation

$$\nabla_w [-2y^T Xw + w^T X^T Xw + \lambda w^T w] = 0$$

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

$$X^T Xw + \lambda w = X^T y$$

$$(X^T X + \lambda I)w = X^T y$$

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

| Scalar derivative                |  | Vector derivative                                                       |  |
|----------------------------------|--|-------------------------------------------------------------------------|--|
| $f(x) \rightarrow \frac{df}{dx}$ |  | $f(\mathbf{x}) \rightarrow \frac{df}{d\mathbf{x}}$                      |  |
| $bx \rightarrow b$               |  | $\mathbf{x}^T \mathbf{B} \rightarrow \mathbf{B}$                        |  |
| $bx \rightarrow b$               |  | $\mathbf{x}^T \mathbf{b} \rightarrow \mathbf{b}$                        |  |
| $x^2 \rightarrow 2x$             |  | $\mathbf{x}^T \mathbf{x} \rightarrow 2\mathbf{x}$                       |  |
| $bx^2 \rightarrow 2bx$           |  | $\mathbf{x}^T \mathbf{B} \mathbf{x} \rightarrow 2\mathbf{B} \mathbf{x}$ |  |

# Shrinkage Properties

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

$$w \in \mathbb{R}^{d \times 1}$$

$$X \in \mathbb{R}^{n \times d}$$

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Hand-drawn diagram illustrating the matrix dimensions in the ridge regression formula:

- $X^T$  is a  $1 \times n$  matrix (horizontal rectangle).
- $X$  is an  $n \times d$  matrix (vertical rectangle).
- $\lambda I$  is a  $d \times d$  matrix (small square).
- The term  $(X^T X + \lambda I)^{-1}$  is the inverse of the sum of  $X^T X$  and  $\lambda I$ .
- $X^T y$  is an  $n \times 1$  matrix (vertical rectangle).

- When  $\lambda = 0$ , this gives the least squares model
- This defines a family of models hyper-parametrized by  $\lambda$
- Large  $\lambda$  means more regularization and simpler model
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# What problem does this solve?

Hand-drawn diagram illustrating the matrix dimensions in the ridge regression formula. The expression is  $(\mathbf{X}^T \mathbf{X} + \lambda I)^{-1} \mathbf{X}^T \mathbf{y}$ . The matrix  $\mathbf{X}^T \mathbf{X}$  is represented by a rectangle labeled  $d \times d$ . The identity matrix  $I$  is represented by a smaller rectangle labeled  $d \times d$ . The vector  $\mathbf{X}^T \mathbf{y}$  is represented by a tall rectangle labeled  $n \times 1$ . The entire expression is enclosed in large parentheses with a superscript  $-1$ .

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Hand-drawn diagram illustrating the matrix dimensions in the ridge regression formula. The expression is  $(\mathbf{X}^T \mathbf{X} + \lambda I)^{-1} \cdot \mathbf{X}^T \mathbf{y}$ . The dimensions are indicated by rectangles and labels:  $\mathbf{X}^T$  is a horizontal rectangle labeled  $d \times n$ ,  $\mathbf{X}$  is a vertical rectangle labeled  $n \times d$ ,  $\lambda I$  is a small square labeled  $d \times d$ , and the result  $\mathbf{X}^T \mathbf{y}$  is a vertical rectangle labeled  $n \times 1$ .

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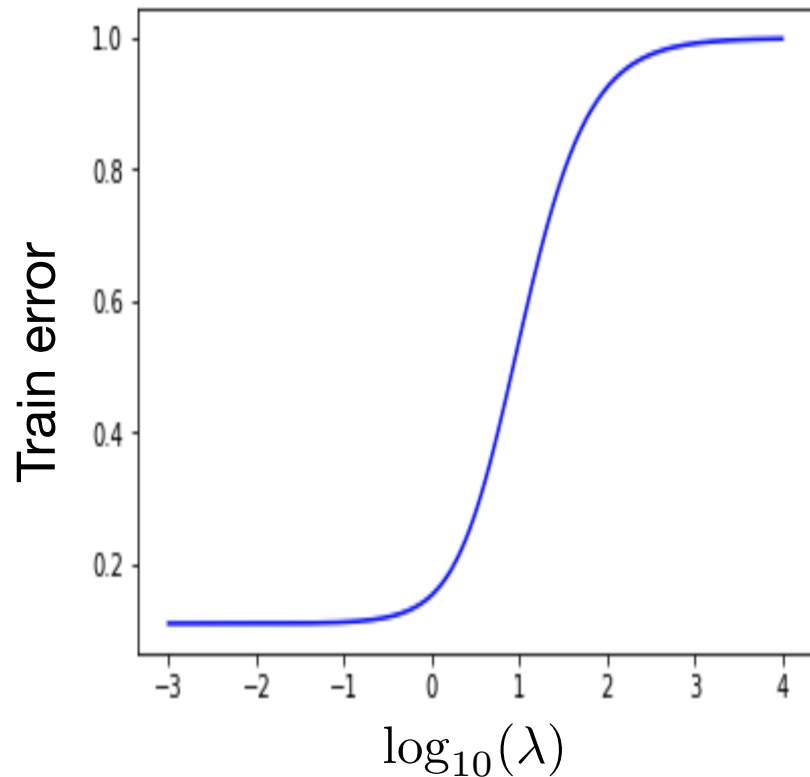
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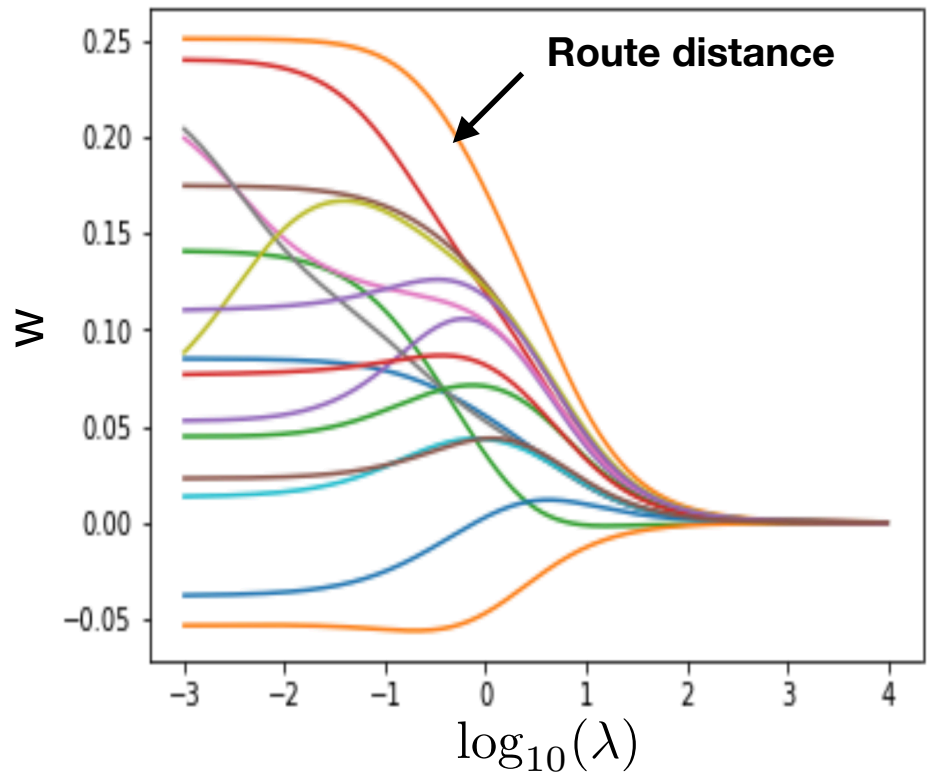
# Optimal  $\lambda$  depends on magnitude of features

