Lecture 4: Cross validation and Bias-Variance Tradeoff

- explaining test error using theoretical analysis

Cross-validation

Leave-one-out Cross Validation and k-fold Cross Validation

LOO cross validation

Leave-one-out

LOO Cross validation

(x_1, y_1) . . . . . . (x_n, y_n) Data

Split 1 … i … split n

(x_1,y_1) Validation, $D/1$ Train

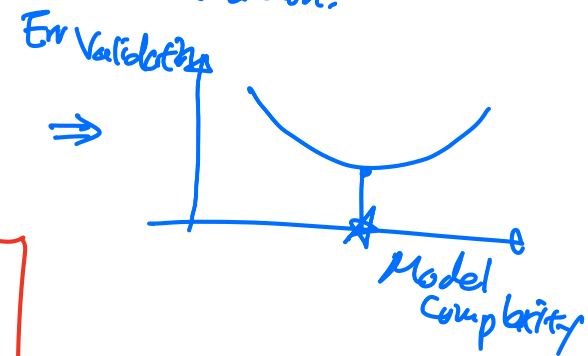
(x_i, y_i) Validation, D/i Train

D/n Train, (x_n, y_n) Validation.

trained model $f_{D/i} : \mathbb{R}^d \to \mathbb{R}$

Repor $\text{Error}_{\text{validation}} \triangleq (y_i - f_{D/i}(x_i))^2 \Rightarrow$

$\triangleq$ denotes definition



Pro: Each $f_{D/i}$ uses $n-1$ samples

↳ performance close to f_D

Con: n models trained

$\Rightarrow$ Very slow

k-fold Cross validation

$\shortparallel$
3

D_1 | D_2 | D_3

Split 1 … split i … split K

D_1 Val, D_2 D_3 Train

Train f_{D/D_2}

Report $\text{Error}_{\text{validation}} \triangleq \sum_{(x,y)\in D_2} (y - f_{D/D_2}(x))^2$

Pro: only K models Trained ($K \overset{\shortparallel}{=} 5$)

$\Rightarrow$ much faster.

Con: f_{D/D_i} uses $(1-\frac{1}{K})n$ samples

might not $\Leftarrow$ be representative of f_D

LOO cross validation is (almost) unbiased estimate!

> When computing **LOOCV error, we only use $n - 1$ data points**
  - So it's not estimate of true error of learning with n data points
  - learning with less data typically gives worse answer $\Rightarrow$ Usually validation error is **pessimistic**
  - but that bias is small, since $n - 1$ is very close to n

in the validation error. $\mathbb{E}[(\hat{f}_D(x)-y)^2] \approx \mathbb{E}[(\hat{f}_{D/i}(x)-y)^2]$

> LOO is almost unbiased and it is common to use LOO error for **model class** selection
  - E.g., picking degree is a model class selection since, for example, a set of all degree-5 polynomial functions is a **model class**

> But, LOOCV requires a lot of computational time
  - Suppose you have $\underbrace{100{,}000}_{=n}$ data points
  - You implemented a great version of your learning algorithm that 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 $f_{D\backslash D_i}$ using data point not in D_i
  – Estimate error of $\boxed{f_{D\backslash D_i}}$ on validation set D_i:

1	2	3	4	5
Train	Train	Validation	Train	Train

f_{D/D_1} f_{D/D_2} f_{D/D_3} . . f_{D/D_k}

$\underbrace{\mathrm{error}_{D_i}(f_{D/D_i}) \;\; . \;\; . \;\; . \;\; .}$

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

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

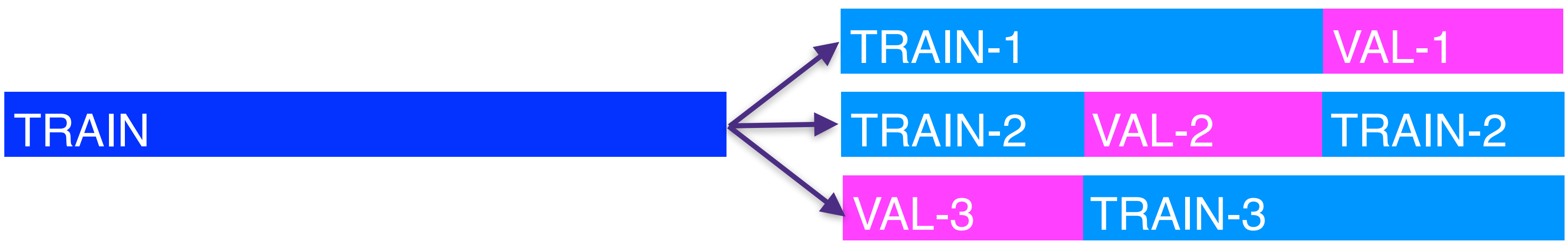
$$\mathrm{error}_{k\text{-fold}} = \frac{1}{k}\sum_{i=1}^{k}\mathrm{error}_{D_i}(f_{D\setminus D_i})$$

> k-fold cross validation properties:
  – Much faster to compute than LOO ← only K models trained
  – More (pessimistically) biased – using much less data, only $\frac{k-1}{k}n = n - \frac{n}{k}$: k-fold
    $n-1$: LOO
  – 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 degree



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

- **Never train or choose hyper-parameters based on the test data**

Example 1

- 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
- 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 entire dataset:

50 indices j that have largest $$\frac{\left|\sum_{i=1}^n x_{i,j} y_i\right|}{\sqrt{\sum_{i=1}^n x_{i,j}^2}}$$

> After picking our 50 features, we then break data into train and test dataset.

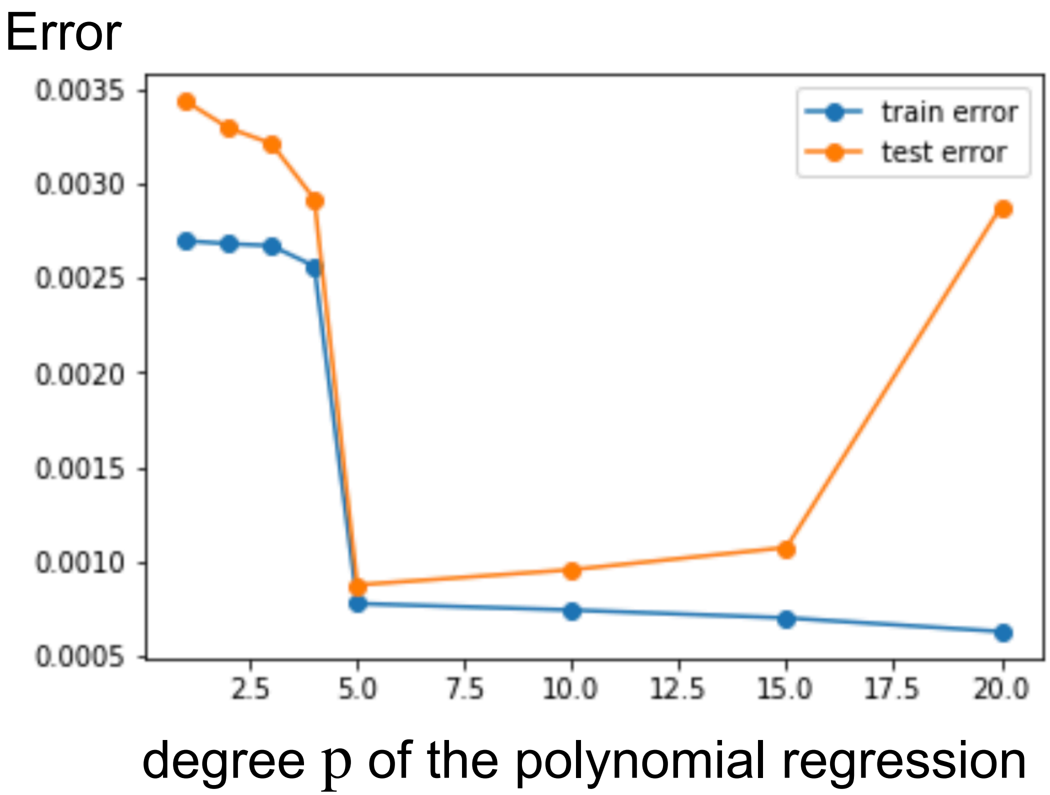
> We train linear regression on these selected features on the training set. We compute the test error and report it

