Bias-Variance

Features	Train MSE	Test MSE
All	2640	3224
S5 and BMI	3004	3453
S5	3869	4227
BMI	3540	4277
S4 and S3	4251	5302
S4	4278	5409
S3	4607	5419
None	5524	6352

- **test MSE is the primary criteria for model selection**
- Using only 2 features (S5 and BMI), one can get very close to the prediction performance of using all features
- Combining S3 and S4 does not give any performance gain

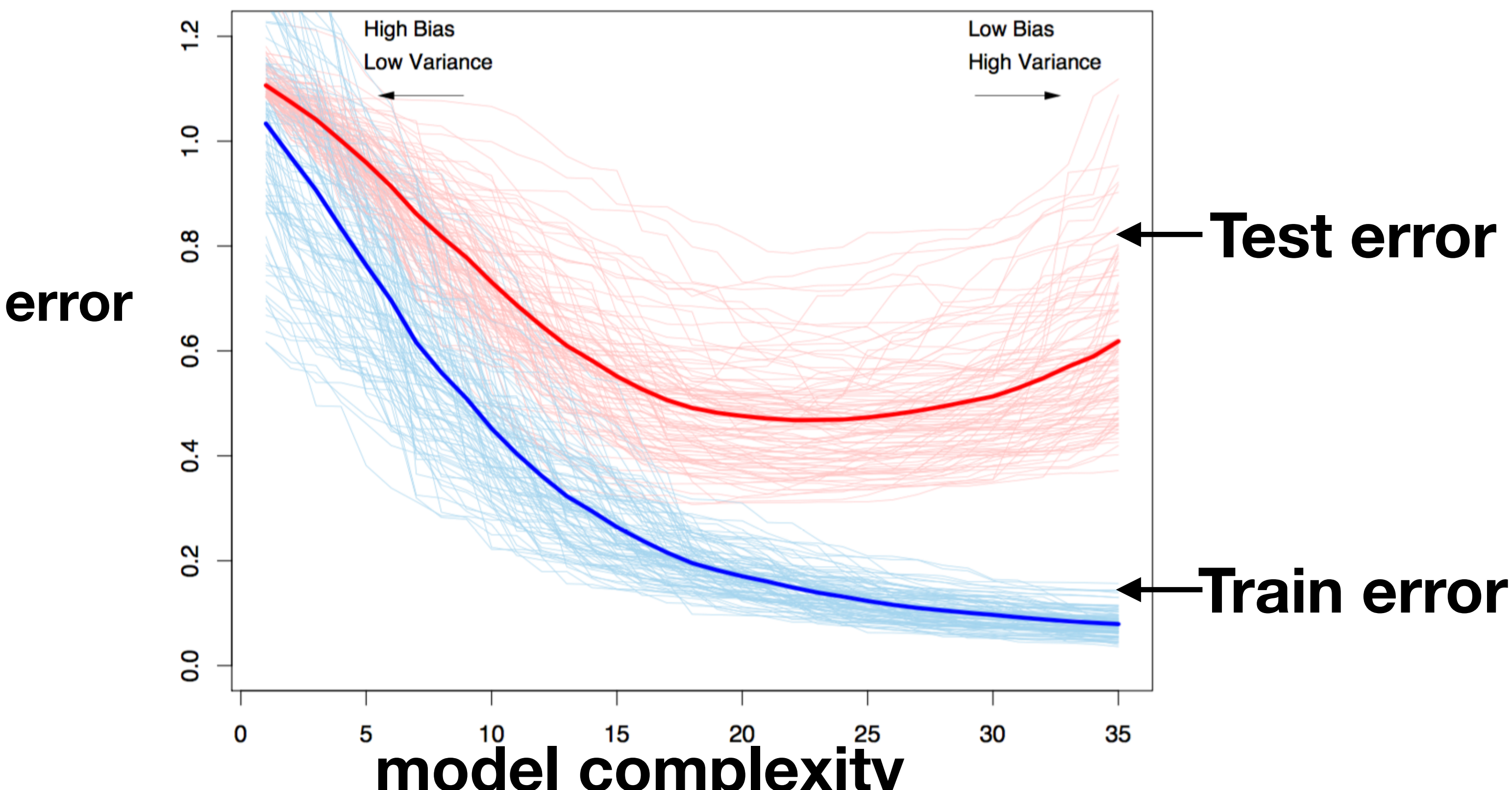
demo3_diabetes.ipynb

What does the bias-variance theory tell us?

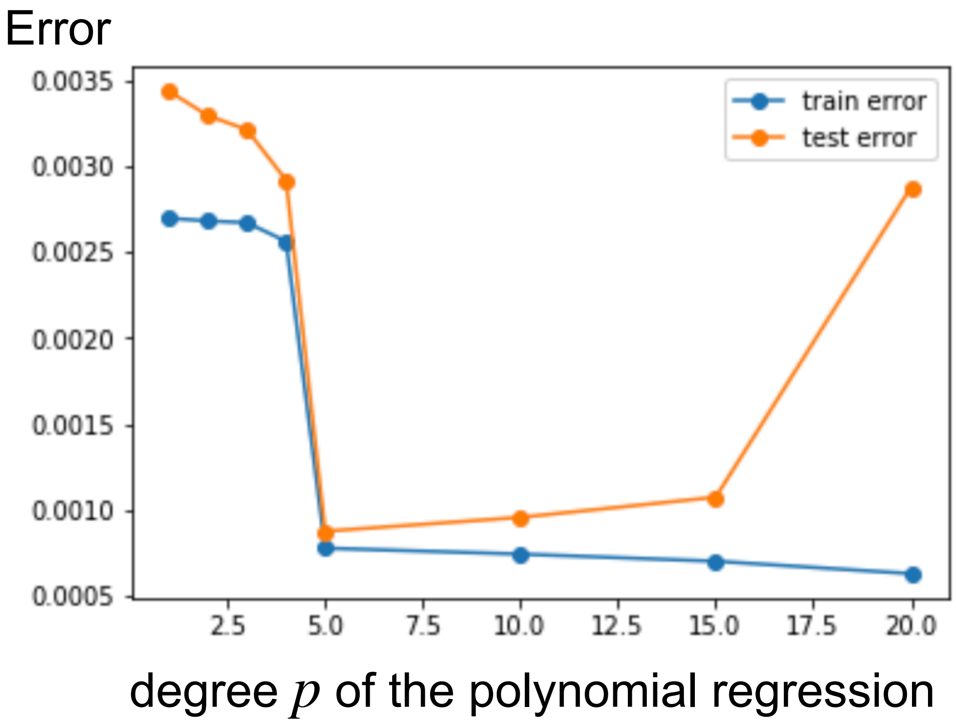
- **Train error** (random variable, randomness from $\mathcal{D}$)
  - Use $\mathcal{D} = \{(x_i, y_i)\}_{i=1}^{n} \sim P_{X,Y}$ to find $\widehat{w}$
  - Train error: $\mathcal{L}_{\text{train}}(\widehat{w}_{\text{LS}}) = \frac{1}{|\mathcal{D}|} \sum_{(x_i,y_i)\in\mathcal{D}} (y_i - \widehat{w}^T x_i)^2$
- recall the **test error** is an unbiased estimator of the **true error**
- **True error** (random variable, randomness from $\mathcal{D}$)
  - True error: $\mathcal{L}_{\text{true}}(\widehat{w}) = \mathbb{E}_{(x,y)\sim P_{X,Y}}[(y - \widehat{w}^T x)^2]$
- **Test error** (random variable, randomness from $\mathcal{D}$ and $\mathcal{T}$)
  - Use $\mathcal{T} = \{(x_i, y_i)\}_{i=1}^{m} \sim P_{X,Y}$
  - Test error: $\mathcal{L}_{\text{test}}(\widehat{w}) = \frac{1}{|\mathcal{T}|} \sum_{(x_i,y_i)\in\mathcal{T}} (y_i - \widehat{w}^T x_i)^2$
- theory explains **true error**, and hence expected behavior of the (random) **test error**

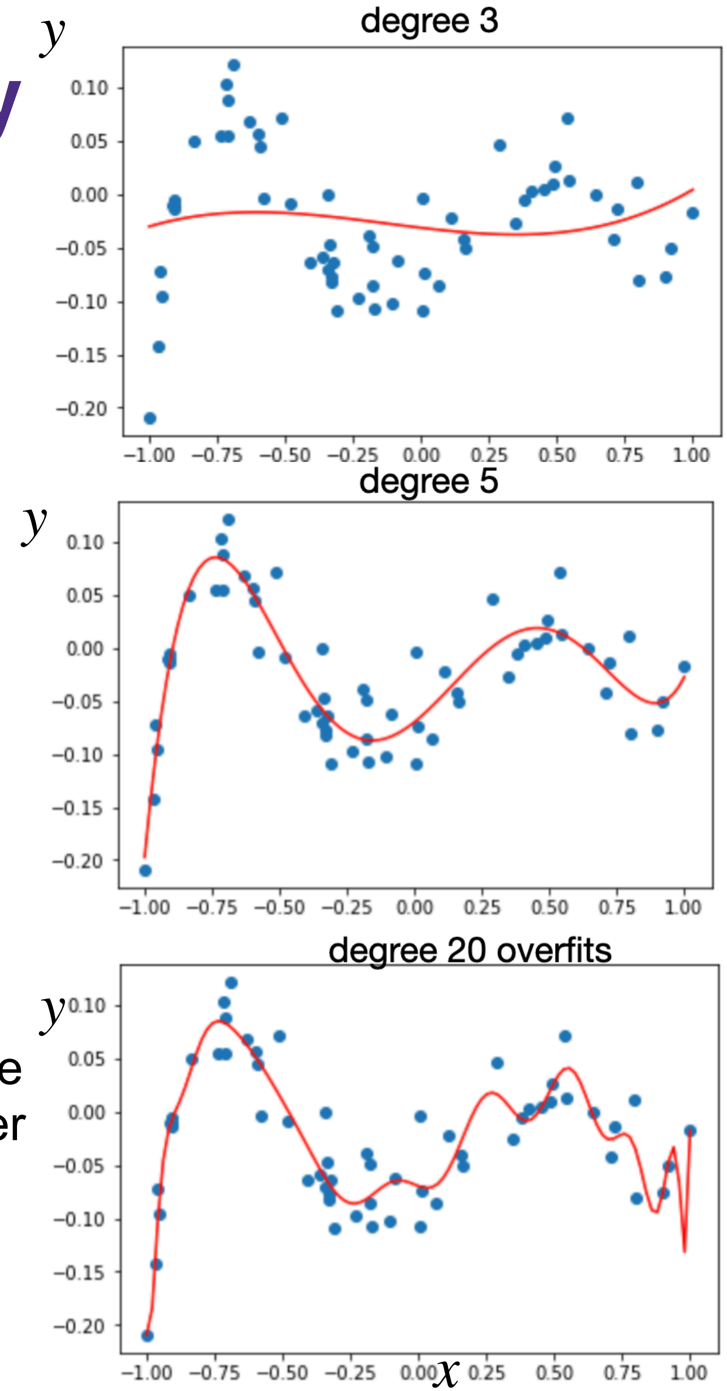
What does bias-variance theory tell us?