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

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



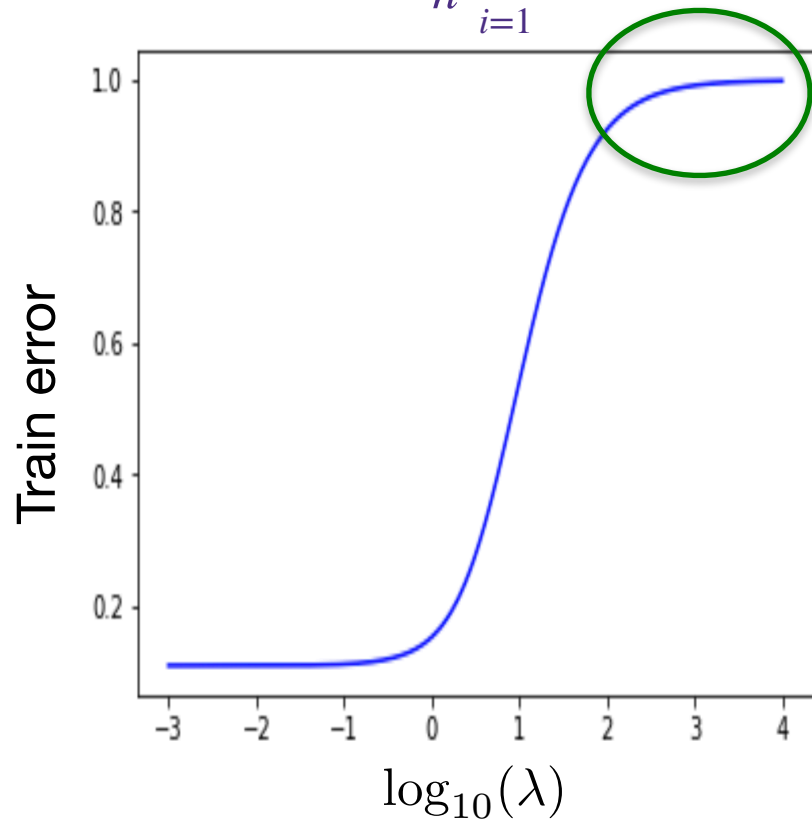
Illustrative potato delivery:  $w_i$



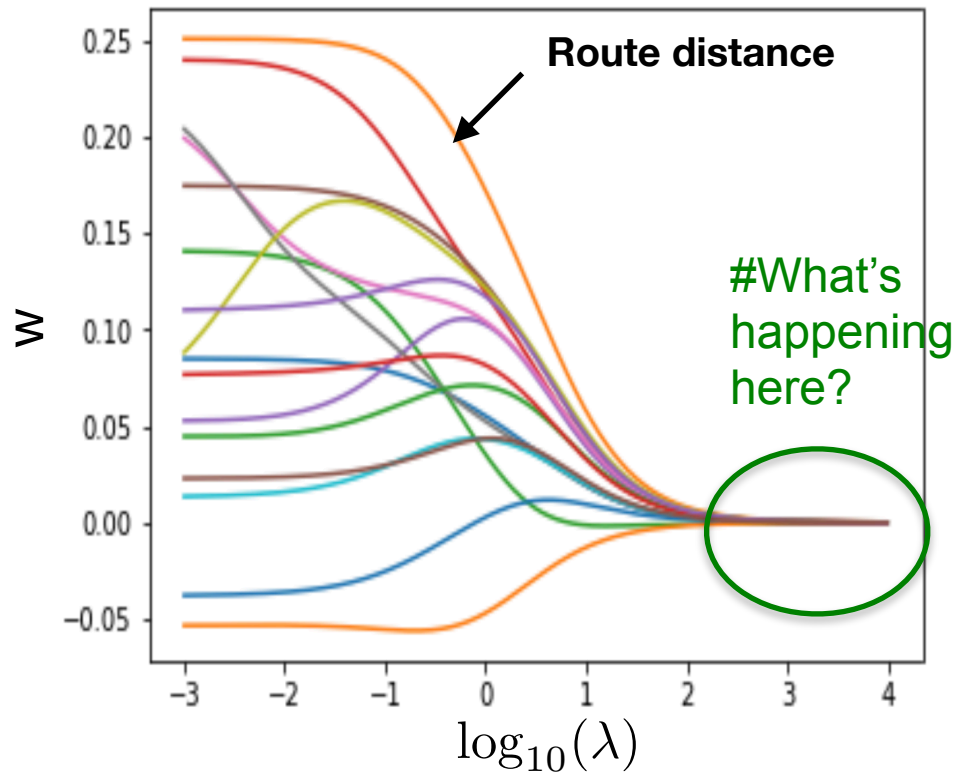
Right plot: called **regularization path**