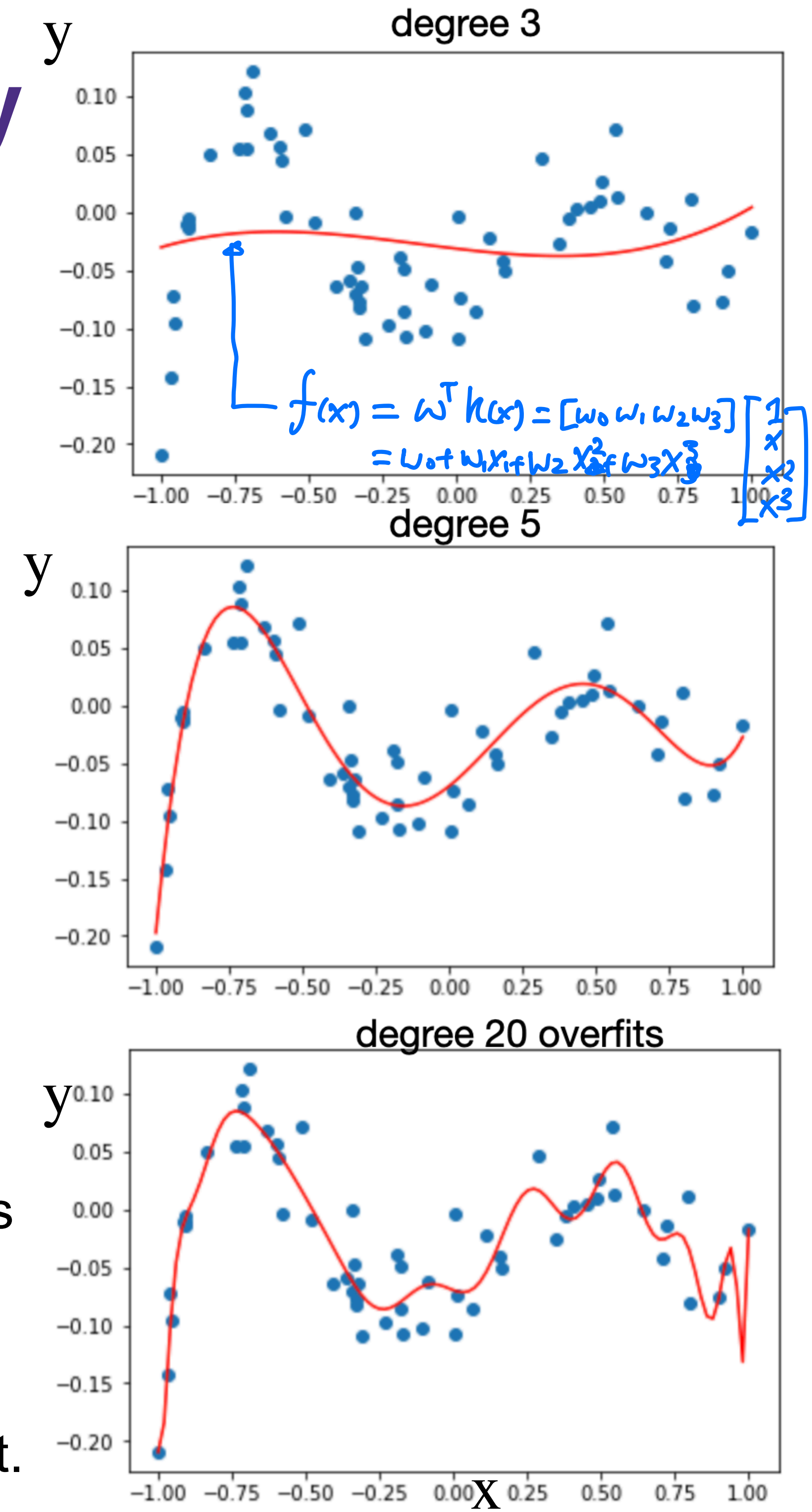
> What's wrong with this procedure?

Bias-Variance Tradeoff

- explaining test error using theoretical analysis

Train/test error vs. complexity





$$f(x) = w^T h(x) = [w_0\ w_1\ w_2\ w_3] \begin{bmatrix} 1 \\ x \\ x^2 \\ x^3 \end{bmatrix} = w_0 + w_1 x + w_2 x^2 + w_3 x^3$$

- **Test error** has a U shape as we change the **model complexity**
- We want to theoretically explain and understand this important phenomenon in machine learning
- This is called **bias-variance tradeoff**
- Let's start with what an **optimal predictor** can achieve, and how practical predictor deviates from it.

Optimal prediction

Typical notation for this lecture:
X denotes a random variable
x denotes a deterministic instance

- Suppose data is generated from a statistical model $(\mathrm{X}, \mathrm{Y}) \sim \mathrm{P}_{\mathrm{X},\mathrm{Y}}$
  - and assume we know $\mathrm{P}_{\mathrm{X},\mathrm{Y}}$ (just for now to explain statistical learning)
- Then **learning** is to find a predictor $\eta : \mathbb{R}^d \to \mathbb{R}$ that minimizes
  $\mathrm{X} \mapsto \eta(\mathrm{X})$
  True Error
  =
  - the expected error $\mathbb{E}_{(\mathrm{X},\mathrm{Y})\sim \mathrm{P}_{\mathrm{X},\mathrm{Y}}}[(\underbrace{\mathrm{Y} - \eta(\mathrm{X})}_{\text{error}})^2]$
  - think of this random (X, Y) as a new sample you will encounter when you deployed your learned model, and we care about its average performance

Optimal prediction

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- Suppose data is generated from a statistical model $(X, Y) \sim P_{X,Y}$
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- Then **learning** is to find a predictor $\eta : \mathbb{R}^d \to \mathbb{R}$ that minimizes
  - the expected error $\mathbb{E}_{(X,Y)\sim P_{X,Y}}[(Y - \eta(X))^2]$
  - think of this random (X, Y) as a new sample you will encounter when you deployed your learned model, and we care about its average performance
- Since, we do not assume anything about the function $\eta(x)$, it can take any value for each $X = x$,

  in order to derive "optimal prediction"
  - for example $\eta(1.0)$ has nothing to do with $\eta(1.1)$
- hence we can try to find the optimal prediction $\eta(x)$ for each value of $X = x$ separately

Optimal prediction

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  - think of this random (X, Y) as a new sample you will encounter when you deployed your learned model, and we care about its average performance
- Since, we do not assume anything about the function $\eta(x)$, it can take any value for each $X = x$, hence we can try to find the optimal prediction $\eta(x)$ for each value of $X = x$ separately
  - $$\mathbb{E}_{(X,Y)\sim P_{X,Y}}[(Y - \eta(X))^2] = \mathbb{E}_{X\sim P_X}\boxed{\mathbb{E}_{Y\sim P_{Y|X}}[(Y - \eta(x))^2 \,|\, X = x]}$$
$$= \int \mathbb{E}_{Y\sim P_{Y|X}}[(Y - \eta(x))^2 \,|\, X = x]\, \underline{P_X(x)\, dx}$$

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

separately derive optimal $\eta(x)$ for each x

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

Optimal prediction

- To find an optimal predictor, we can solve the optimization for each $X = x$ separately
  - $\eta(x) = \arg\min_{a_x \in \mathbb{R}} \mathbb{E}_{Y \sim P_{Y|X}}[(Y - a_x)^2 \mid X = x]$
- The optimal solution is $\eta(x) = \mathbb{E}_{Y \sim P_{Y|X}}[Y \mid X = x]$, which is the best prediction in ℓ_2-loss/Mean Squared Error
- Claim: $\mathbb{E}_{Y \sim P_{Y|X}}[Y \mid X = x] = \arg\min_{a_x \in \mathbb{R}} \underbrace{\mathbb{E}_{Y \sim P_{Y|X}}[(Y - a_x)^2 \mid X = x]}_{f(a_x)}$
- Proof: $\frac{\partial f(a_x)}{\partial a_x} = \mathbb{E}_{Y \sim P_{Y|X}}\left[\cancel{+2}(Y - a_x) \mid X = x\right] = 0$

$$\Rightarrow \mathbb{E}_{Y \sim P_{Y|X}}[Y \mid X = x] = \mathbb{E}_{P_{Y|X}}[a_x \mid X = x] = a_x$$

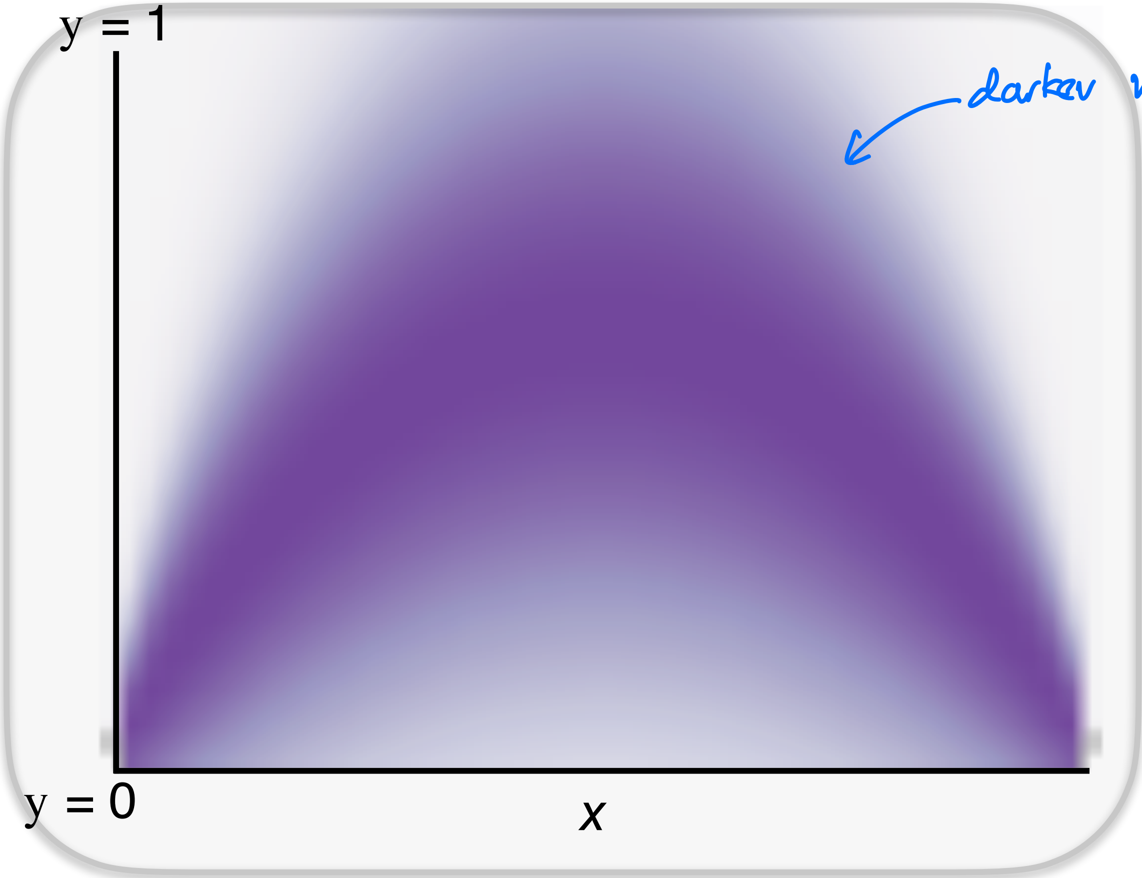
- Note that this optimal statistical estimator $\eta(x) = \mathbb{E}[Y \mid X = x]$ cannot be implemented as we do not know $P_{X,Y}$ in practice
- This is only for the purpose of conceptual understanding