- Train error is optimistically biased (i.e. smaller) because the trained model is minimizing the train error
- Test error is unbiased estimate of the true error, if test data is never used in training a model or selecting the model complexity
- Each line is an i.i.d. instance of $\mathscr{D}$ and $\mathscr{T}$



Train/test error vs. complexity





- **Model complexity** e.g., degree p of the polynomial model, number of features used in diabetes example
  - Related to the dimension of the model parameter
- **Train error** monotonically decreases with model complexity
- **Test error** has a U shape

Statistical learning

Typical notation:
X denotes a random variable
x denotes a deterministic instance

- Suppose data is generated from a statistical model $(X, Y) \sim P_{X,Y}$
  - and assume we know $P_{X,Y}$ (just for now to explain statistical learning)
- **learning** aims to find a predictor $\eta : \mathbb{R}^d \to \mathbb{R}$ that minimizes
  - expected error $\mathbb{E}_{(X,Y)\sim P_{X,Y}}[(Y - \eta(X))^2]$
  - think of random (X, Y) as a new sample you will encounter when you deployed your learned model, and we care about its average performance
- We assume the function $\eta(x)$ could be anything
  - it can take any value for each $X = x$
- So the optimization can be done separately for each $X = x$
  - $$\mathbb{E}_{(X,Y)\sim P_{X,Y}}[(Y - \eta(X))^2] = \mathbb{E}_{X\sim P_X}\Big[\mathbb{E}_{Y\sim P_{Y|X}}[(Y - \eta(x))^2 \,|\, X = x]\Big]$$
    $$= \int \mathbb{E}_{Y\sim P_{Y|X}}[(Y - \eta(x))^2 \,|\, X = x]\, P_X(x)\, dx$$

Or for discrete X,
$$= \sum_x P_X(x)\, \mathbb{E}_{Y\sim P_{Y|X}}[(Y - \eta(x))^2 \,|\, X = x]$$

Where we used the chain rule: $\mathbb{E}_{X,Y}[f(X,Y)] = \mathbb{E}_X\Big[\,\mathbb{E}_{Y|X}[f(x,Y) \,|\, X = x]\Big]$

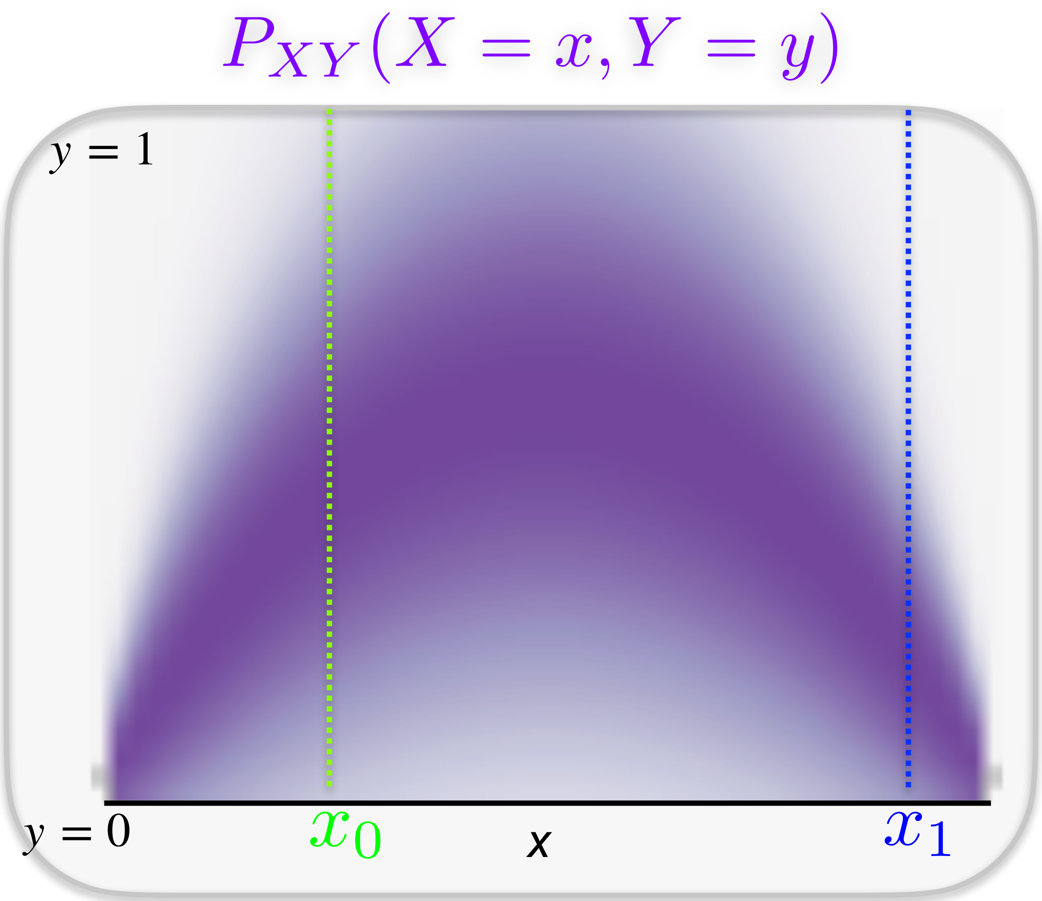
Statistical learning

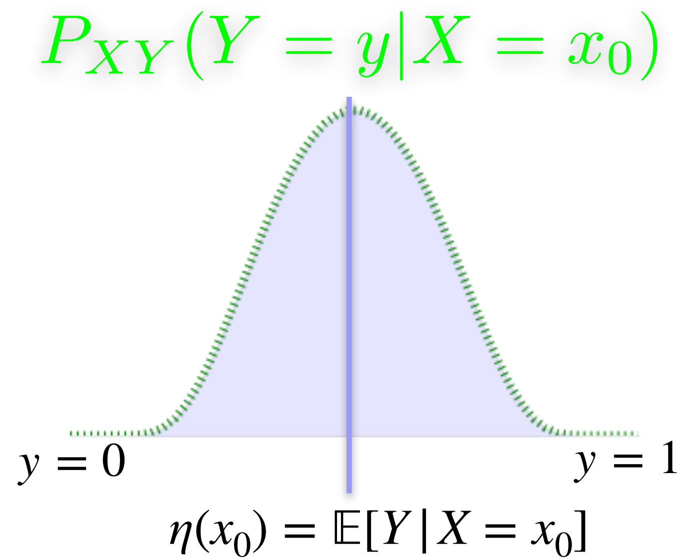
- The optimal predictor sets its value for each $X = x$ separately
  - $\eta(x) \; = \; \arg\min_{a \in \mathbb{R}} \mathbb{E}_{Y \sim P_{Y|X}}[(Y - a)^2 \,|\, X = x]$
- The optimal solution is $\eta(x) = \mathbb{E}_{Y \sim P_{Y|X}}[Y \,|\, X = x]$,
  which is the best prediction in ℓ_2-loss/Mean Squared Error
- Claim: $\mathbb{E}_{Y \sim P_{Y|X}}[Y \,|\, X = x] \; = \; \arg\min_{a \in \mathbb{R}} \mathbb{E}_{Y \sim P_{Y|X}}[(Y - a)^2 \,|\, X = x]$
- Proof:
- Can't implement optimal statistical estimator $\eta(x) = \mathbb{E}[Y \,|\, X = x]$
  - as we do not know $P_{X,Y}$ in practice
- This is only for the purpose of conceptual understanding

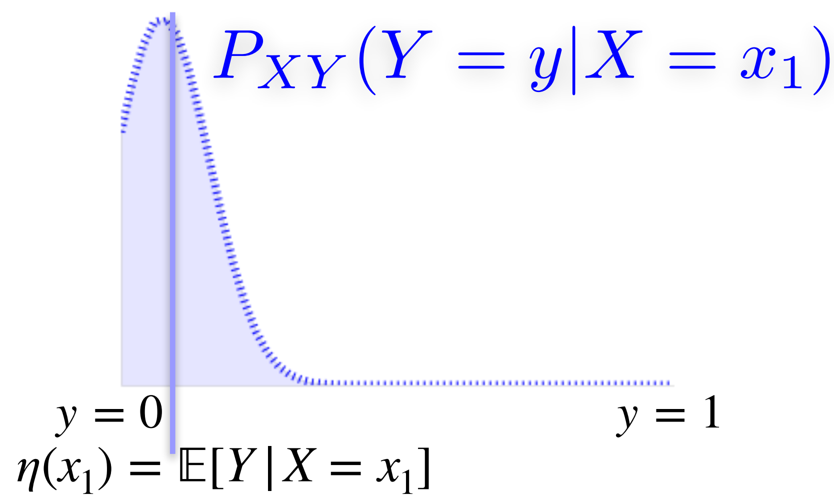
Statistical Learning

Ideally, we want to find:

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

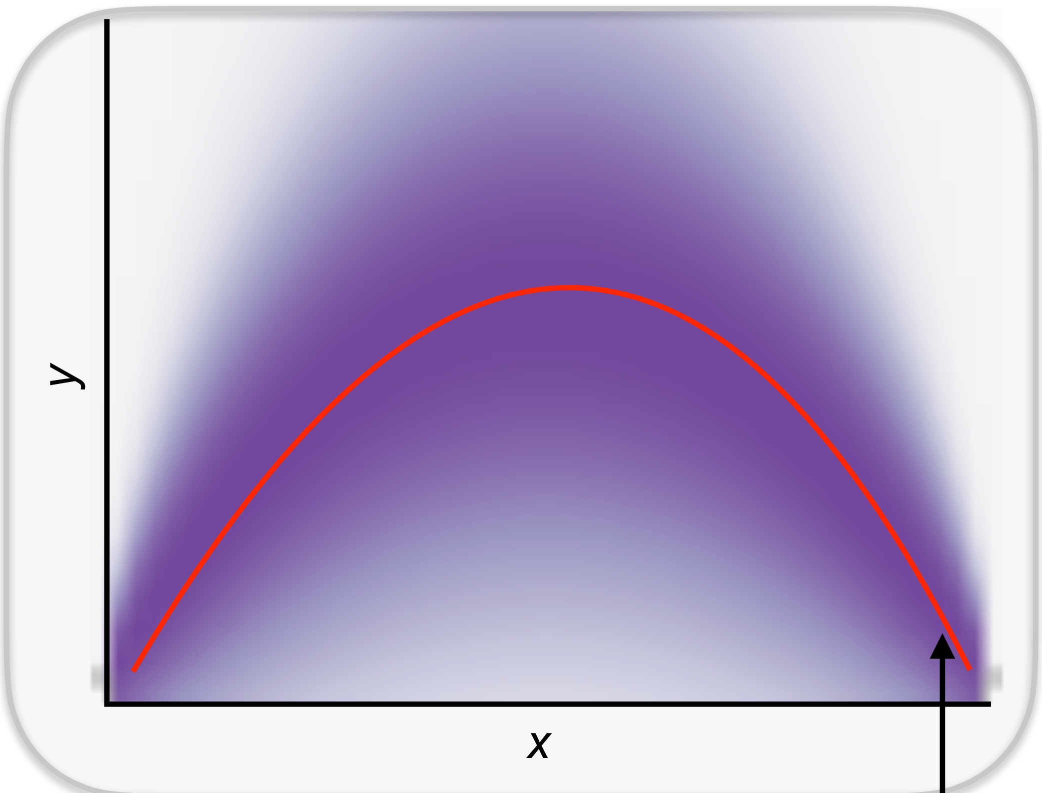






Statistical Learning

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



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

Ideally, we want to find:

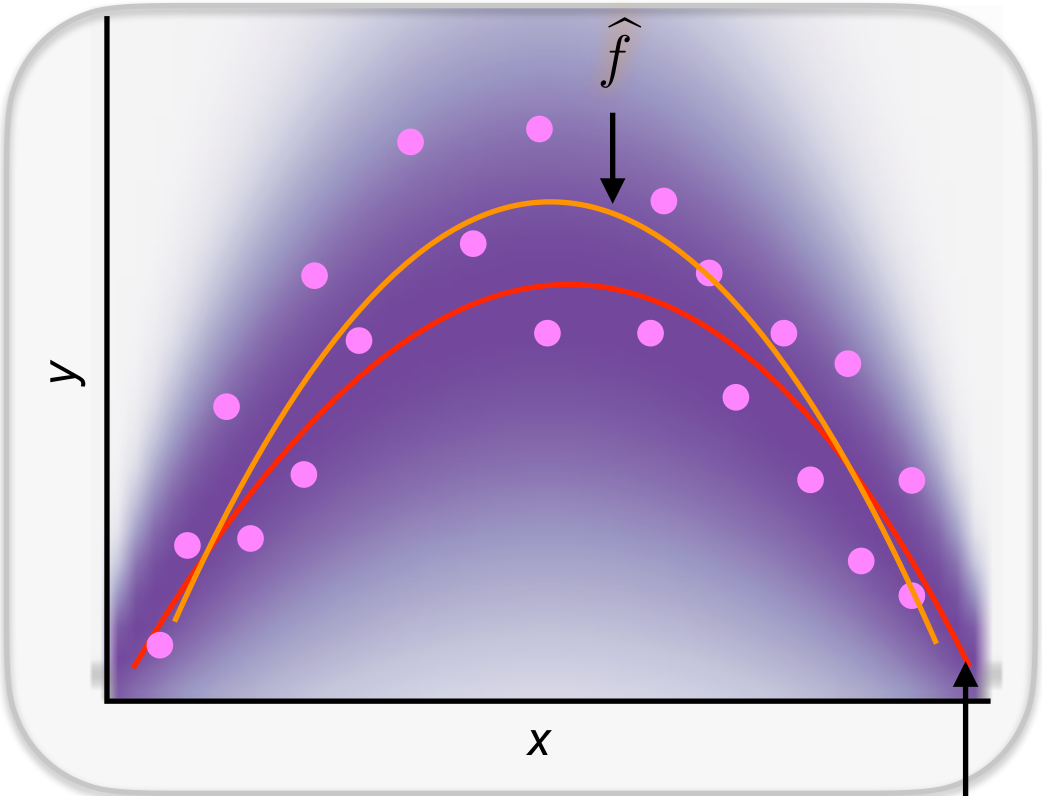
$$\eta(x) = \mathbb{E}_{Y|X}[Y|X = x]$$

But we do not know $P_{X,Y}$

We only have samples.

Statistical Learning

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



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

Ideally, we want to find:

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

But we only have samples:

$$(x_i, y_i) \overset{i.i.d.}{\sim} P_{XY} \quad \text{for } i = 1, \ldots, n$$

So we need to restrict our predictor to a function class (e.g., linear, degree-p polynomial) to avoid overfitting:

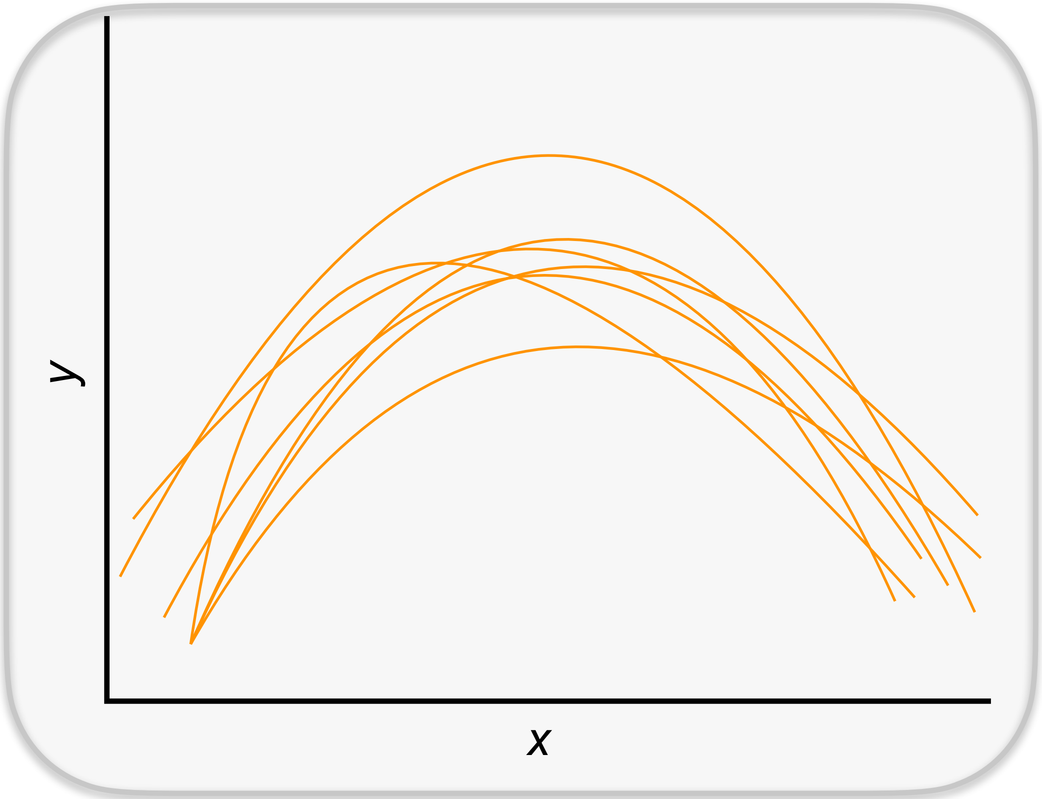
$$\widehat{f} = \arg\min_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^{n} (y_i - f(x_i))^2$$

We care about how our predictor performs on future unseen data

True Error of $\hat{f}$: $\mathbb{E}_{X,Y}[(Y - \hat{f}(X))^2]$

Future prediction error $\mathbb{E}_{X,Y}[(Y - \hat{f}(X))^2]$ is random because $\hat{f}$ is random (whose randomness comes from training data $\mathscr{D}$)

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



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

Bias-variance tradeoff

Notation:
I use predictor/model/estimate, interchangeably

Ideal predictor

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

Learned predictor

$$\hat{f}_{\mathcal{D}} = \arg\min_{f \in \mathcal{F}} \frac{1}{|\mathcal{D}|} \sum_{(x_i, y_i) \in \mathcal{D}} (y_i - f(x_i))^2$$

- We are interested in the **True Error** of a (random) learned predictor:

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

- But the analysis can be done for each $X = x$ separately, so we analyze the **conditional true error**:

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

- And we care about the **average conditional true error**, averaged over training data:

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

written compactly as $= \mathbb{E}[(Y - \hat{f}_{\mathcal{D}}(x))^2]$

Bias-variance tradeoff

Ideal predictor

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

Learned predictor

$$\hat{f}_{\mathcal{D}} = \arg\min_{f \in \mathcal{F}} \frac{1}{|\mathcal{D}|} \sum_{(x_i, y_i) \in \mathcal{D}} (y_i - f(x_i))^2$$

- **Average conditional true error**:

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

Bias-variance tradeoff

Ideal predictor

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

Learned predictor

$$\hat{f}_{\mathcal{D}} = \arg\min_{f \in \mathcal{F}} \frac{1}{|\mathcal{D}|} \sum_{(x_i, y_i) \in \mathcal{D}} (y_i - f(x_i))^2$$

- **Average conditional true error**:

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

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

$$= \mathbb{E}_{Y|x}[(Y - \eta(x))^2] + 2\mathbb{E}_{\mathcal{D},Y|x}[\underbrace{(Y - \eta(x))}_{=0}(\eta(x) - \hat{f}_{\mathcal{D}}(x))] + \mathbb{E}_{\mathcal{D}}[(\eta(x) - \hat{f}_{\mathcal{D}}(x))^2]$$

(this follows from independence of $\mathcal{D}$ and (X, Y) and $\mathbb{E}_{Y|x}[Y - \eta(x)] = \mathbb{E}[Y|X = x] - \eta(x) = 0$)

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

Irreducible error
(a) Caused by stochastic label noise in $P_{Y|X=x}$
(b) cannot be reduced

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

Bias-variance tradeoff

Ideal predictor

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

Learned predictor

$$\hat{f}_{\mathcal{D}} = \arg\min_{f \in \mathcal{F}} \frac{1}{|\mathcal{D}|} \sum_{(x_i, y_i) \in \mathcal{D}} (y_i - f(x_i))^2$$

- **Average learning error**:

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

Bias-variance tradeoff

Ideal predictor

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

Learned predictor

$$\hat{f}_{\mathcal{D}} = \arg\min_{f \in \mathcal{F}} \frac{1}{|\mathcal{D}|} \sum_{(x_i, y_i) \in \mathcal{D}} (y_i - f(x_i))^2$$

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- **Average learning error**:

Bias-variance tradeoff

Ideal predictor

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

Learned predictor

$$\hat{f}_{\mathscr{D}} = \arg\min_{f \in \mathscr{F}} \frac{1}{|\mathscr{D}|} \sum_{(x_i, y_i) \in \mathscr{D}} (y_i - f(x_i))^2$$