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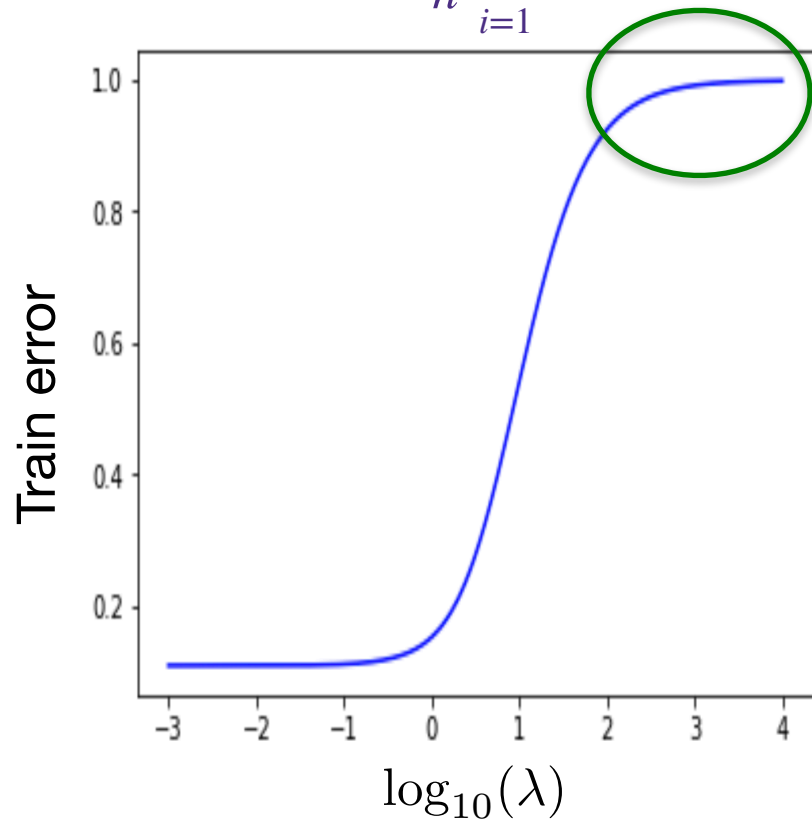
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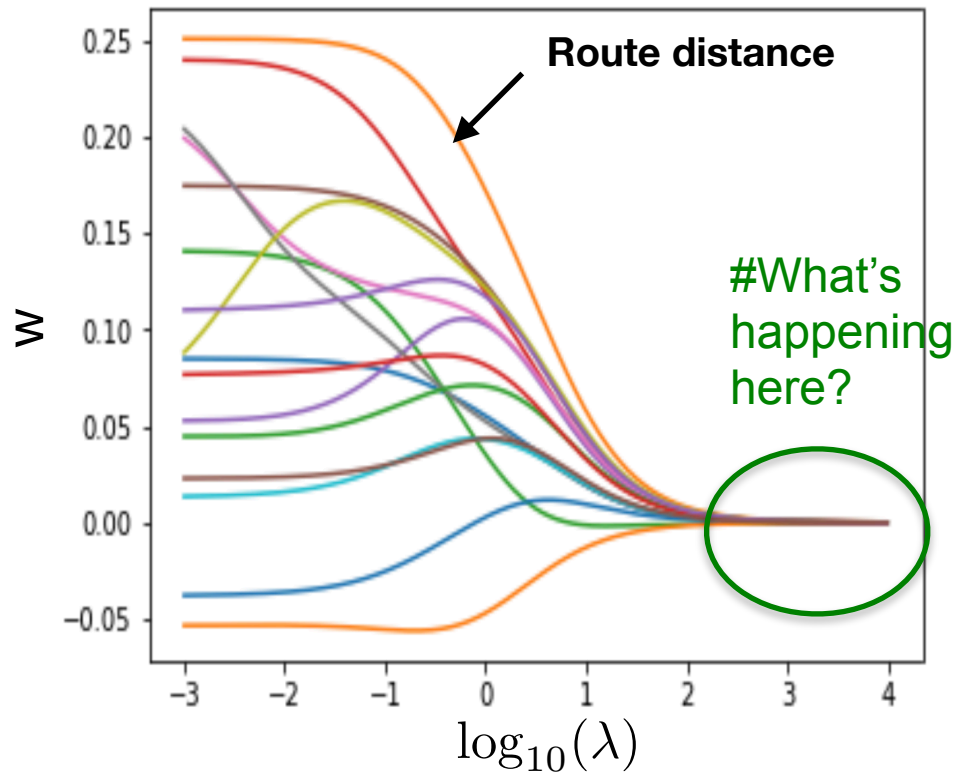
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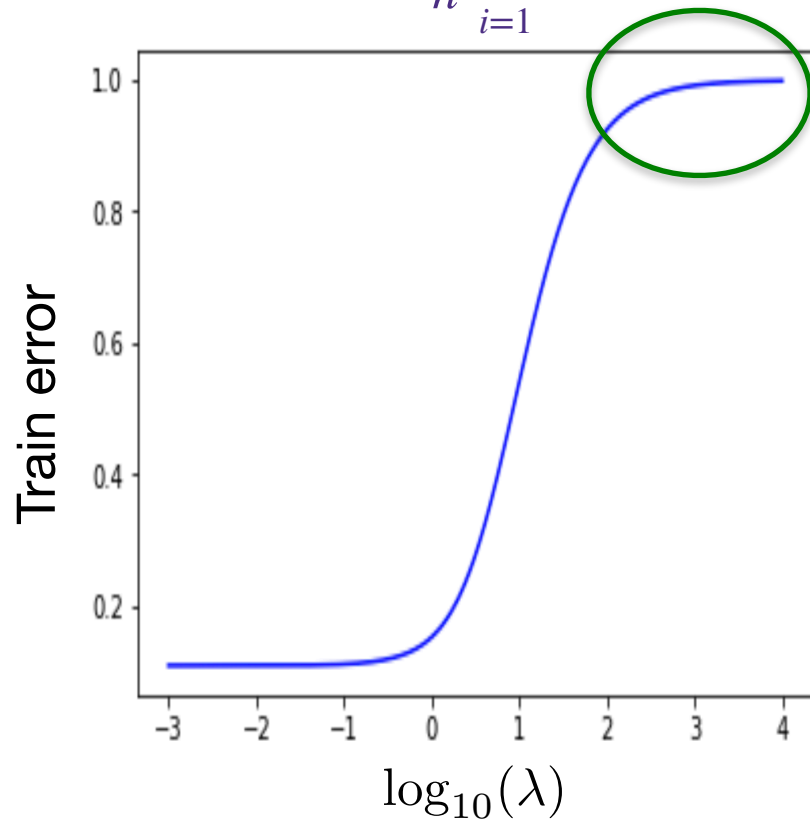