Statistical Learning

= learning from samples

- Consider a joint distribution $P_{XY}(x, y)$
- Our goal is to find the optimal predictor $\eta(x)$ to minimize $\mathbb{E}_{(X,Y)\sim P_{XY}}[(Y - \eta(X))^2]$

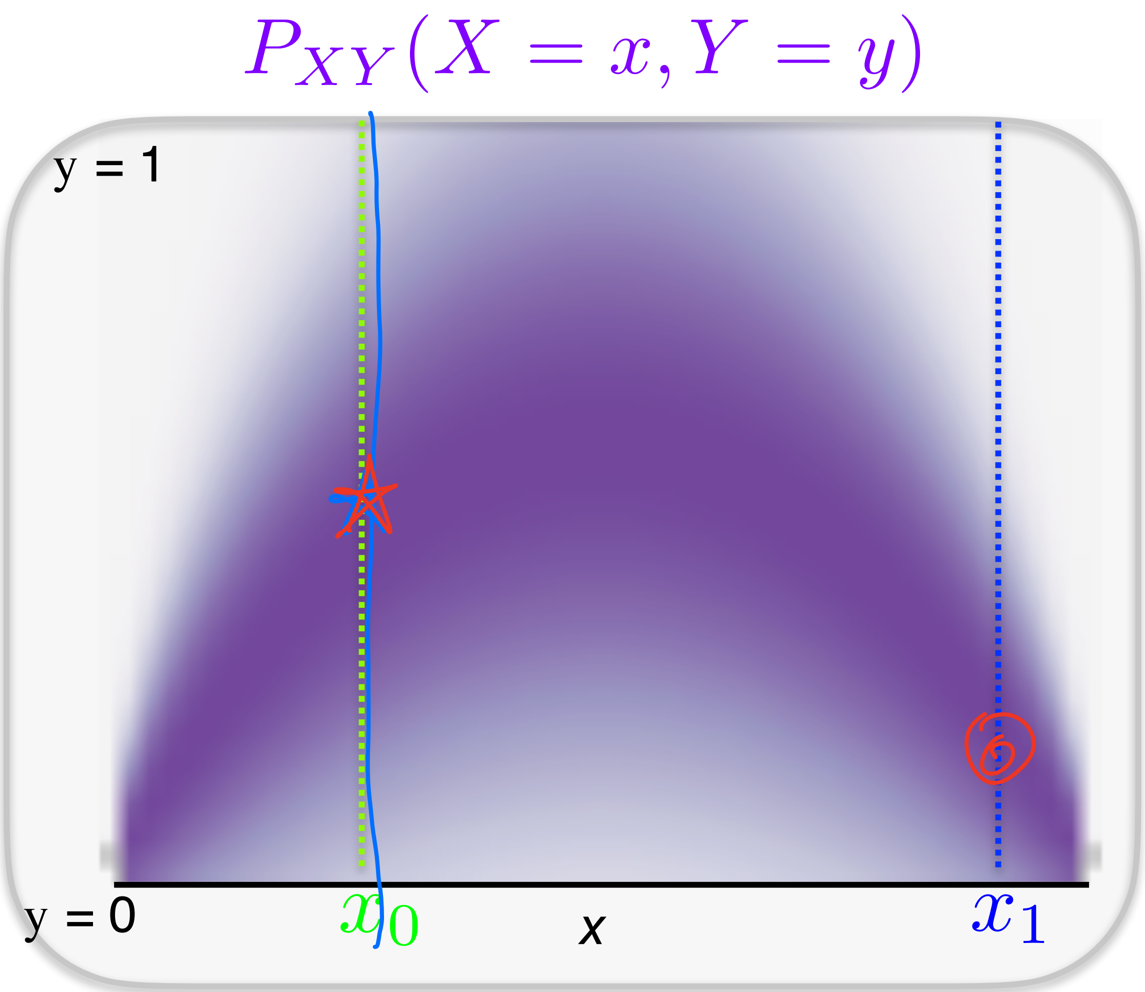
$$P_{XY}(X = x, Y = y)$$

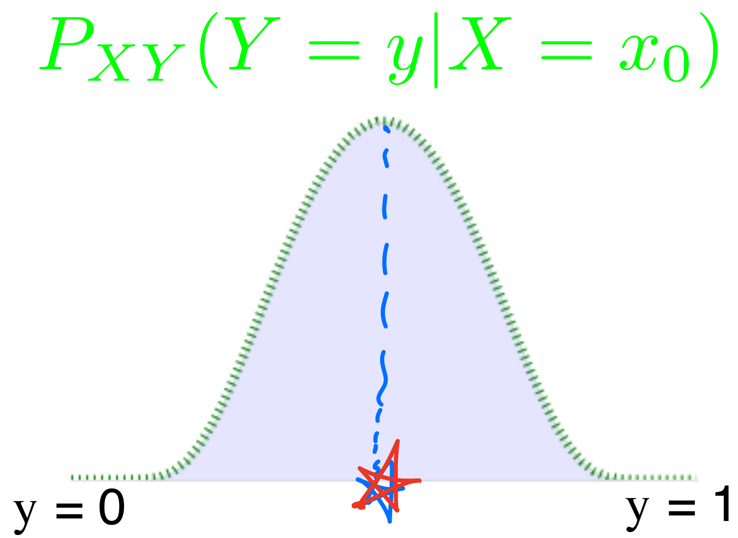


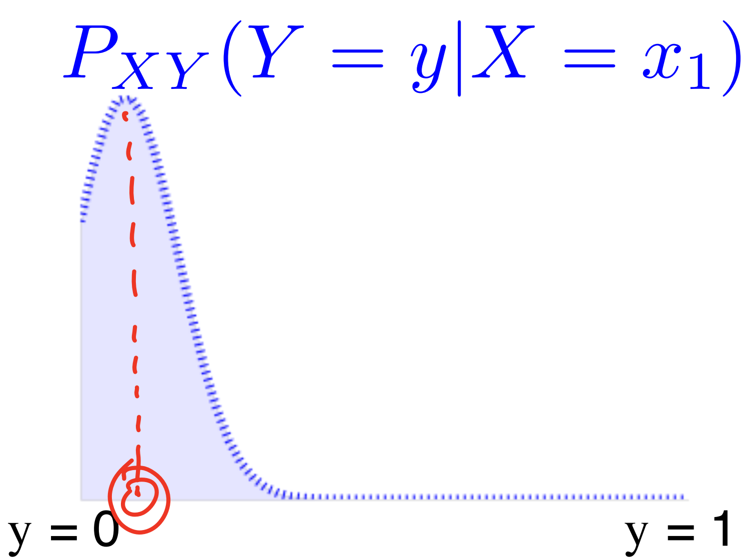
darker means $P_{XY}(x,y) \uparrow$

Statistical Learning

- The optimal predictor is given by $\eta(x) = \mathbb{E}_{P_{Y|X}}[Y \mid X = x]$