- **Average learning error**:

$$\mathbb{E}_{\mathscr{D}}[(\eta(x) - \hat{f}_{\mathscr{D}}(x))^2] = \mathbb{E}_{\mathscr{D}}\left[\left(\eta(x) - \mathbb{E}_{\mathscr{D}}[\hat{f}_{\mathscr{D}}(x)] + \mathbb{E}_{\mathscr{D}}[\hat{f}_{\mathscr{D}}(x)] - \hat{f}_{\mathscr{D}}(x) \right)^2 \right]$$

Bias-variance tradeoff

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

Bias-variance tradeoff

Ideal predictor

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

Learned predictor

$$\hat{f}_{\mathcal{D}} = \arg\min_{f \in \mathcal{F}} \frac{1}{|\mathcal{D}|} \sum_{(x_i, y_i) \in \mathcal{D}} (y_i - f(x_i))^2$$

- **Average learning error**:

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

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

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

Bias-variance tradeoff

Ideal predictor

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

Learned predictor

$$\hat{f}_{\mathcal{D}} = \arg\min_{f \in \mathcal{F}} \frac{1}{|\mathcal{D}|} \sum_{(x_i, y_i) \in \mathcal{D}} (y_i - f(x_i))^2$$

- **Average learning error**:

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

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

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

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

Bias-variance tradeoff

Ideal predictor

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

Learned predictor

$$\hat{f}_{\mathcal{D}} = \arg\min_{f \in \mathcal{F}} \frac{1}{|\mathcal{D}|} \sum_{(x_i, y_i) \in \mathcal{D}} (y_i - f(x_i))^2$$

- **Average learning error**:

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

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

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

biased squared **variance**

Bias-variance tradeoff

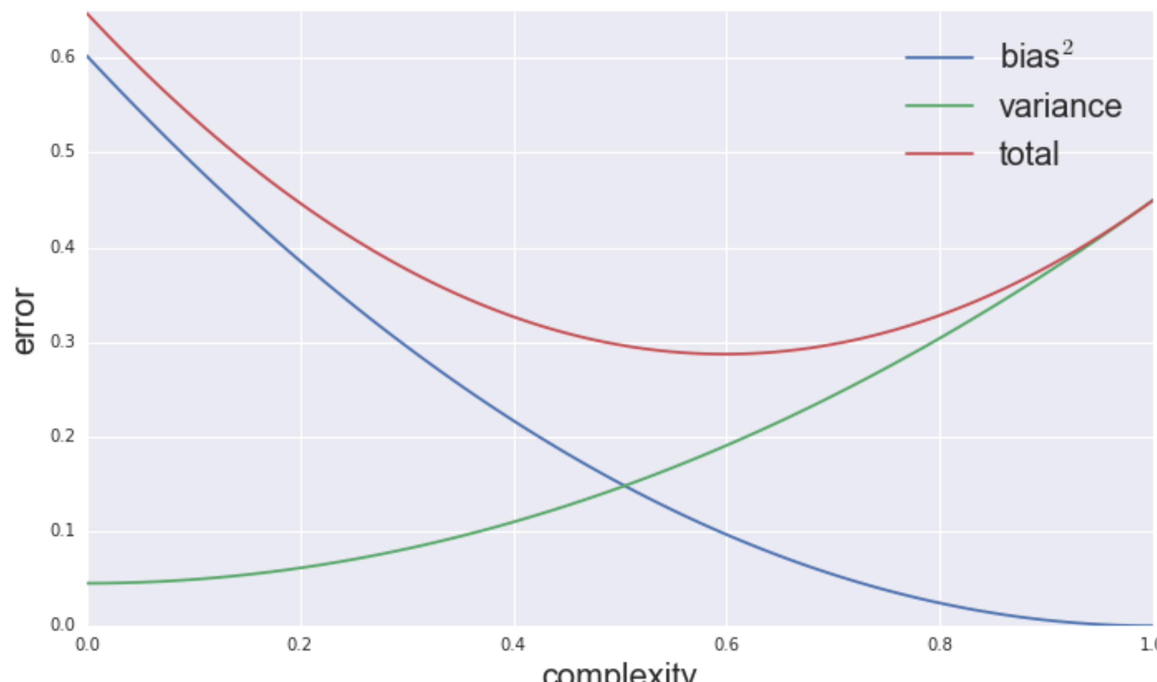
- **Average conditional true error**:

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

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

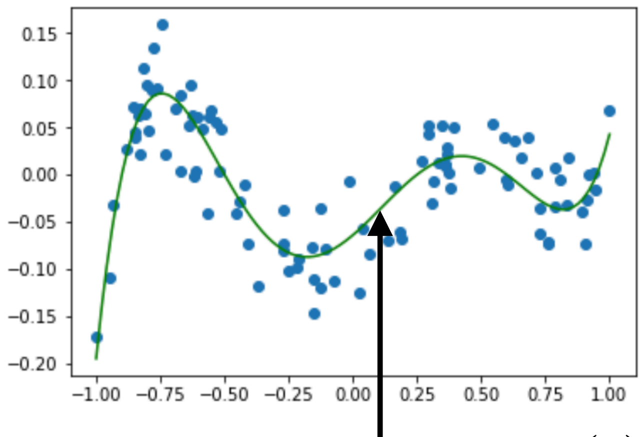
Bias squared:
measures how the predictor is mismatched with the best predictor in expectation

variance:
measures how the predictor varies each time with a new training datasets



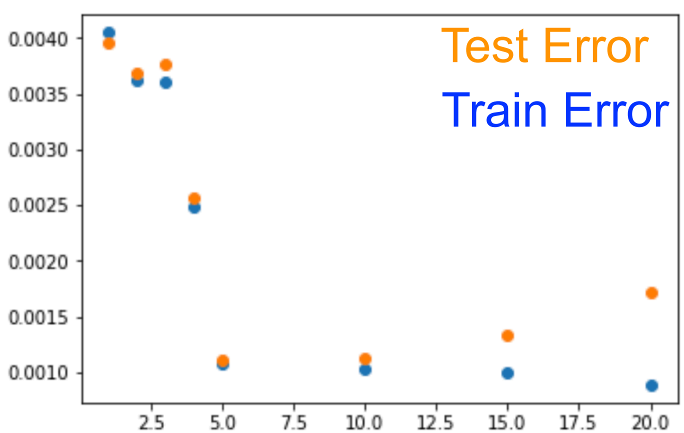
Questions?