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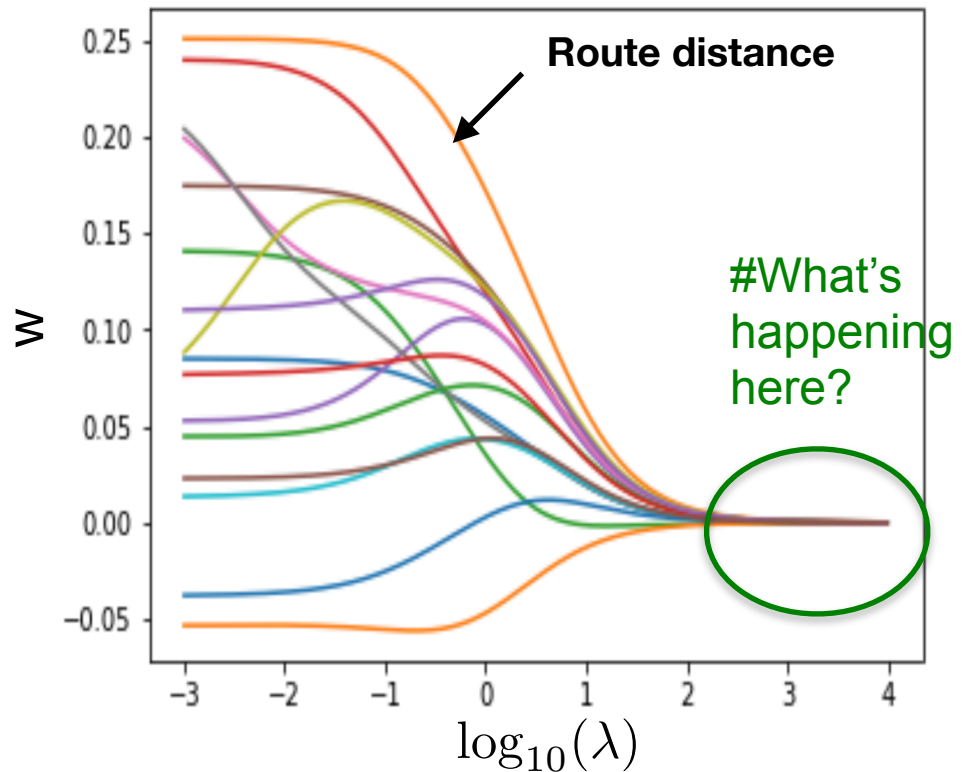
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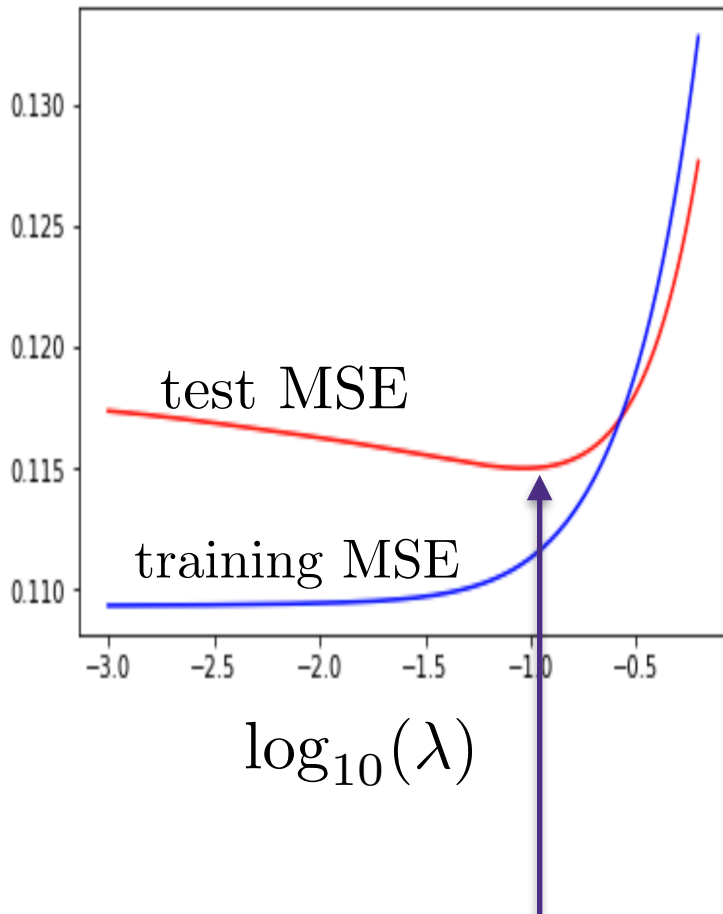


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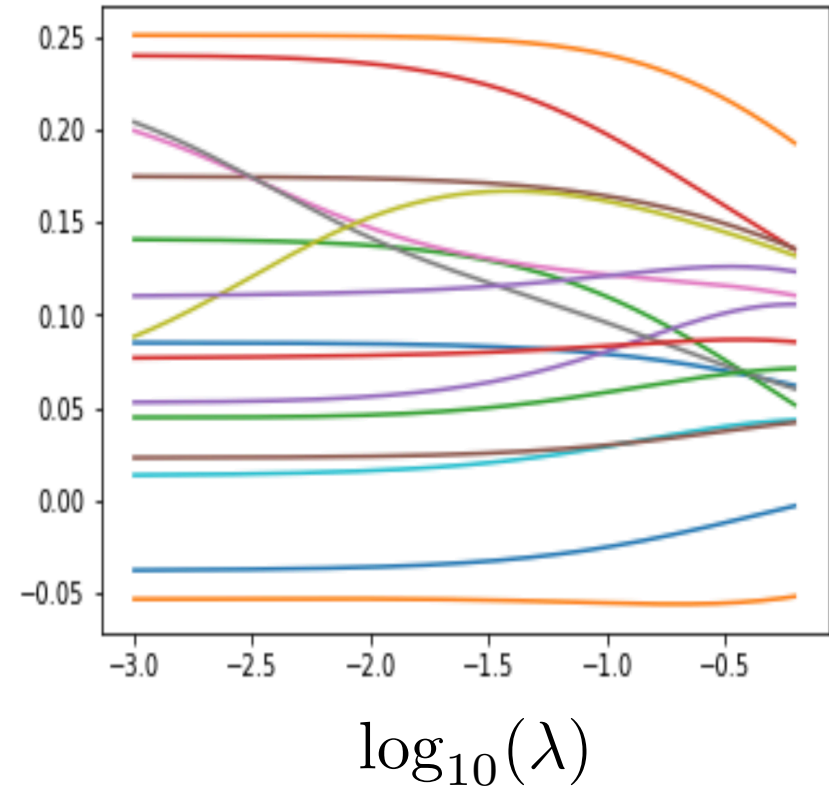
# Route-distance coefficient shrinks slowly in this example