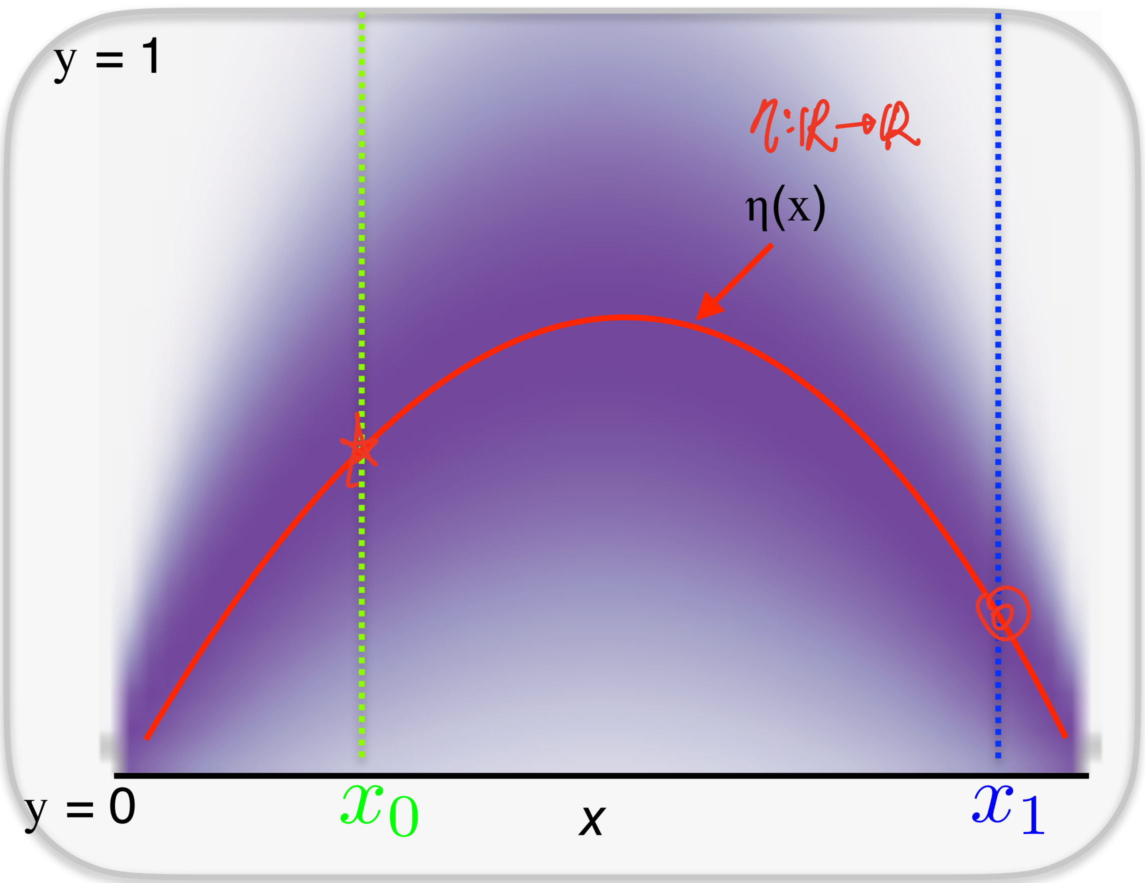




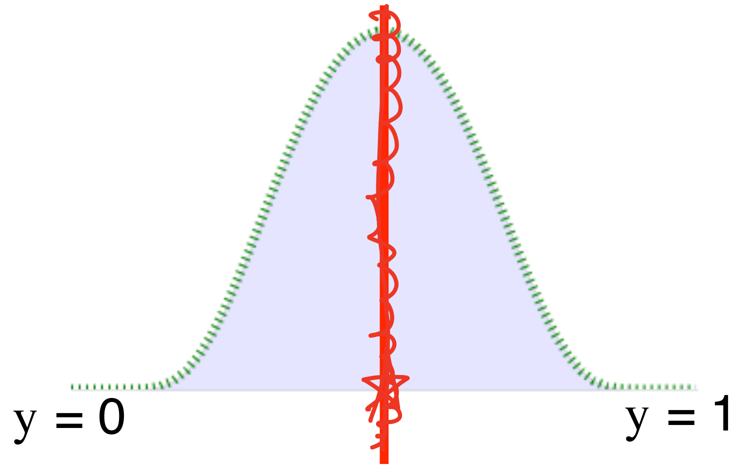
Statistical Learning

- The optimal predictor is given by $\eta(x) = \mathbb{E}_{P_{Y|X}}[Y \mid X = x]$