Test error vs. model complexity



Optimal predictor $\eta(x)$ is degree-5 polynomial

Error

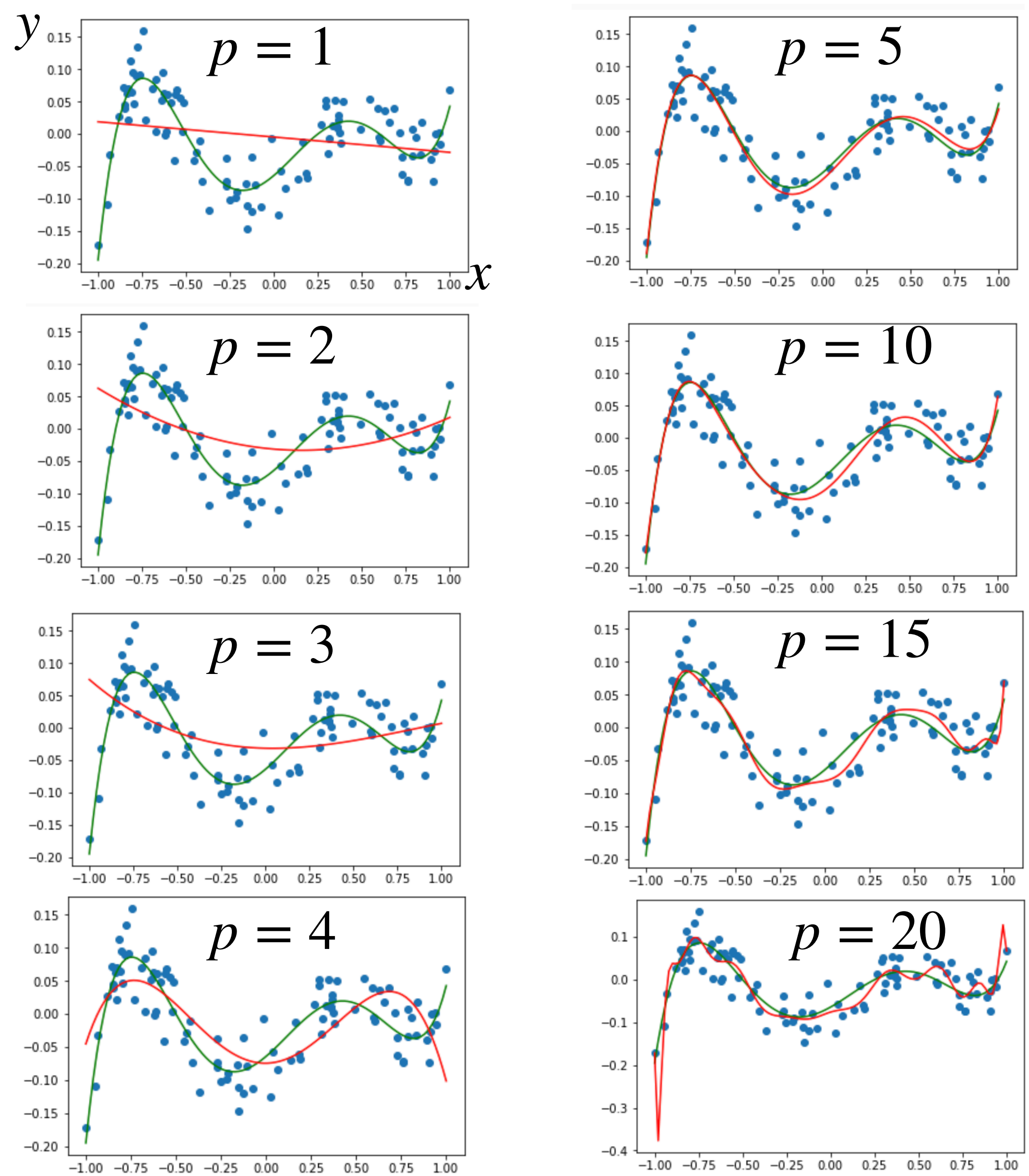


degree p of the polynomial regression

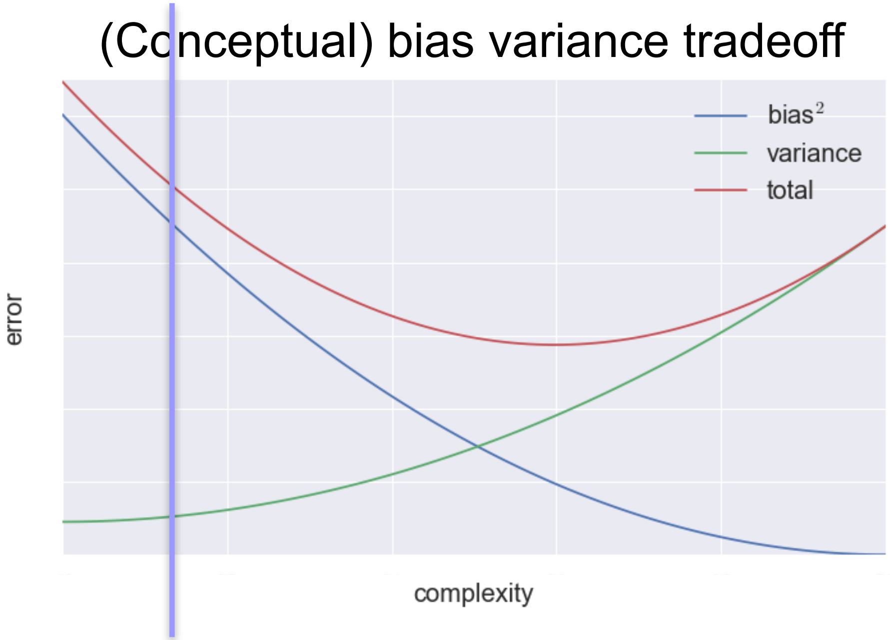
demo4_tradeoff.ipynb

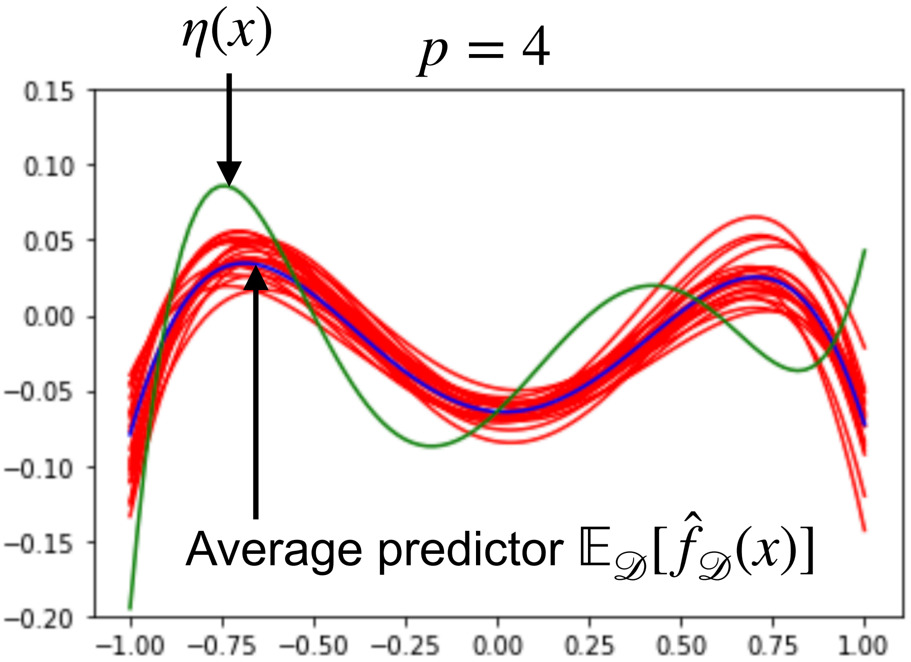
Simple model:
Model complexity is below the complexity of $\eta(x)$

Complex model:



Recap: Bias-variance tradeoff with simple model

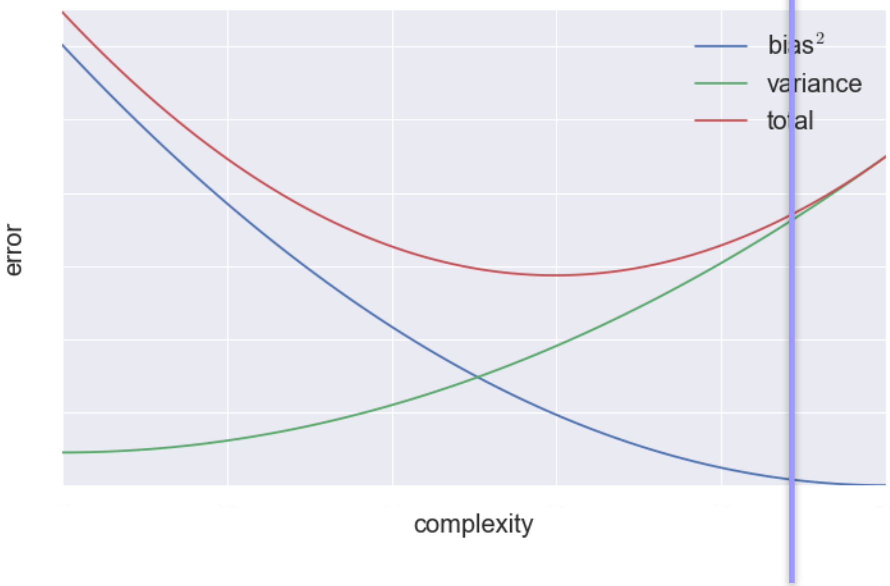


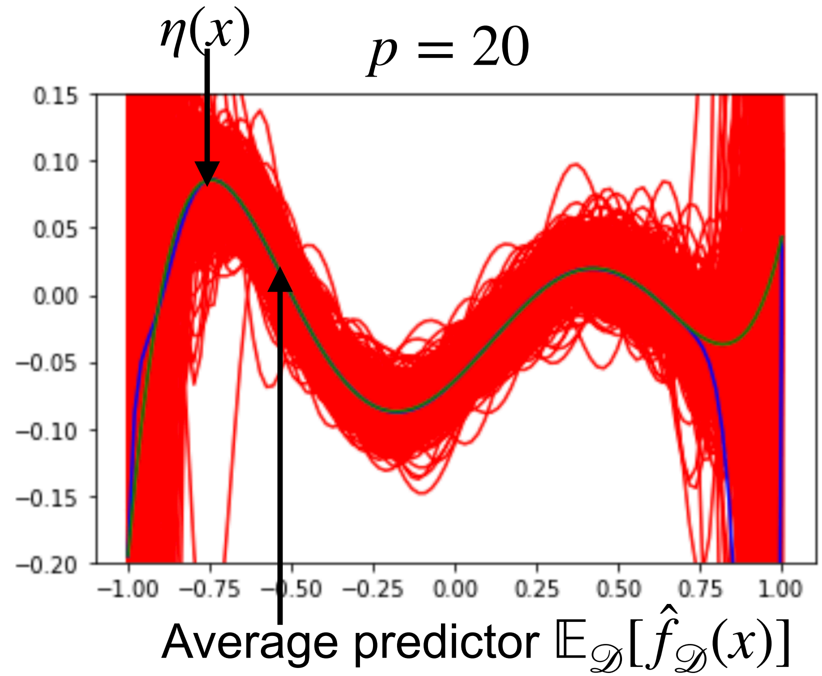


- When model **complexity is low** (lower than the optimal predictor $\eta(x)$)
  - Bias^2 of our predictor, $\left(\eta(x) - \mathbb{E}_{\mathcal{D}}[\hat{f}_{\mathcal{D}}(x)]\right)^2$, is large
  - Variance of our predictor, $\mathbb{E}_{\mathcal{D}}\left[\left(\mathbb{E}_{\mathcal{D}}[\hat{f}_{\mathcal{D}}(x)] - \hat{f}_{\mathcal{D}}(x)\right)^2\right]$, is small
  - If we have more samples, then
    - Bias
    - Variance
    - Because Variance is already small, overall test error

Recap: Bias-variance tradeoff with simple model

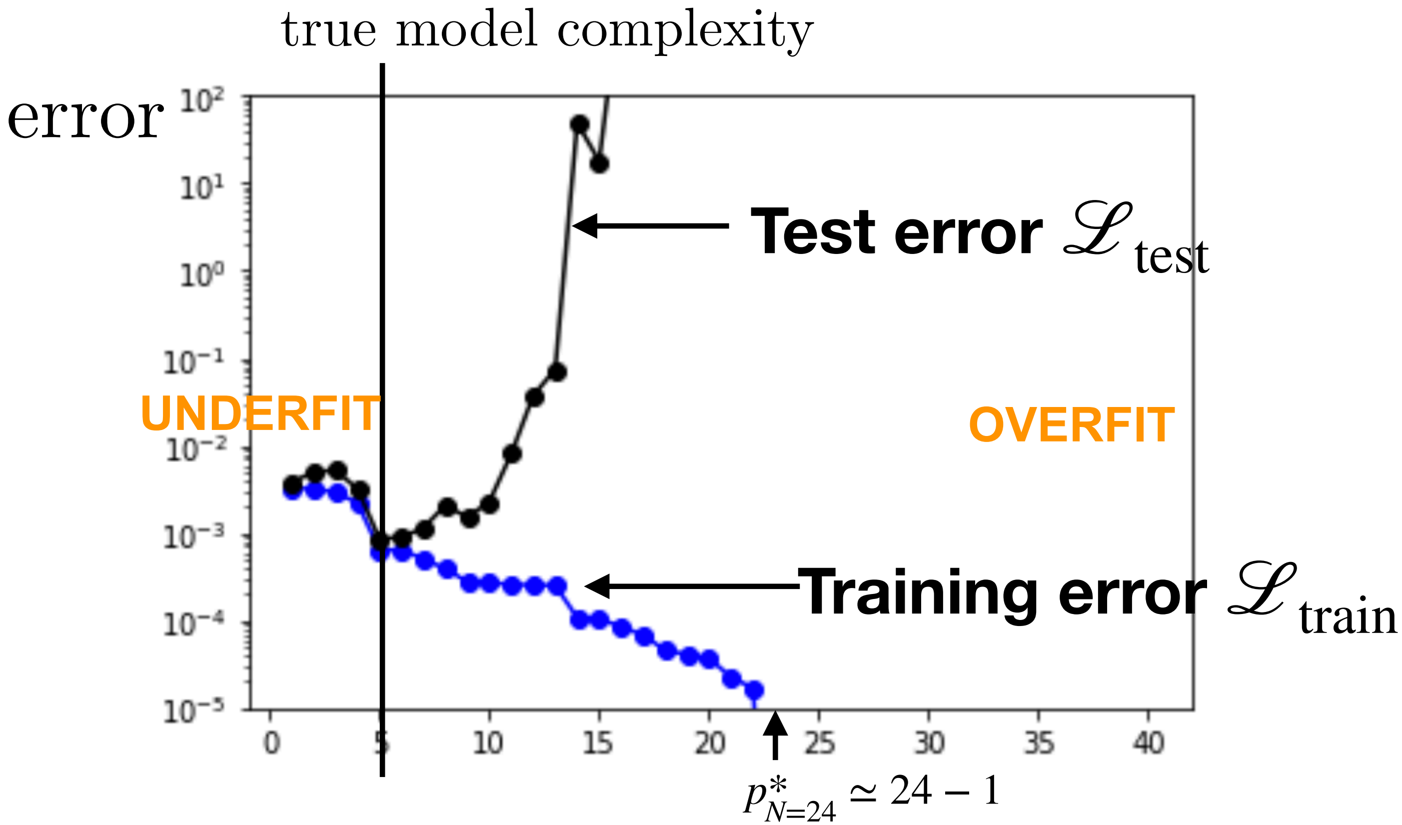
(Conceptual) bias variance tradeoff





- When model complexity is high (higher than the optimal predictor $\eta(x)$)
  - Bias of our predictor, $\left(\eta(x) - \mathbb{E}_{\mathcal{D}}[\hat{f}_{\mathcal{D}}(x)]\right)^2$, is small
  - Variance of our predictor, $\mathbb{E}_{\mathcal{D}}\left[\left(\mathbb{E}_{\mathcal{D}}[\hat{f}_{\mathcal{D}}(x)] - \hat{f}_{\mathcal{D}}(x)\right)^2\right]$, is large
  - If we have more samples, then
    - Bias
    - Variance
    - Because Variance is dominating, overall test error