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

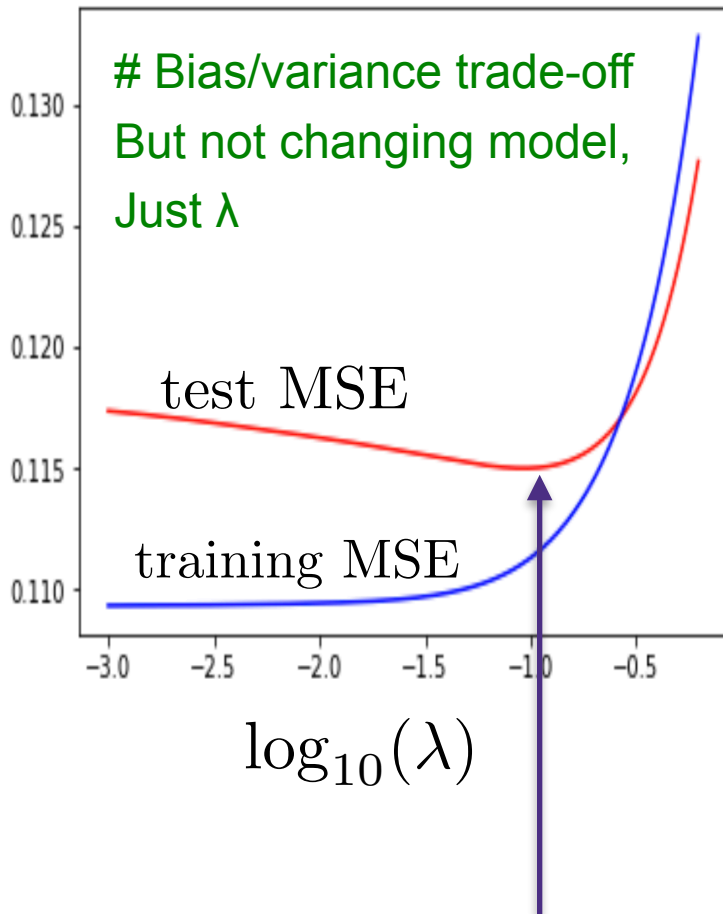
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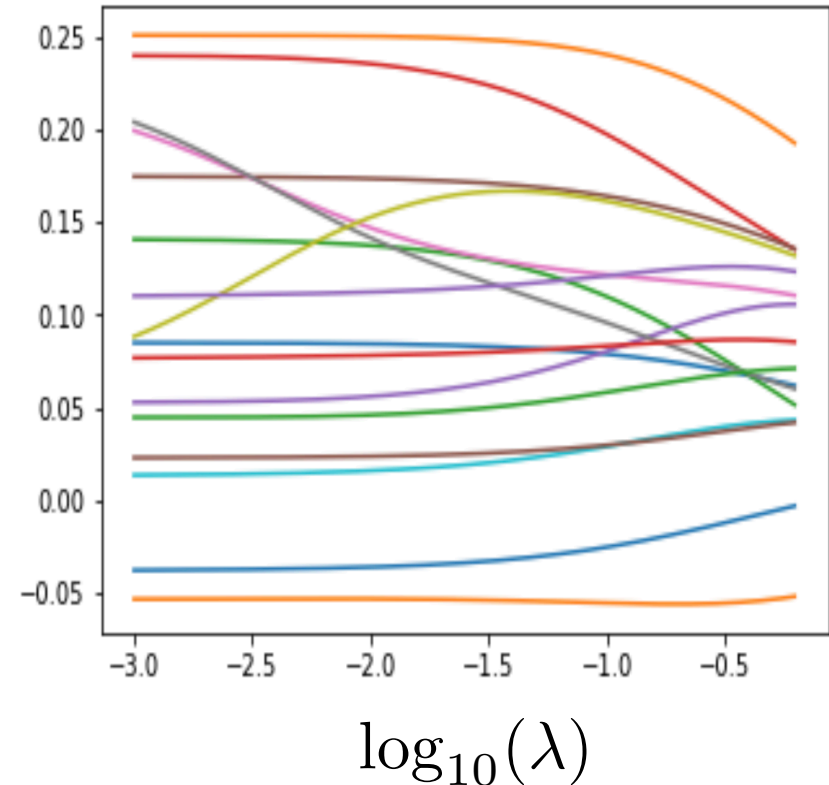
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# Bias-Variance Properties

---

- 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:  $x_i \sim P_X$ ,  $\mathbf{y} = \mathbf{X}w + \epsilon$ ,  $\epsilon \sim \mathcal{N}(0, \sigma^2 \mathbf{I})$  for some ground truth model parameter  $w$
- The true error at a sample with feature  $x$  is 
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$$= \underbrace{\mathbb{E}_{y|x} [(y - \mathbb{E}[y|x])^2 | x]}_{\text{Irreducible Error}} + \underbrace{\mathbb{E}_{\mathcal{D}_{\text{train}}} [(\mathbb{E}[y|x] - x^T \hat{\mathbf{w}}_{\text{ridge}})^2 | x]}_{\text{Learning Error}}$$

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Irreduc. Error

Bias-squared

Variance

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

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

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

# Not realistic but pretend we're sampling independent Gaussians

$$= \frac{n}{n + \lambda} w + \frac{1}{n + \lambda} \mathbf{X}^T \epsilon \quad \# \lambda \text{ trades off weight on data vs. noise}$$

# Bias-Variance Properties

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

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

- 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

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

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

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

(verify at home)

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

Irreduc. Error

Bias-squared

Variance

# Bias-Variance Properties

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

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- $\lambda$  trades off bias + variance

Irreduc. Error

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Variance

# Bias-Variance Properties

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- Larger  $\lambda \rightarrow$

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(verify at home)

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Irreduc. Error

Bias-squared

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- $\lambda$  trades off bias + variance
- Larger  $\lambda \rightarrow$ 
  - Bigger bias

# Bias-Variance Properties

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Irreduc. Error

Bias-squared

Variance

- $\lambda$  trades off bias + variance
- Larger  $\lambda \rightarrow$ 
  - Bigger bias
  - Smaller variance

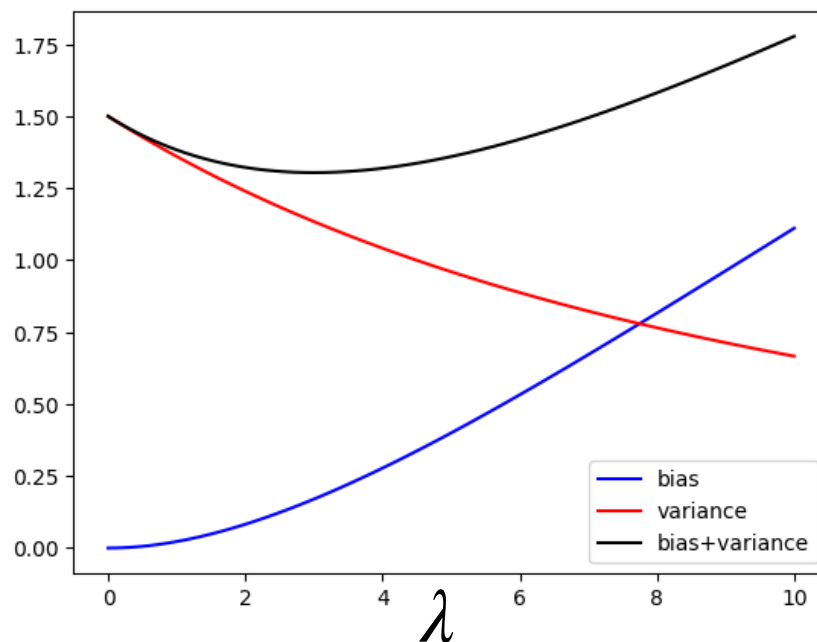
# Bias-Variance Properties

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

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

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

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



as  $\lambda \rightarrow 0$ ,

$$\hat{w}_{ridge} \rightarrow \hat{w}_{LS}$$

as  $\lambda \rightarrow \infty$

$$\hat{w}_{ridge} \rightarrow 0$$

# 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!

# What you need to know...

---

## > Regularization

- Penalizes complex models towards preferred, simpler models

## > Ridge regression

- $L_2$  penalized least-squares regression  $\lambda \|w\|_2^2$
- Regularization parameter trades off model complexity with training error
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# Simple Variable Selection