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

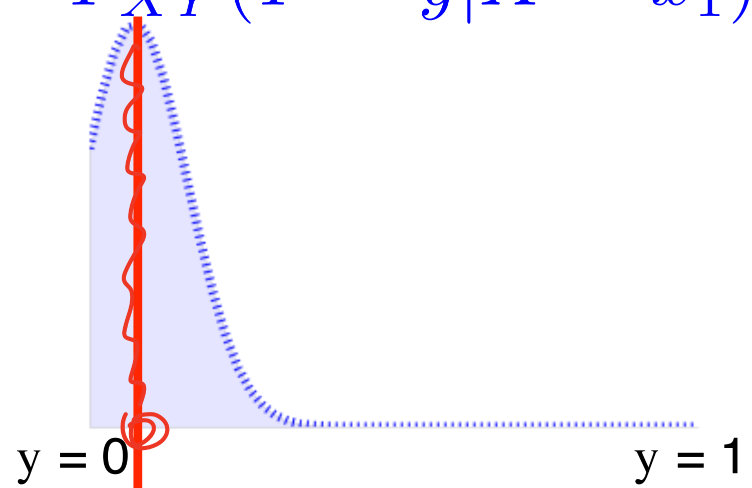


$$P_{XY}(Y = y | X = x_0)$$



$\eta(x_0) = \mathbb{E}[Y \mid X = x_0]$

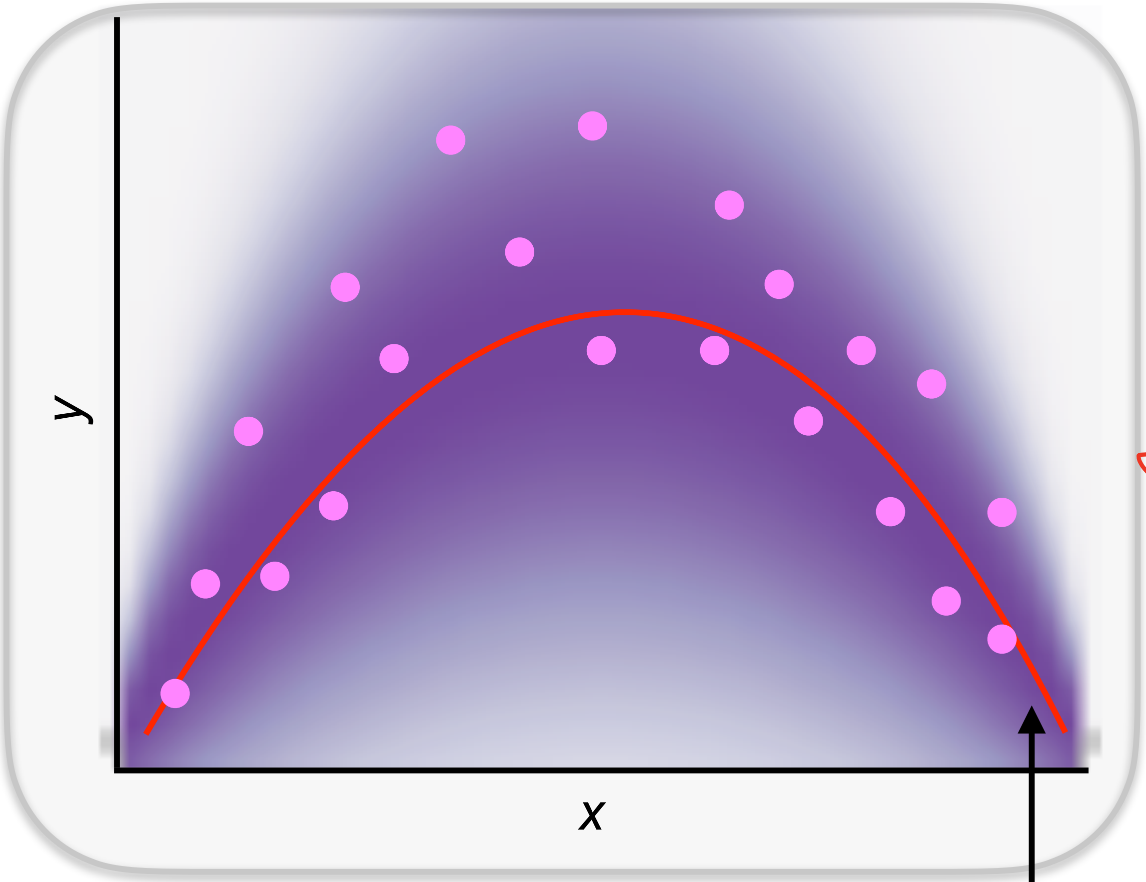
$$P_{XY}(Y = y | X = x_1)$$



$\eta(x_1) = \mathbb{E}[Y \mid X = x_1]$

Statistical Learning

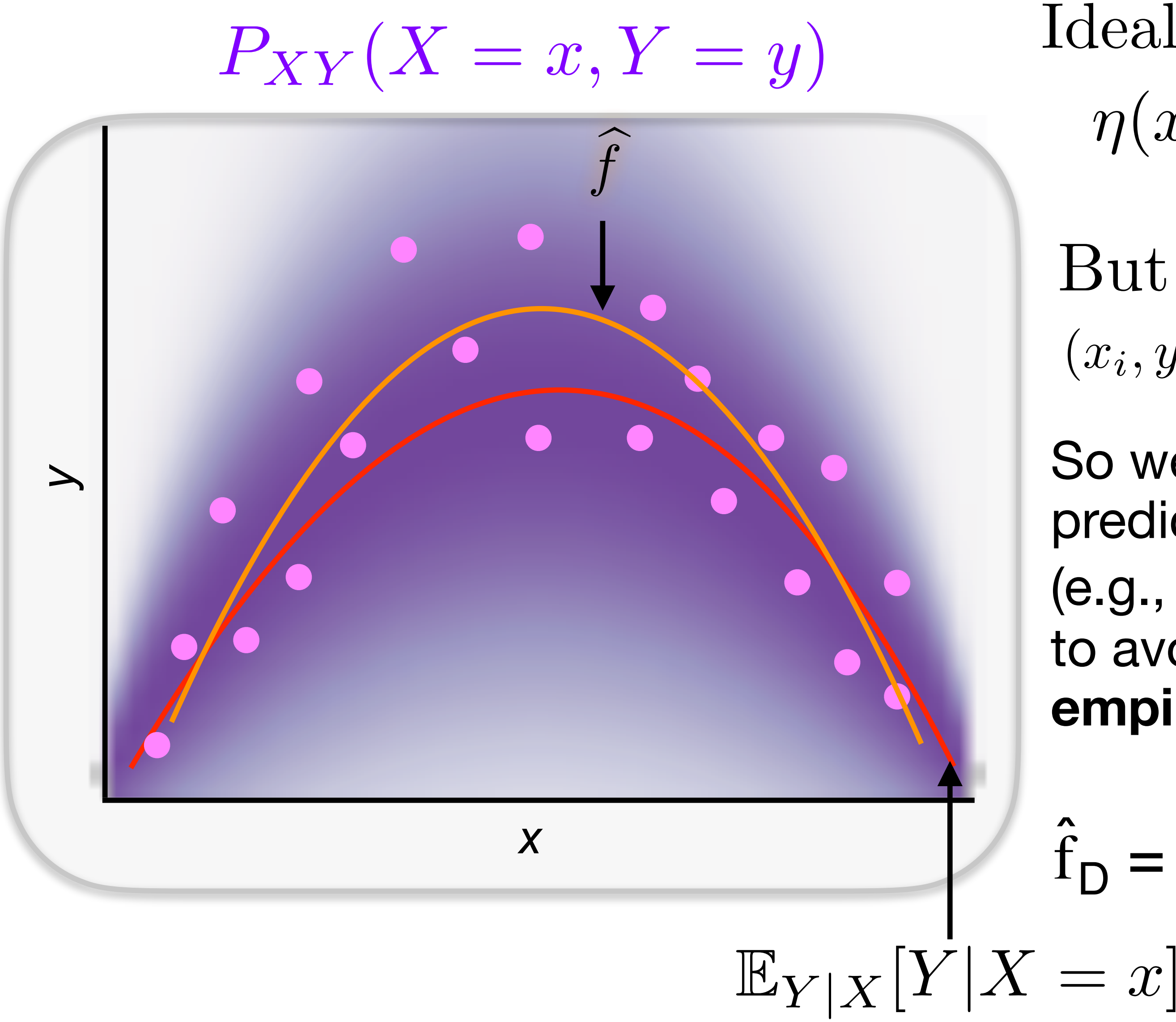
$$P_{XY}(X = x, Y = y)$$



But we do not know $P_{X,Y}$,
and so we cannot compute $\eta(x)$
We only have samples.
What can we do?

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

Statistical Learning



Ideally, we want to find:

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

But we only have samples:

$(x_i, y_i) \overset{i.i.d.}{\sim} P_{XY}$ 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 and **minimize empirical error**:

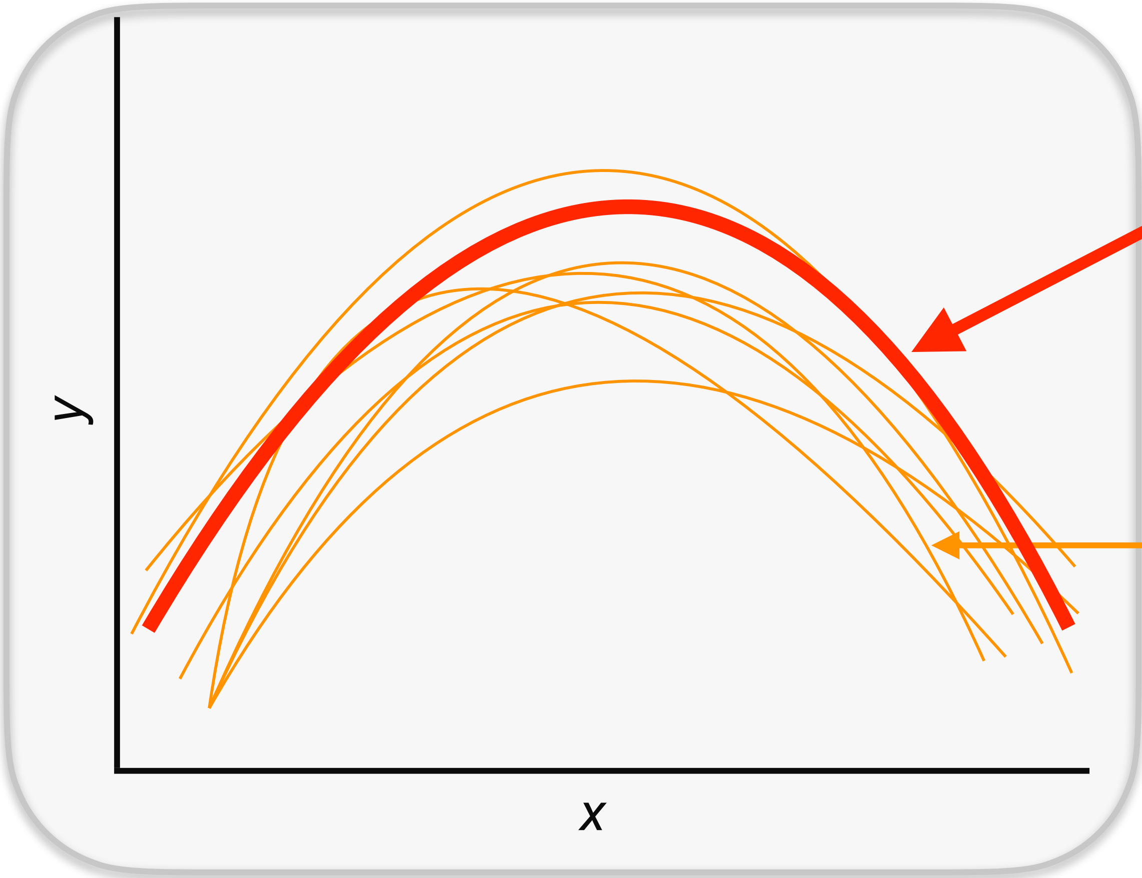
1 2

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

We care about how our predictor performs on future unseen data

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

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



Optimal predictor

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

Learned predictor

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

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

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

R.V.
= Random Variable.

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

Demo bias-variance trade-off

Exercise: Given joint distribution $(X, Y) \sim \mathcal{N}\left([\mu_X, \mu_Y], \begin{bmatrix} \Sigma_X, \Sigma_{XY} \\ \Sigma_{XY}, \Sigma_Y \end{bmatrix}\right)$,

- is $E_{X,Y}[X + Y]$ a random variable or not? $\mu_X + \mu_Y$, No
- is $E_{X|Y}[X + Y \mid Y]$ a random variable or not? $E_{X|Y}[X \mid Y] + Y$, Yes $= \mu_X + \Sigma_{XY}\Sigma_{YY}^{-1}(Y - \mu_Y)$
- is $E_{X|Y}[X + Y \mid Y = y]$ a random variable or not? $E_{X|Y}[X \mid Y = y] + y$, No.

Random (Y) deterministic. (y)

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

- 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**:

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

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

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

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

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

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

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

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

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

written compactly as

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

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

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

Bias-variance tradeoff

for zero mean A, B, indep. $\mathbb{E}[(A+B)^2]$

$= \mathbb{E}A^2 + \mathbb{E}[AB] + \mathbb{E}B^2$

$= \mathbb{E}A^2 + \overset{0}{\mathbb{E}A\,\mathbb{E}B} + \mathbb{E}B^2$

$= \mathbb{E}[A^2] + \mathbb{E}[B^2]$

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**:

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

$$= \underbrace{\mathbb{E}[(Y - \eta(x))^2]}_{\text{Irreducible Error.}} + \underbrace{\mathbb{E}[(\eta(x) - \hat{f}_{\mathcal{D}}(x))^2]}_{\text{Average Learning Error.}}$$

Variance/Randomness in Y → Irreducible Error.