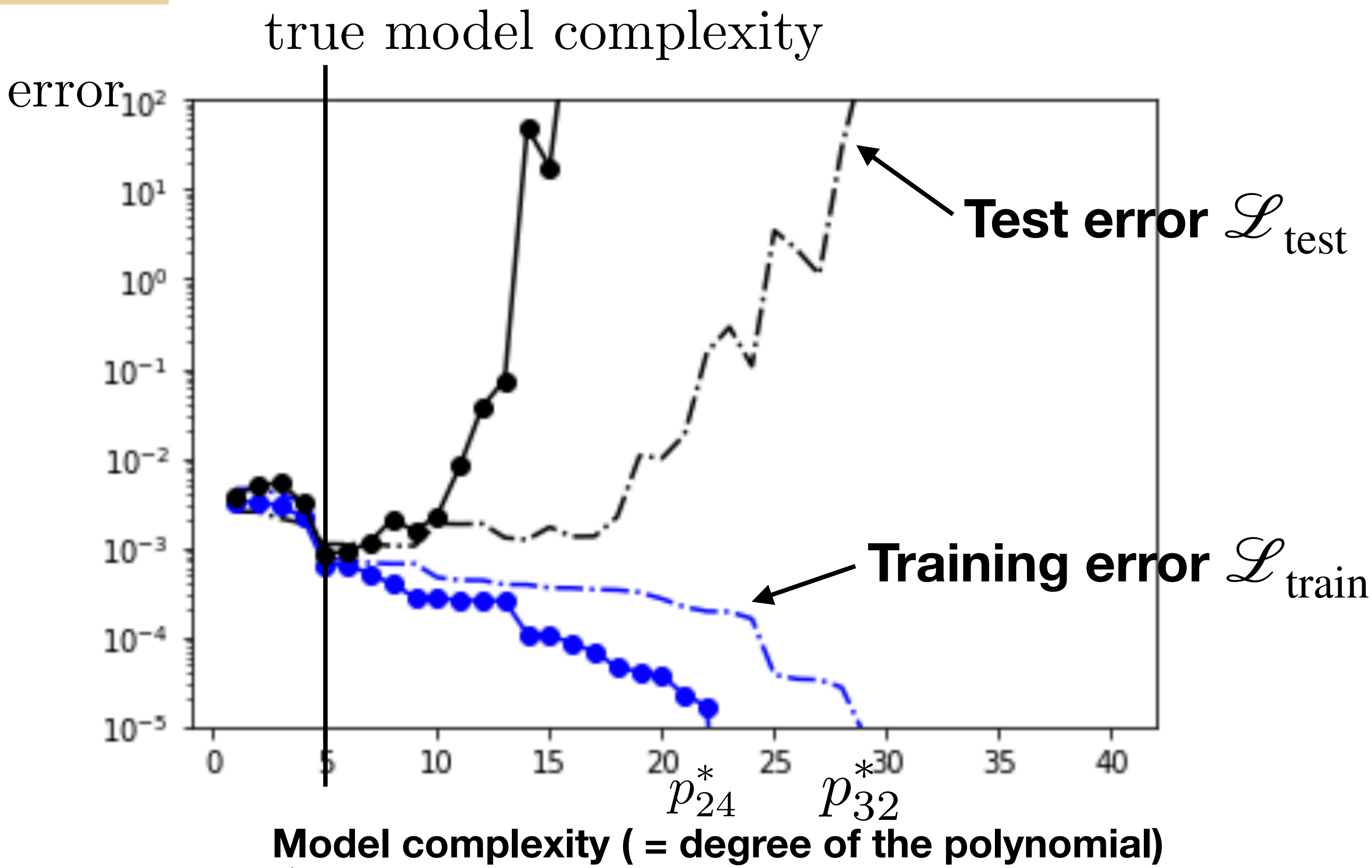
- let us first fix sample size ***N=30***, collect one dataset of size N i.i.d. from a distribution, and fix one training set S_{train} and test set S_{test} via 80/20 split
- then we run multiple validations and plot the computed MSEs for all values of ***p*** that we are interested in



Model complexity (= degree of the polynomial)

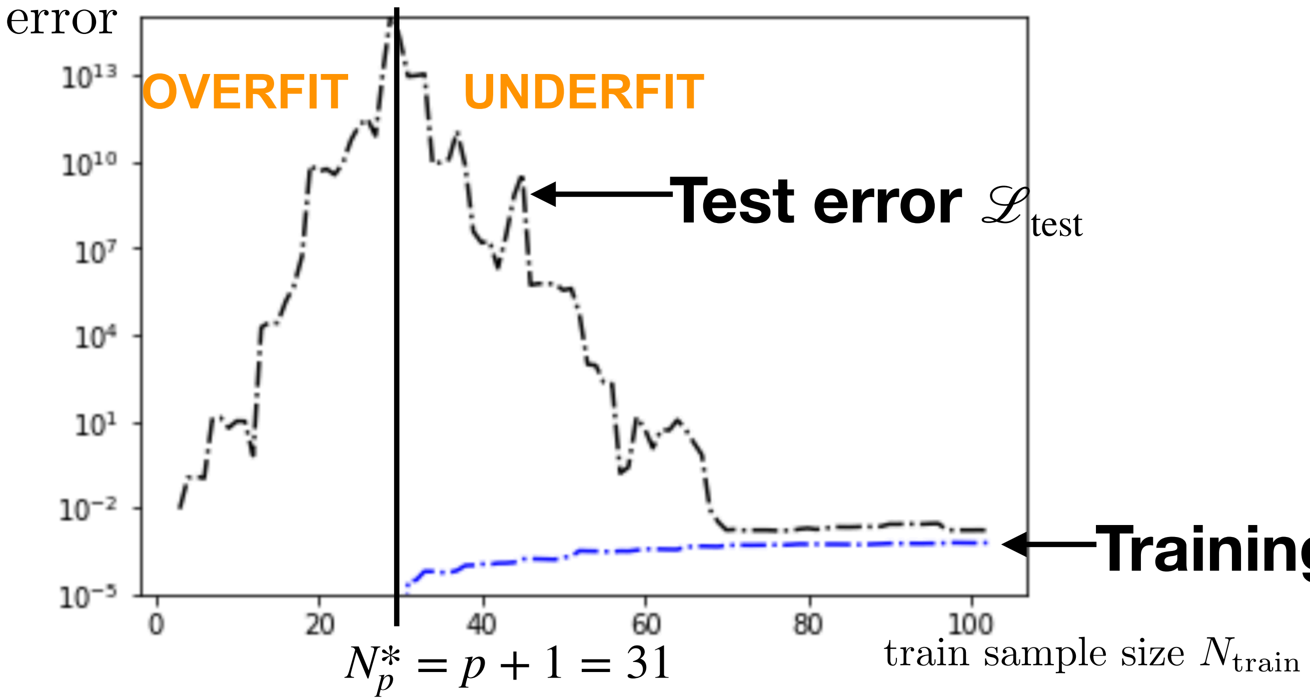
- Given sample size N there is a threshold, p_N^*, where training error is zero
- Training error is **always** monotonically non-increasing
- Test error has a trend of going down and then up, but fluctuates

- let us now repeat the process changing the sample size to **N=40** , and see how the curves change



- The threshold, p^*_N, moves right
- Training error tends to increase, because more points need to fit
- Test error tends to decrease, because Variance decreases

- let us now fix predictor model complexity ***p=30***, collect multiple datasets by starting with 3 samples and adding one sample at a time to the training set, but keeping a large enough test set fixed
- then we plot the computed MSEs for all values of train sample size ***Ntrain*** that we are interested in



- There is a threshold, N_p^*, below which training error is zero (extreme overfit)
- Below this threshold, test error is meaningless, as we are overfitting and there are multiple predictors with zero training error some of which have very large test error
- Test error tends to decrease
- Training error tends to increase

lecture2_polynomialfit.ipynb

Bias-variance tradeoff for linear models

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

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

$$\widehat{w}_{\text{MLE}} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y} =$$

$$=$$

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

$$\hat{f}_{\mathcal{D}}(x) = x^T \widehat{w}_{\text{MLE}} =$$

Bias-variance tradeoff for linear models

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

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

$$\widehat{w}_{\text{MLE}} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T(\mathbf{X}w^* + \epsilon)$$

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

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

$$\hat{f}_{\mathcal{D}}(x) = x^T \widehat{w}_{\text{MLE}} = x^T w^* + x^T(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\epsilon$$

- Irreducible error: $\mathbb{E}_{X,Y}[(Y - \eta(x))^2 \mid X = x] =$
- Bias squared: $\left(\eta(x) - \mathbb{E}_{\mathcal{D}}[\hat{f}_{\mathcal{D}}(x)]\right)^2 =$
  (is independent of the sample size!)