## LASSO: Sparse Regression

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# Sparsity

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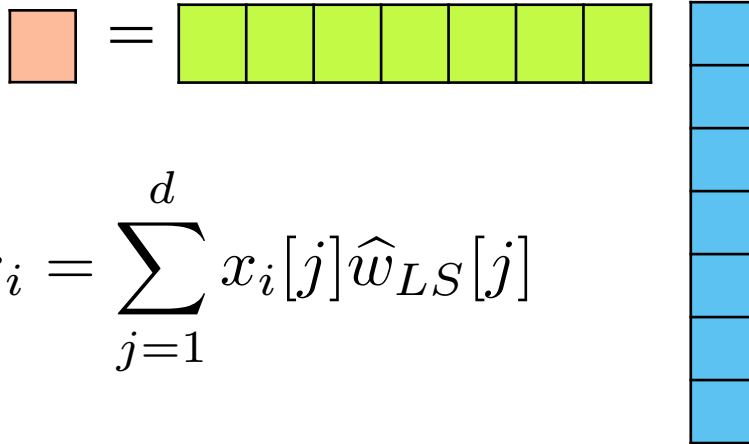
$$\hat{w}_{LS} = \arg \min_w \sum_{i=1}^n (y_i - x_i^T w)^2$$

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

# Sparsity

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

- **Vector  $w$  is sparse, if many entries are zero**
  - **Efficiency:** If  $\text{size}(w) = 100$  Billion, each prediction is expensive:
    - If  $w$  is sparse, prediction computation only depends on number of non-zeros



$$\hat{y}_i = \hat{w}_{LS}^T x_i = \sum_{j=1}^d x_i[j] \hat{w}_{LS}[j]$$

# Sparsity

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

- **Vector  $w$  is sparse, if many entries are zero**
  - **Interpretability:** What are the relevant dimension to make a prediction?

**$y$  = delivery time (s)**



**Candidate features  $x$**

Known at prediction time

|                      |                      |
|----------------------|----------------------|
| Route distance (km)  | Traffic forecast     |
| Direct distance (km) | Forecast wind speed  |
| Potato weight (lbs)  | Forecast tailwind    |
| Battery charge (%)   | Forecast rainfall    |
| Package size (L)     | Forecast temperature |
| Planned stops        | Launch queue         |

- How do we find “best” subset among all possible?

Illustrative potato delivery example

# Finding best subset: Exhaustive

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- > Try all subsets of size 1, 2, 3, ... and one that minimizes validation error
- > Problem?

# Finding best subset: Greedy

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## **Forward stepwise:**

Starting from simple model and iteratively add features most useful to fit

## **Backward stepwise:**

Start with full model and iteratively remove features least useful to fit

## **Combining forward and backward steps:**

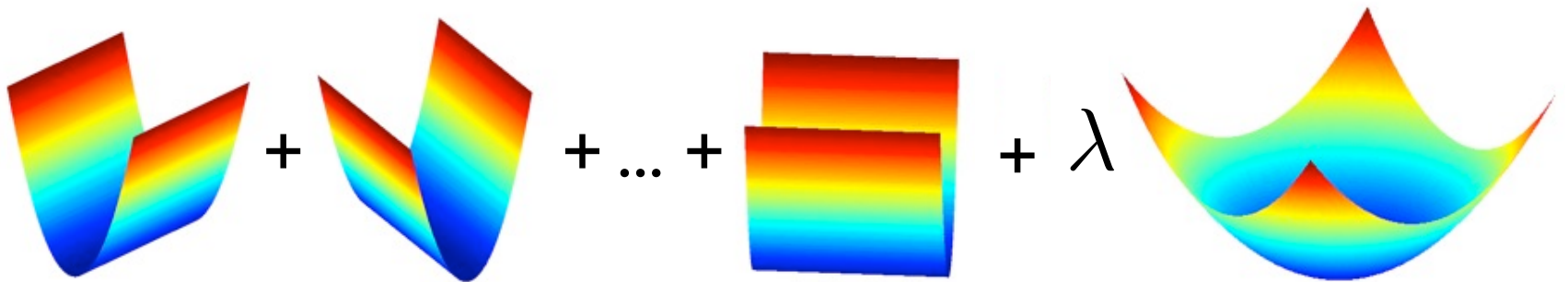
In forward algorithm, insert steps to remove features no longer as important

*Lots of other variants, too.*

# Finding best subset: Regularize

Ridge regression makes coefficients small

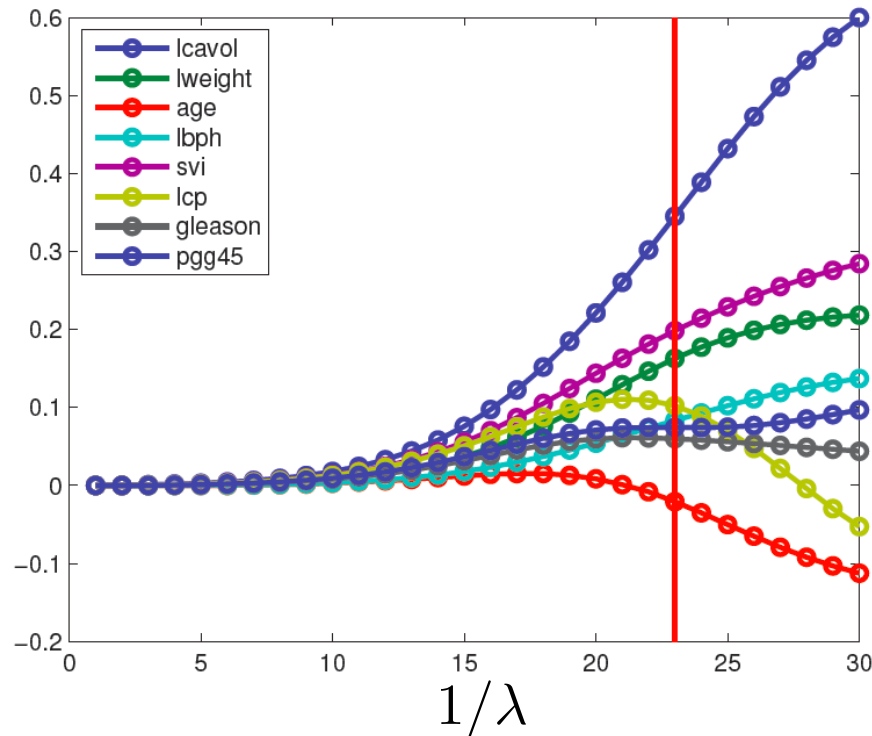
$$\hat{w}_{ridge} = \arg \min_w \sum_{i=1}^n (y_i - x_i^T w)^2 + \lambda ||w||_2^2$$