= error unavoidable by even the optimal est. who knows $P_{X,Y}$

finite sample → Average Learning Error.

model class

Bias-variance tradeoff

Bias-variance tradeoff

Ideal predictor

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Learned predictor

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- **Average conditional true error**:

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

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

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

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

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

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

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

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

- **Average learning error**:

$$\mathbb{E}_{\mathscr{D}}[(\eta(x) - \hat{f}_{\mathscr{D}}(x))^2] = \mathbb{E}_{\mathscr{D}}\left[\left(\overbrace{\eta(x) - \mathbb{E}_{\mathscr{D}}[\hat{f}_{\mathscr{D}}(x)]} + \underbrace{\mathbb{E}_{\mathscr{D}}[\hat{f}_{\mathscr{D}}(x)] - \hat{f}_{\mathscr{D}}(x)}_{B,\ \mathbb{E}[B] = 0}\right)^2\right]$$

$$= \underbrace{\mathbb{E}_{D}[(\underbrace{\eta(x) - \mathbb{E}[\hat{f}(x)]}_{\text{Bias}})^2]}_{\text{Bias squared}} + \underbrace{\mathbb{E}[(\hat{f}_D(x) - \mathbb{E}_{D'}[\hat{f}_{D'}(x)])^2]}_{\text{Variance of } \hat{f}_D(x).}$$

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**:

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

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

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

biased squared **variance**

[Homework 1 Problem B2 derives similar trade-off for a specific estimator]

Bias-variance tradeoff

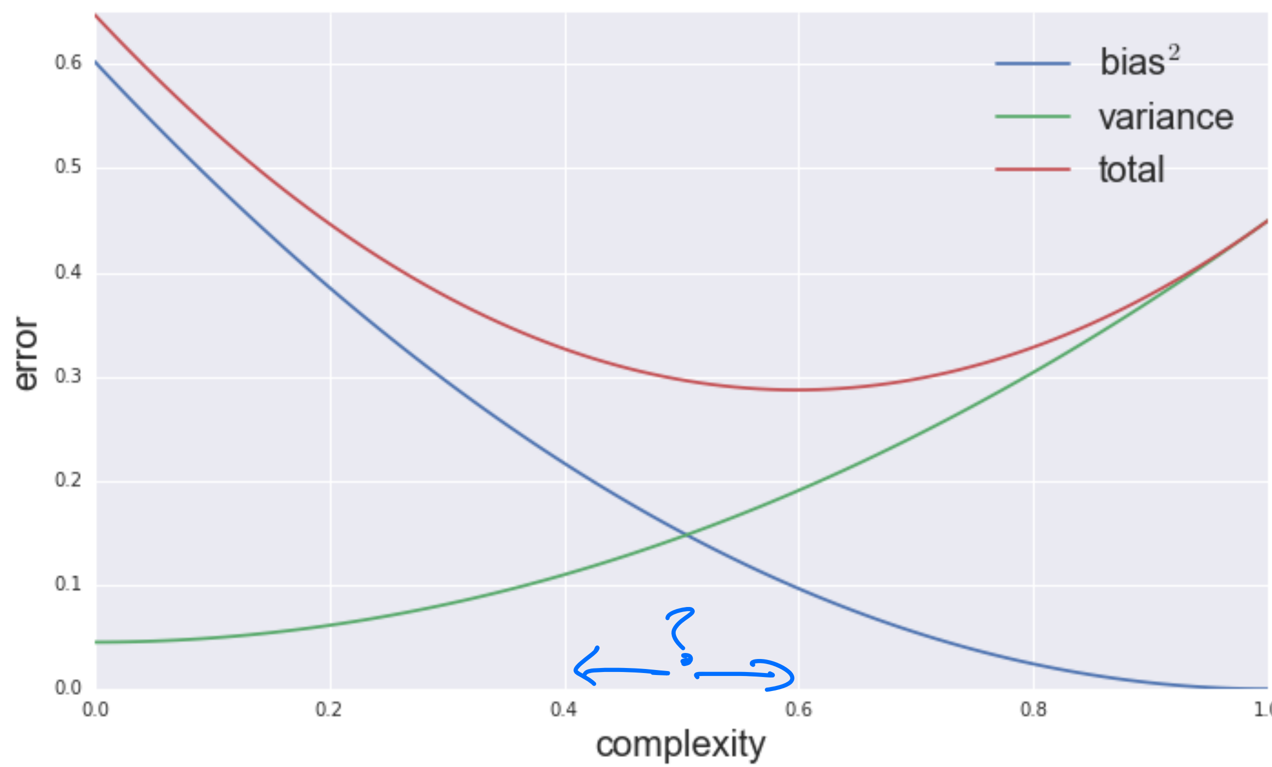
- **Average conditional true error**:

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

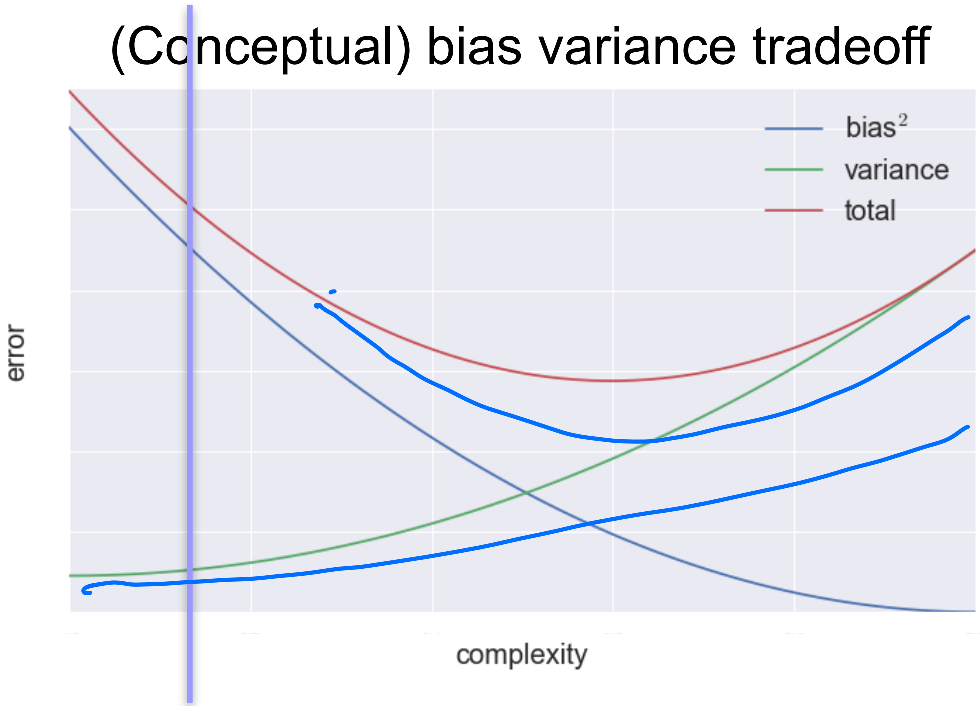
$$+ \underbrace{\eta(x) - \mathbb{E}_{\mathscr{D}}[\hat{f}_{\mathscr{D}}(x)]^2}_{\textbf{biased squared}} + \underbrace{\mathbb{E}_{\mathscr{D}}\, \mathbb{E}_{\mathscr{D}}[\hat{f}_{\mathscr{D}}(x)] - \hat{f}_{\mathscr{D}}(x)^2}_{\textbf{variance}}$$

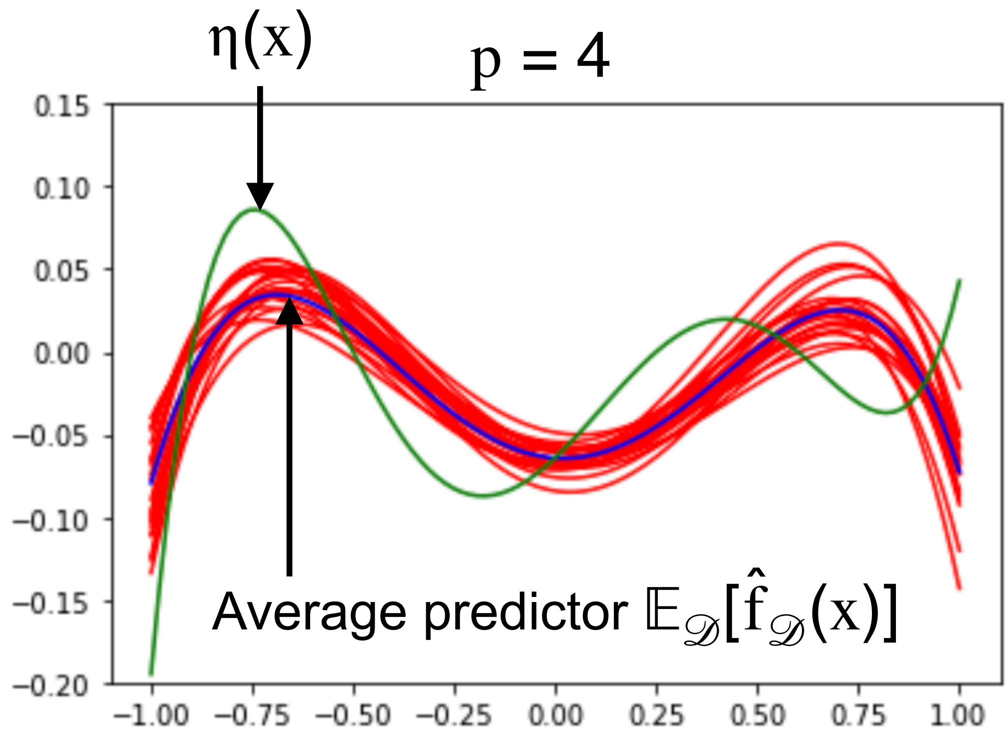
Bias squared:
measures how the predictor is mismatched with the best predictor in expectation