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$$\widehat{w}_{\text{MLE}} = w^* + (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\epsilon$$

$$\eta(x) = x^T w^*$$

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

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

Bias-variance tradeoff for linear models

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

$$\widehat{w}_{\text{MLE}} = w^* + (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\epsilon$$

$$\eta(x) = x^T w^*$$

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

- Variance: $\mathbb{E}_{\mathcal{D}}\Big[\,\big(\hat{f}_{\mathcal{D}}(x) - \mathbb{E}_{\mathcal{D}}[\hat{f}_{\mathcal{D}}(x)]\,\big)^2\,\Big] = \mathbb{E}_{\mathcal{D}}[x^T(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\epsilon\epsilon^T\mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}x]$

$$= \sigma^2\,\mathbb{E}_{\mathcal{D}}[x^T(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}x]$$

$$= \sigma^2\,x^T\mathbb{E}_{\mathcal{D}}[(\mathbf{X}^T\mathbf{X})^{-1}]x$$

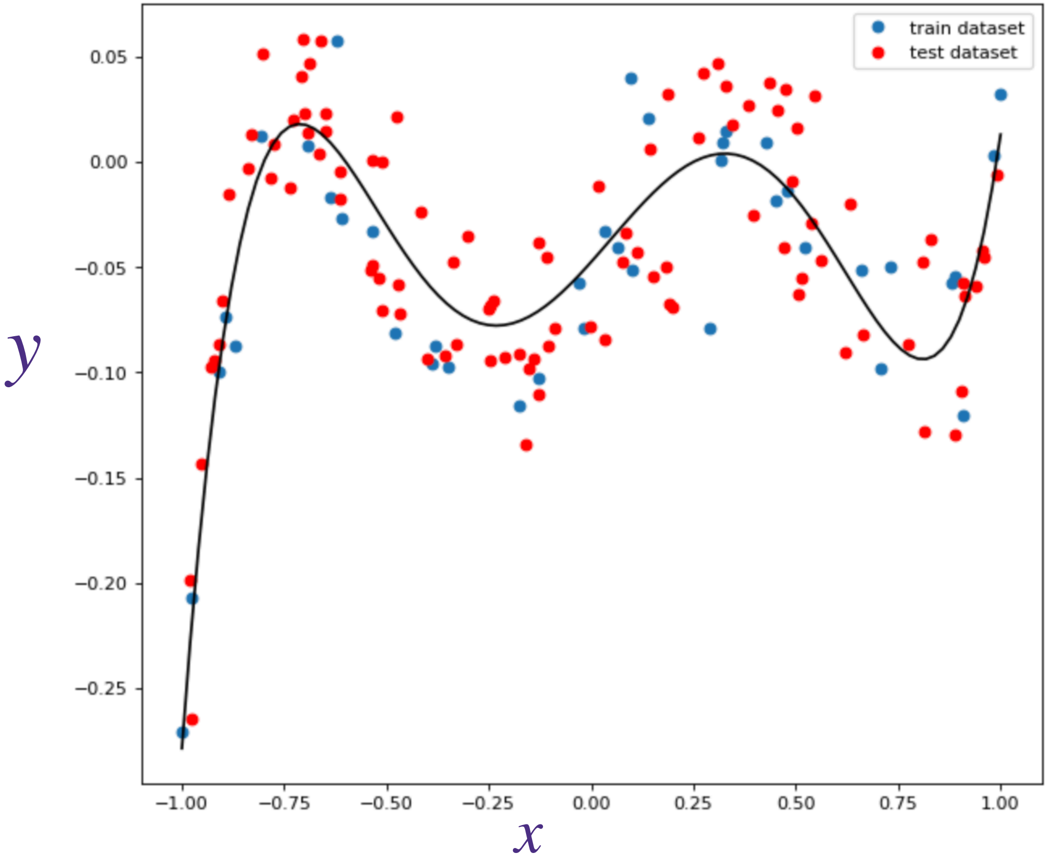
- To analyze this, let's assume that $X_i \sim \mathcal{N}(0,\mathbf{I})$ and number of samples, n, is large enough such that $\mathbf{X}^T\mathbf{X} = n\mathbf{I}$ with high probability and $\mathbb{E}[(\mathbf{X}^T\mathbf{X})^{-1}] \simeq \frac{1}{n}\mathbf{I}$, then
  - Variance is $\frac{\sigma^2 x^T x}{n}$, and decreases with increasing sample size n

Regularization

Recap: bias-variance tradeoff

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

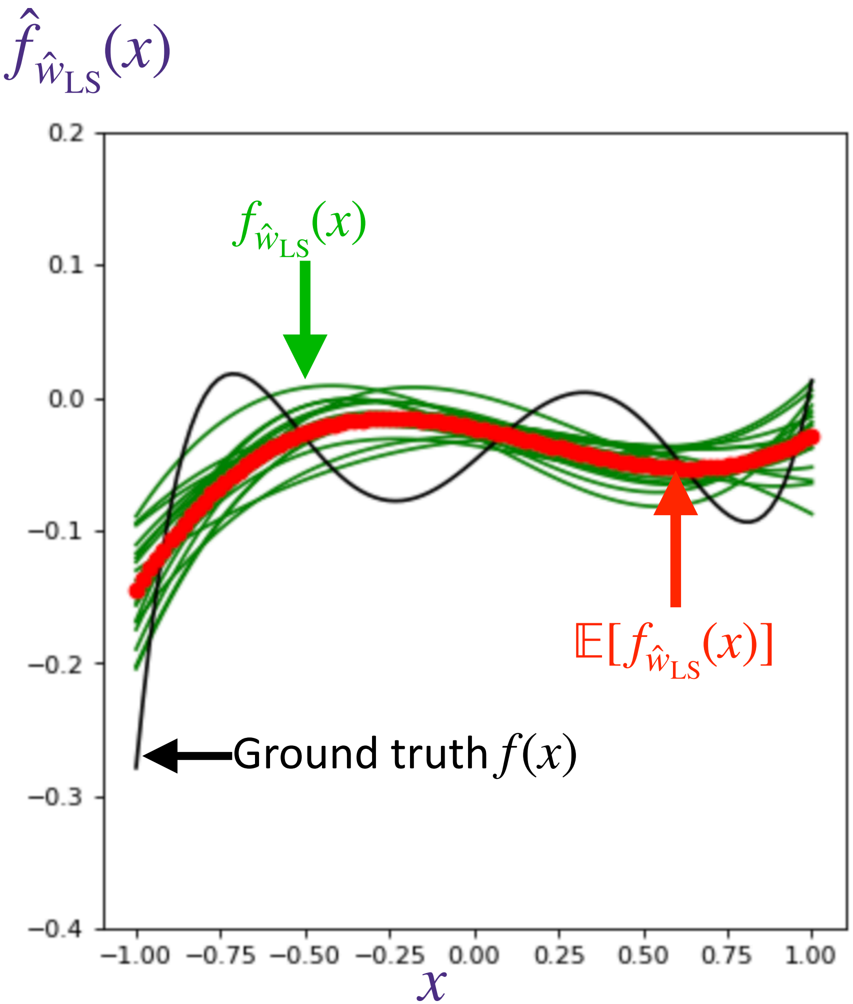
$$f_w(x_i) = b* + w_1^* x_i + w_2^*(x_i)^2 + w_3^*(x_i)^3 + w_4^*(x_i)^4 + w_5^*(x_i)^5$$



This is a linear model with features
$h(x_i) = (x_i, (x_i)^2, (x_i)^3, (x_i)^4, (x_i)^5)$