# Finding best subset: Regularize

Ridge regression makes coefficients small

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

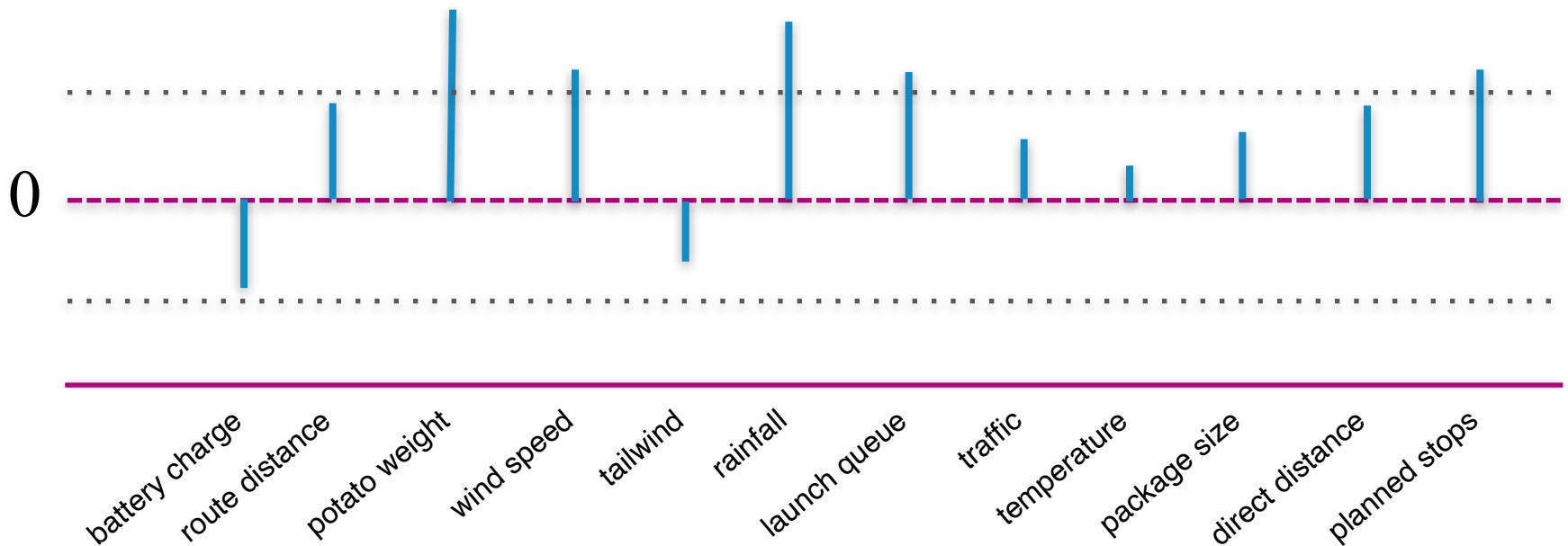


From  
Kevin Murphy  
textbook

# Thresholded Ridge Regression

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

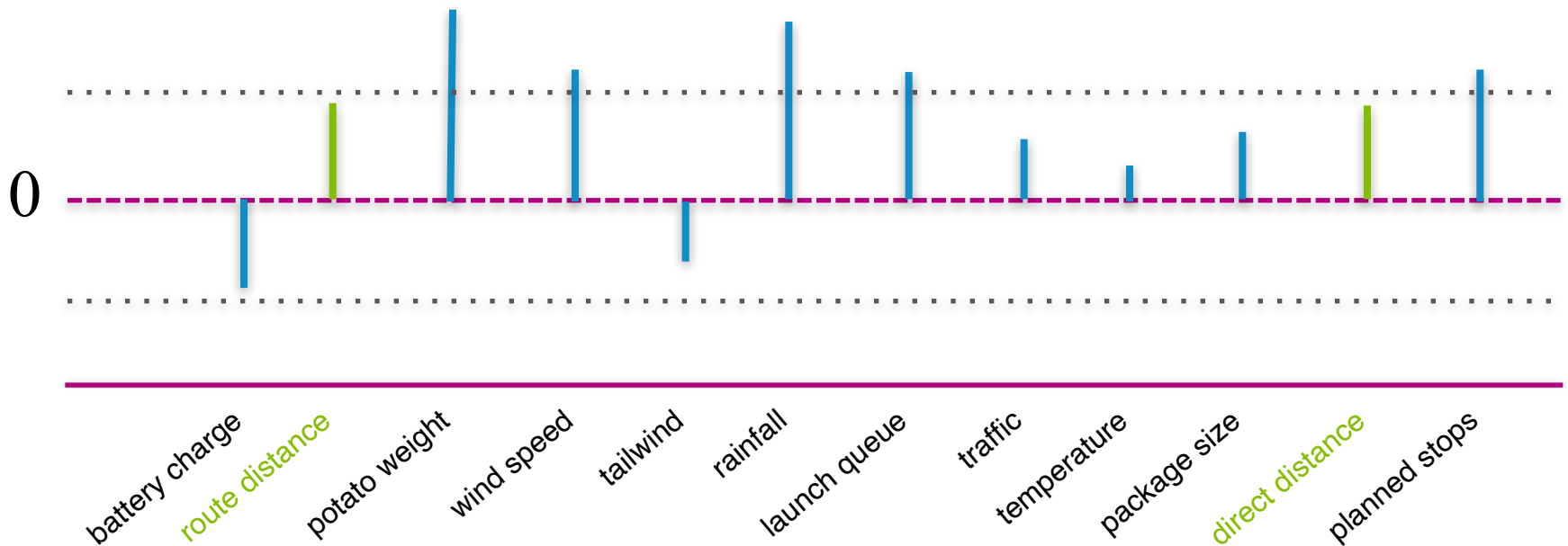
Why don't we just set **small** ridge coefficients to 0?