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



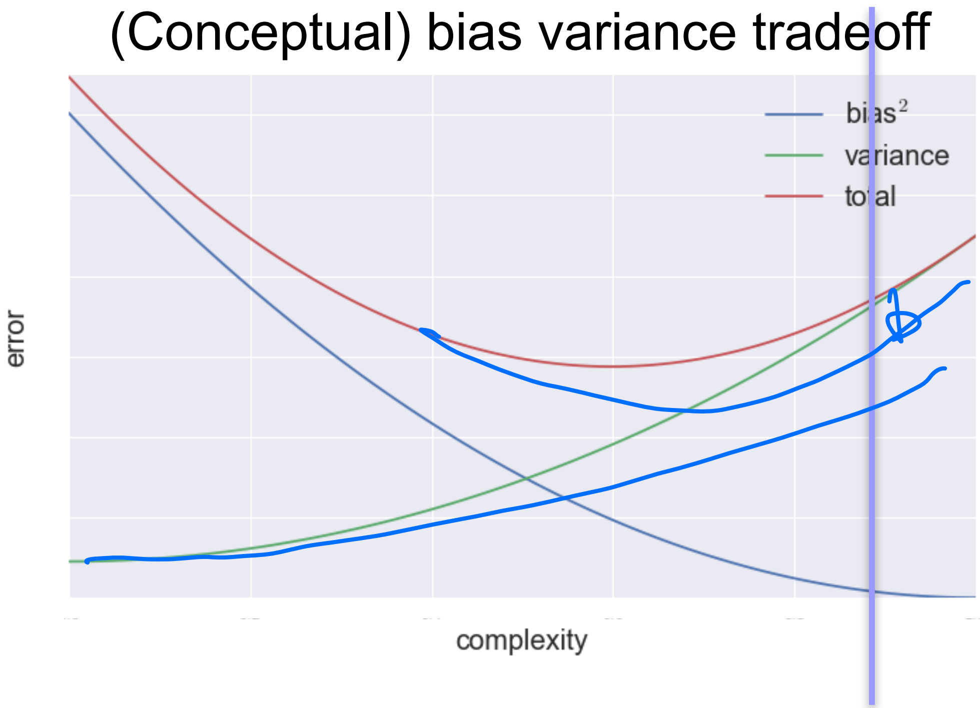
Recap: Bias-variance tradeoff with simple model

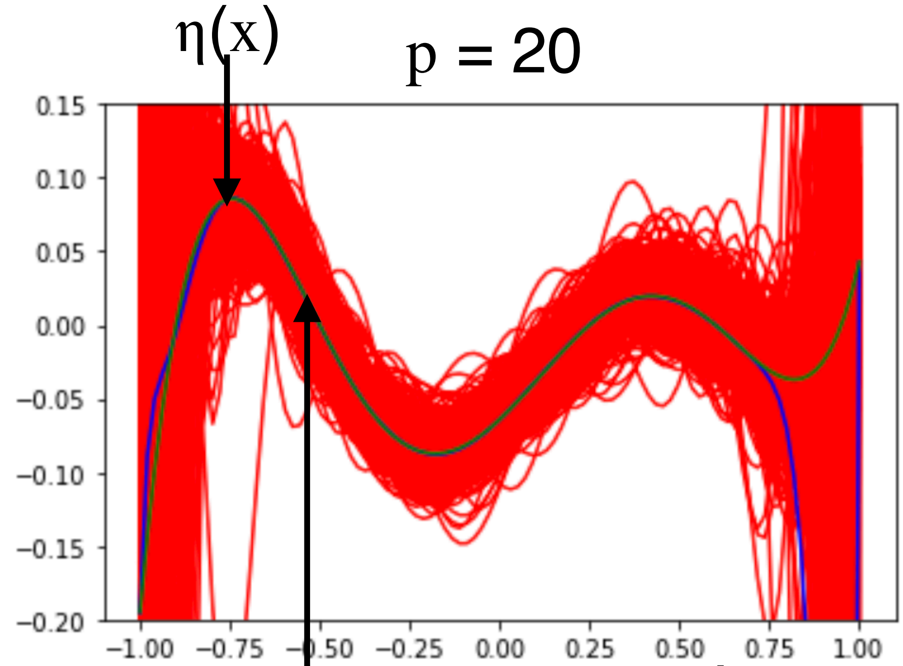




- When model **complexity is low** (lower than the optimal predictor $\eta(x)$)
  - Bias^2 of our predictor, $\eta(x) - \mathbb{E}_{\mathcal{D}}[\hat{f}_{\mathcal{D}}(x)]^2$, is large
  - Variance of our predictor, $\mathbb{E}_{\mathcal{D}}\, \mathbb{E}_{\mathcal{D}}[\hat{f}_{\mathcal{D}}(x)] - \hat{f}_{\mathcal{D}}(x)^2$, is small
  - If we have more samples, then
    - Bias does not change
    - Variance goes down
    - Because Variance is already small, overall test error does not change

Recap: Bias-variance tradeoff with simple model

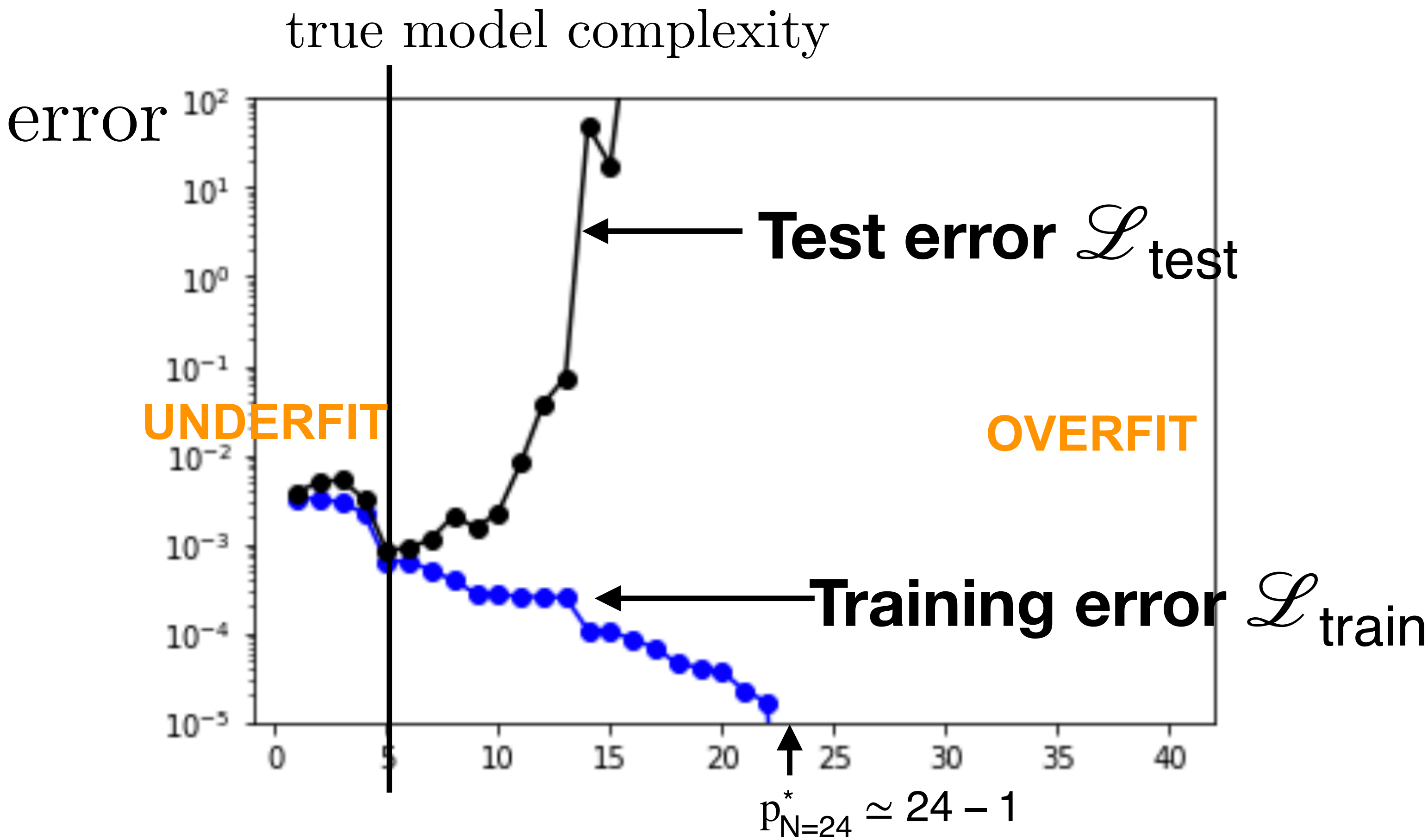




- When model complexity is high (higher than the optimal predictor $\eta(x)$)
  - Bias^2 of our predictor, $\eta(x) - \mathbb{E}_{\mathcal{D}}[\hat{f}_{\mathcal{D}}(x)]^2$, is small
  - Variance of our predictor, $\mathbb{E}_{\mathcal{D}}\, \mathbb{E}_{\mathcal{D}}[\hat{f}_{\mathcal{D}}(x)] - \hat{f}_{\mathcal{D}}(x)^2$, is large
  - If we have more samples, then
    - Bias does not change
    - Variance goes down
    - Because Variance is dominating, overall test error decreases significantly