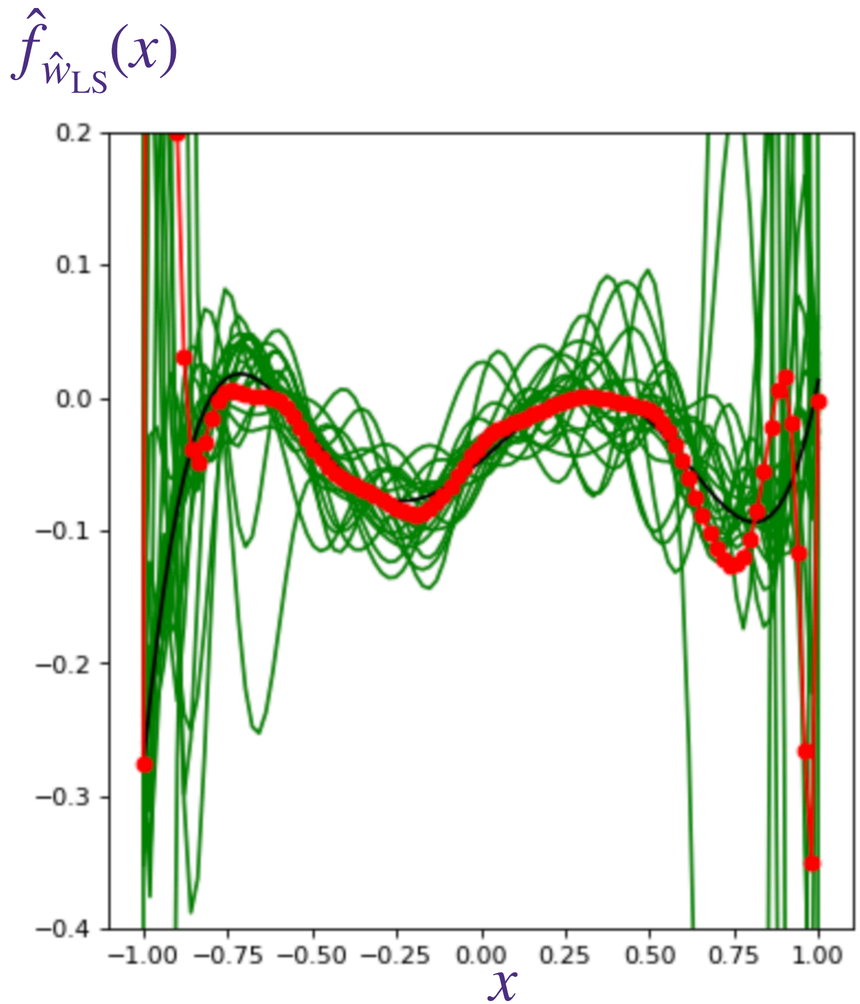
Recap: bias-variance tradeoff

With degree-3 polynomials, we underfit




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

With degree-20 polynomials, we overfit




```
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

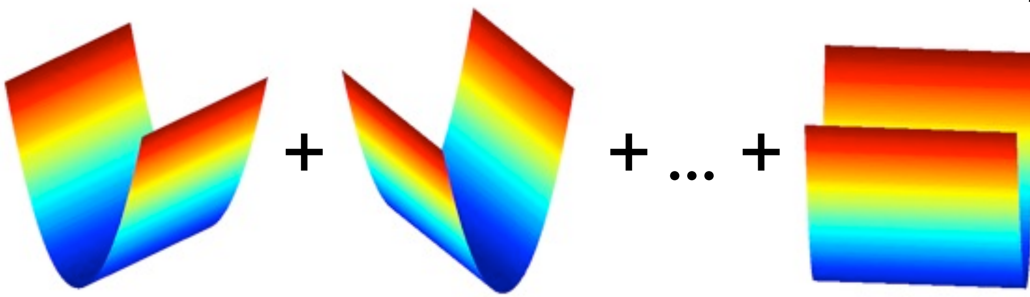
- In **Ridge Regression,** we use a regularizer $||w||_2^2$ to measure and control the sensitivity of the predictor
- And optimize for small loss and small sensitivity, by adding a **regularizer** in the objective (assume no offset for now)

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

Ridge Regression

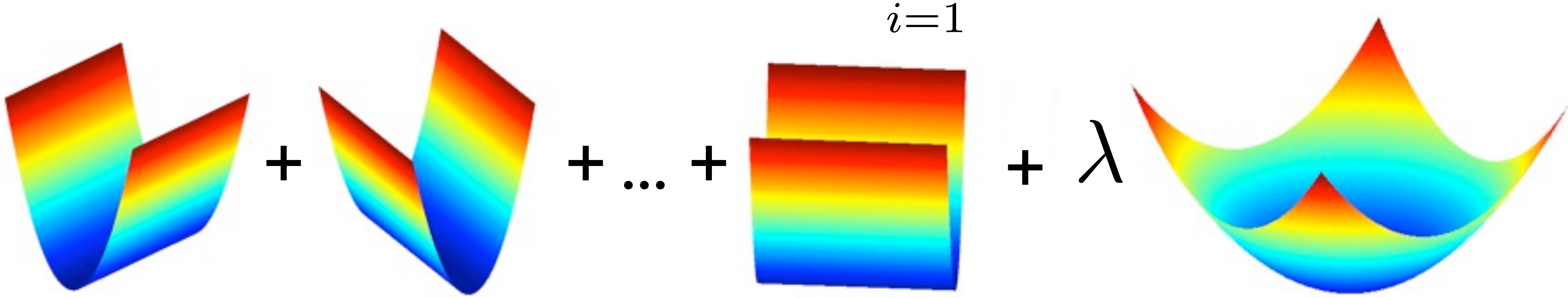
- (Original) Least squares objective:

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



- Ridge Regression objective:

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



Minimizing the Ridge Regression Objective

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

Shrinkage Properties

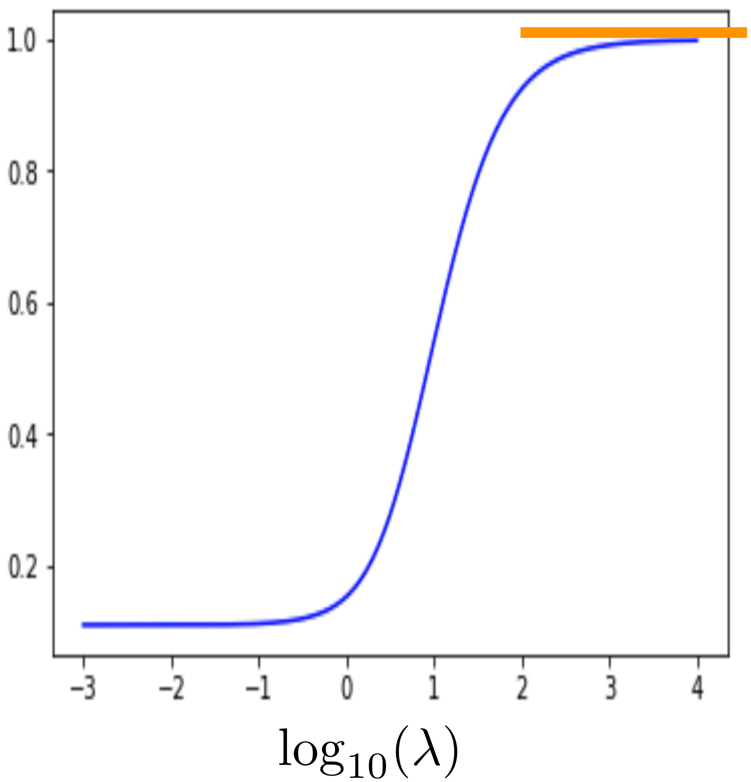
$$\widehat{w}_{ridge} = \arg\min_{w} \sum_{i=1}^{n} \left(y_i - x_i^T w\right)^2 + \lambda ||w||_2^2$$

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

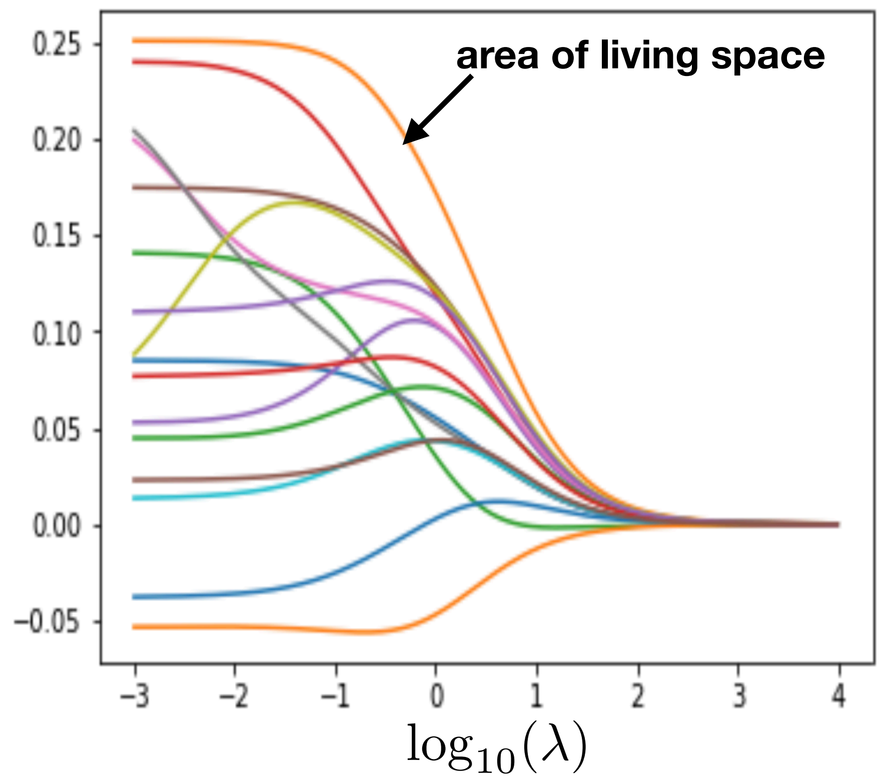
- When $\lambda = 0$, this gives the least squares model
- This defines a family of models hyper-parametrized by λ
- Large λ means more regularization and simpler model
- Small λ means less regularization and more complex model

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

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

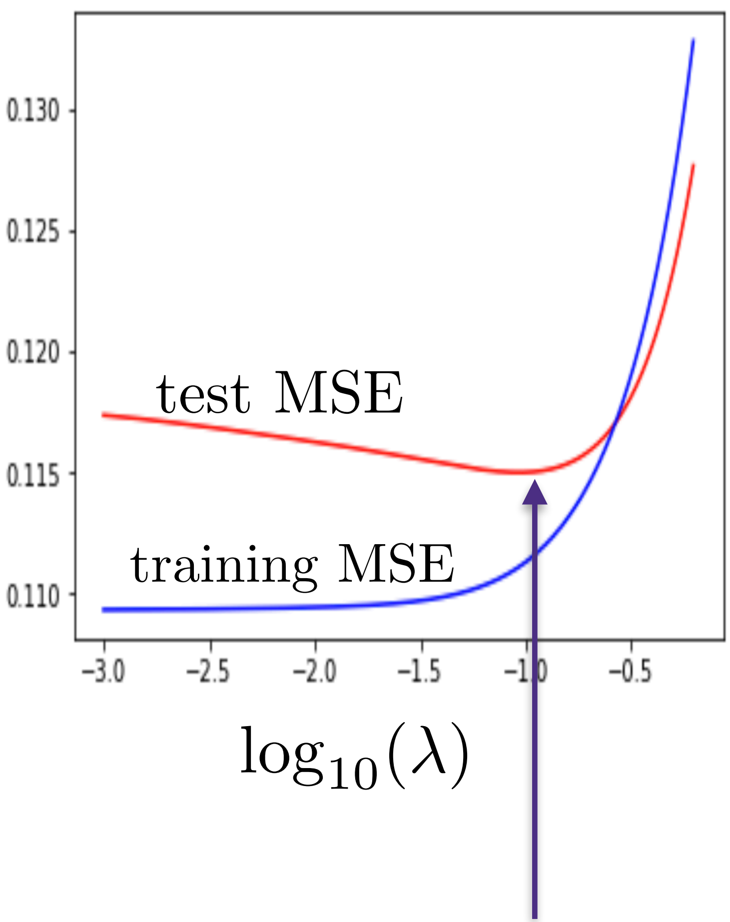


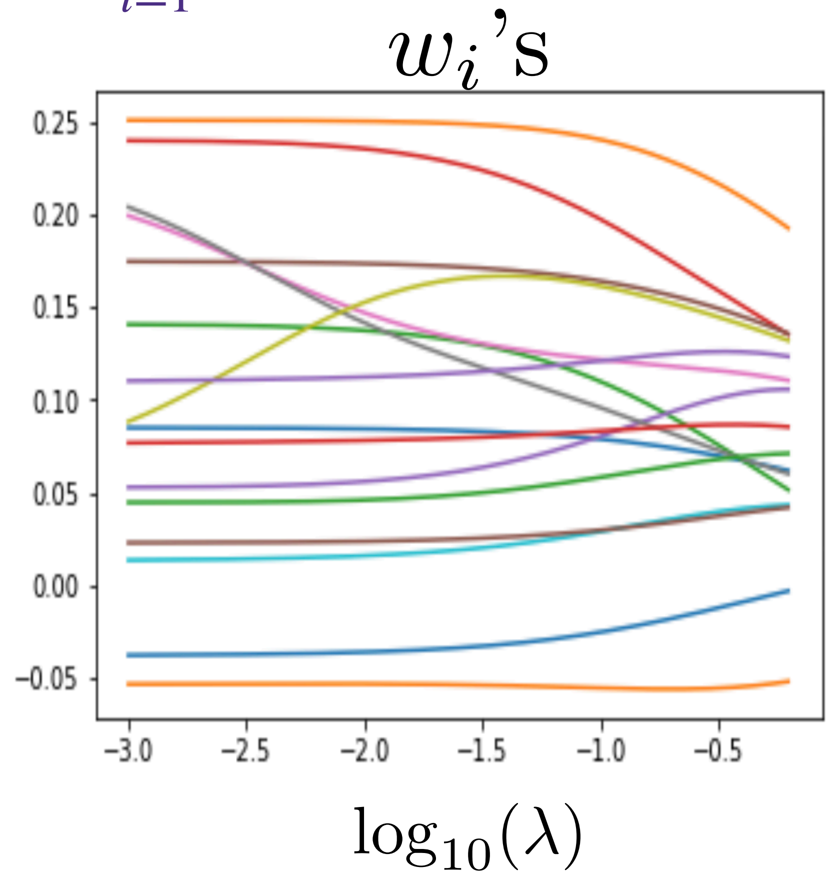
w_i's



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





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

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

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

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

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