# Thresholded Ridge Regression

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

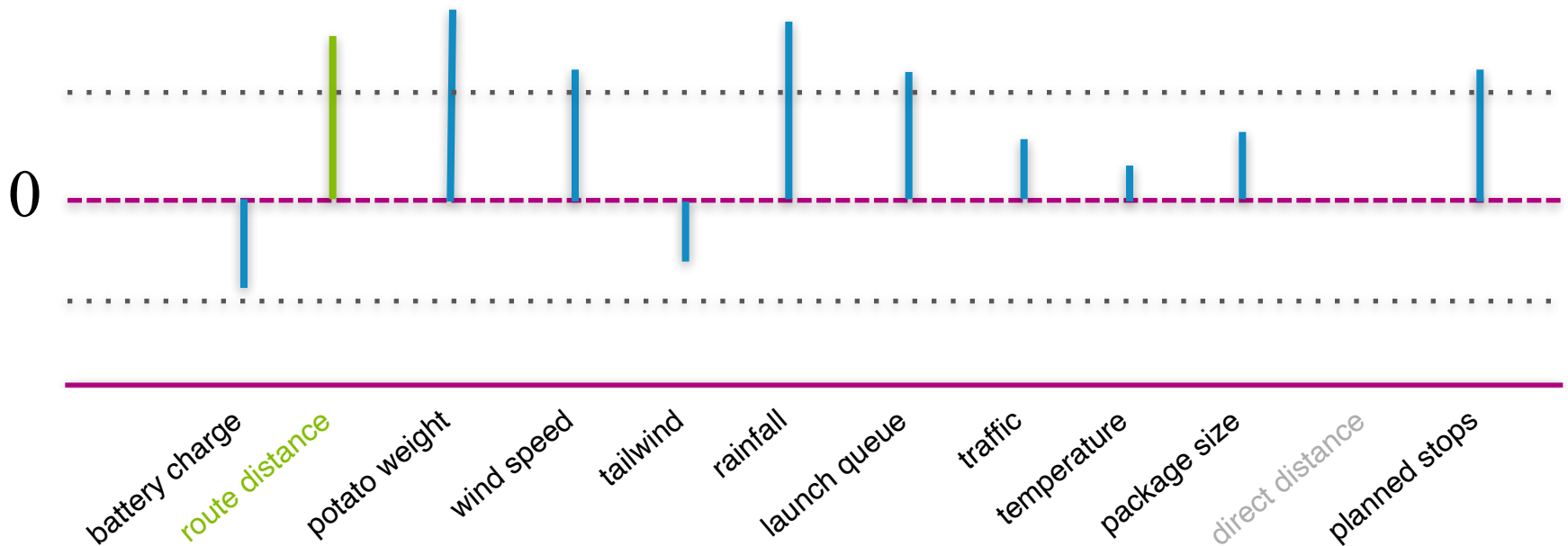
Related features: route distance and direct distance



# Thresholded Ridge Regression

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

Omit direct distance and refit: route-distance weight may rise.



Standardized delivery features

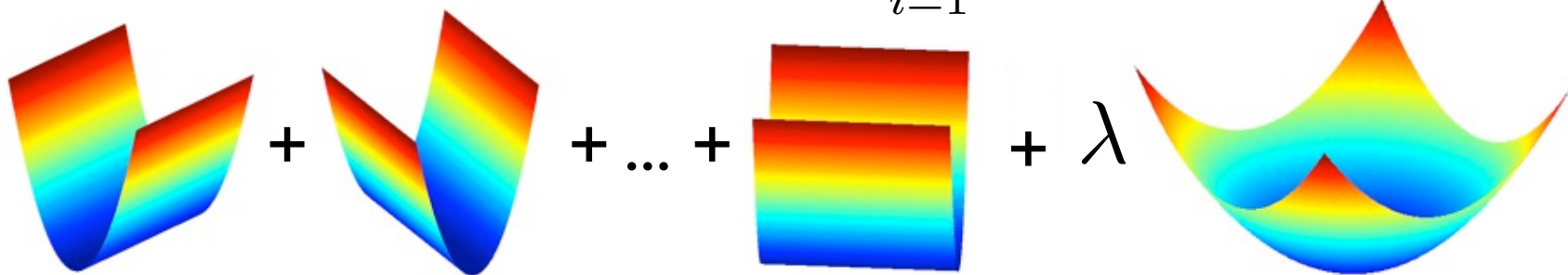
**Can another regularizer perform selection automatically?**

Illustrative

# Recall Ridge Regression

- Ridge Regression objective:

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

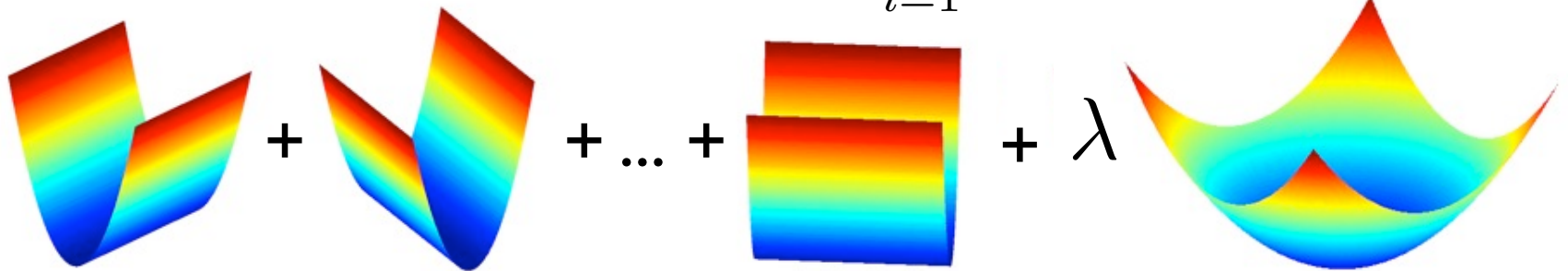


$$||w||_p = \left( \sum_{i=1}^d |w|^p \right)^{1/p}$$

# Ridge vs. Lasso Regression

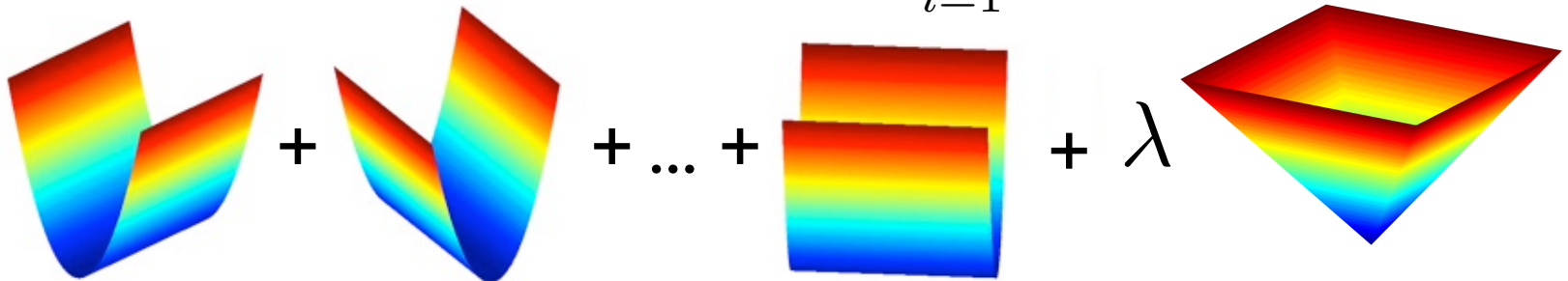
- Ridge Regression objective:

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



- Lasso objective:

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



# Penalized Least Squares

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

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

# Penalized Least Squares

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

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

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

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

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