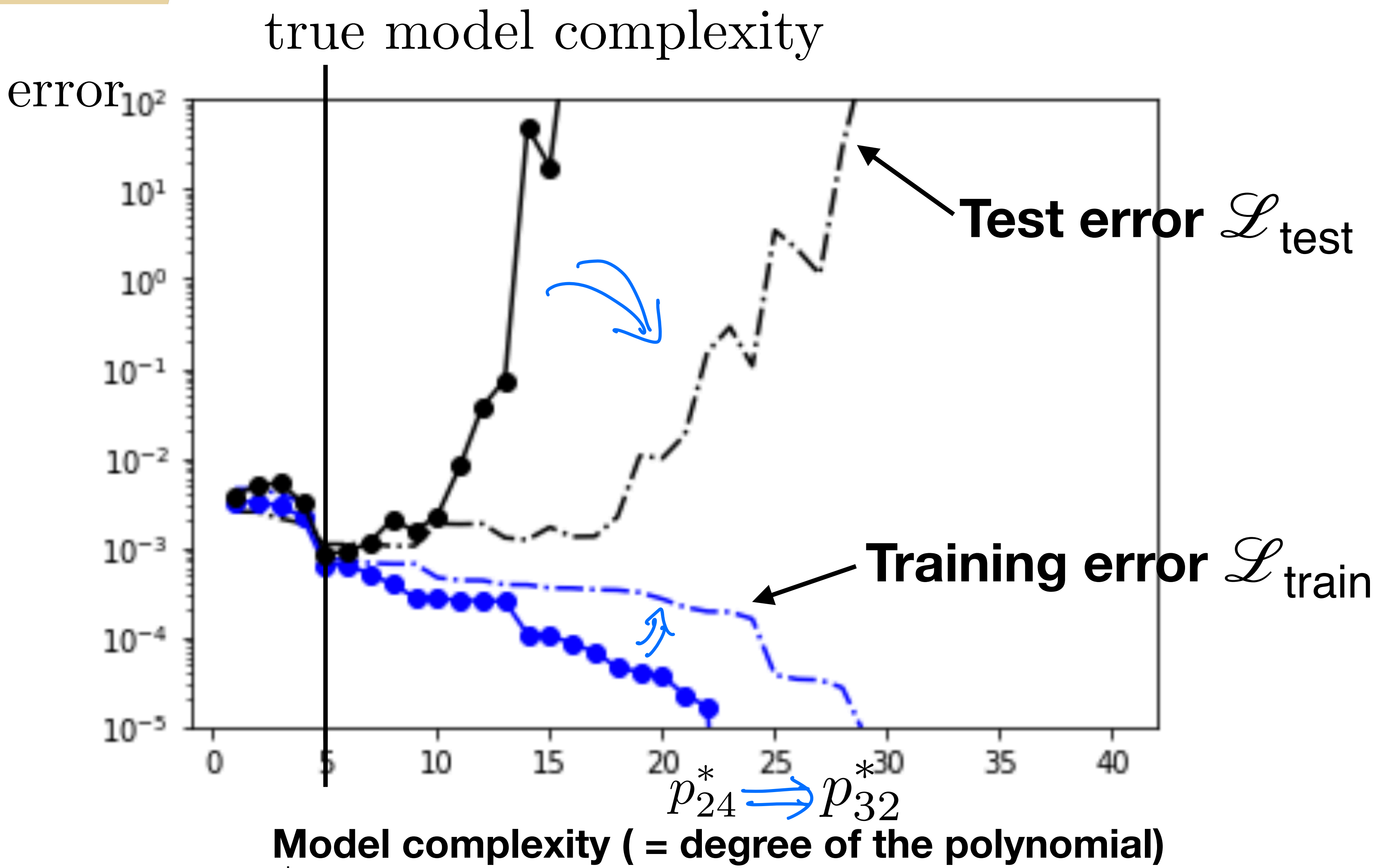
- let us first fix sample size ***N=30***, collect one dataset of size N i.i.d. from a distribution, and fix one training set S_{train} and test set S_{test} via 80/20 split

- then we run multiple validations and plot the computed MSEs for all values of ***p*** that we are interested in



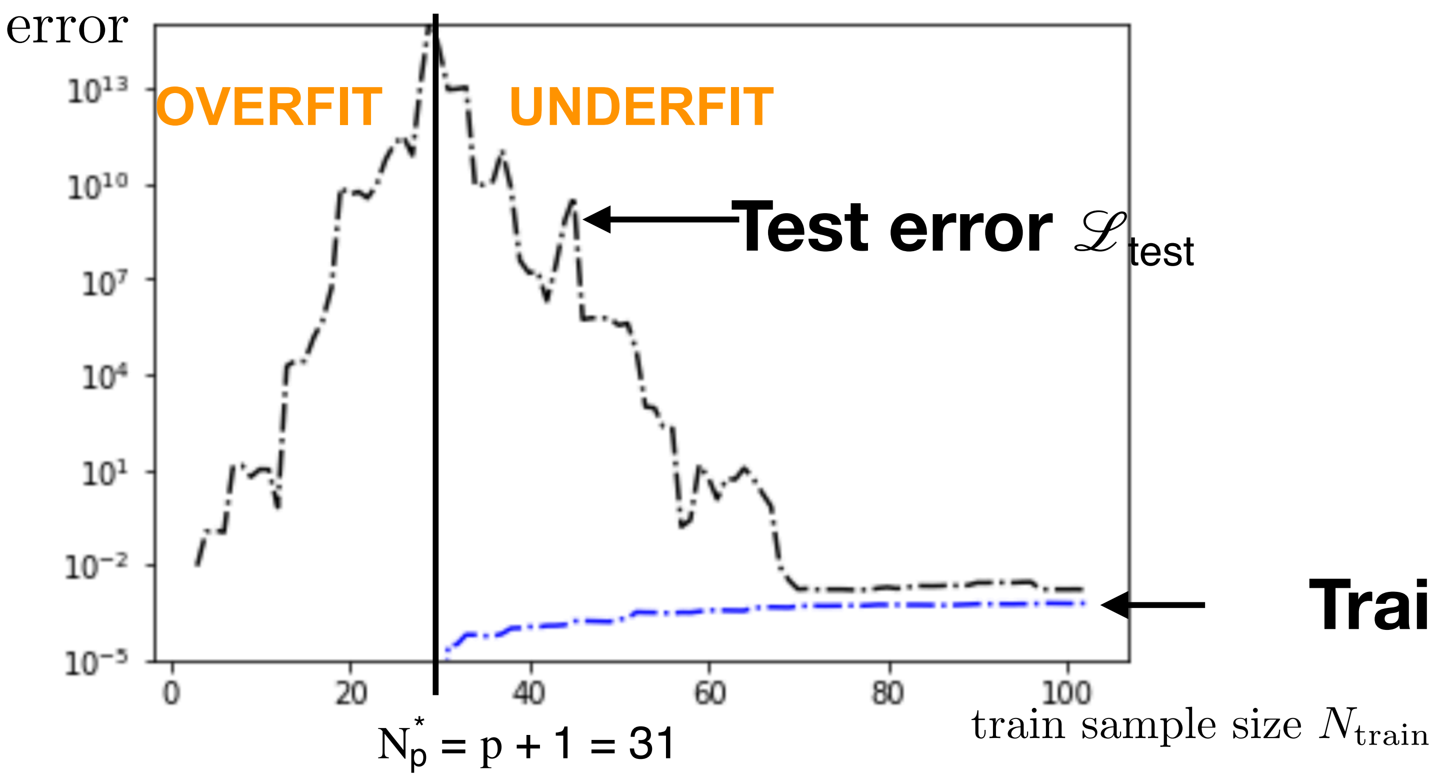
- Given sample size N there is a threshold, p^*_N, where training error is zero
- Training error is **always** monotonically non-increasing
- Test error has a trend of going down and then up, but fluctuates

- 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

Questions?

- Good questions on Ed Discussion
  - Will we be tested in "bias"?
    - Bias shows up in many places, and you will have to know the concept. Anything that is taught in lectures can show up in the exams.
  - Why do we use x to denote a column vector and not a row vector?
  - θ^* is the same as θ_*, it is just my writing that is not always consistent
  - What is θ^*?
    - The reason it is unnatural to think about θ^* is that it is something that does not exist in reality. Only time it exists is when you generate simulated data yourself (like in lecture notes and homework).
    - The right interpretation is that we hypothesize that nature has chosen to generate the data from a distribution, which can be written as $P(\,\cdot\,;\theta^*)$.
    - Whether this assumption is correct or not, we are deciding to go ahead with our MLE process.
    - That gives us some MLE estimate and corresponding distribution $P(\,\cdot\,;\theta^*_{\mathrm{MLE}})$. What we do with it, and what we believe about it is up to us. (Hence you need to check your accuracy on a holdout set, which we will learn later)

[Homework 1 Problem A4 analyzes similar bias-variance tradeoffs]