Bias and Variance and Overfitting

5A

CS 3244
Machine Learning

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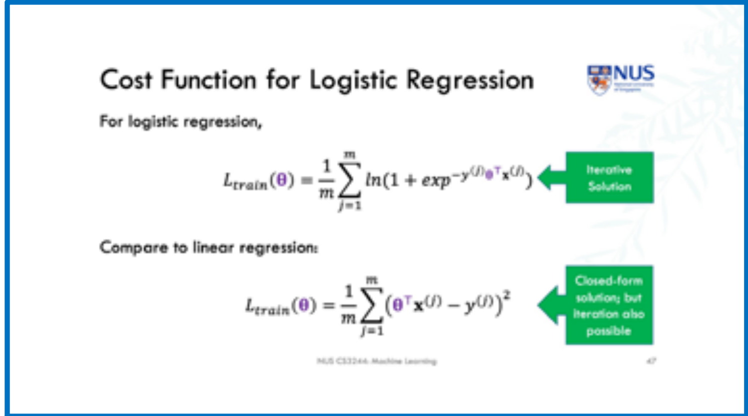
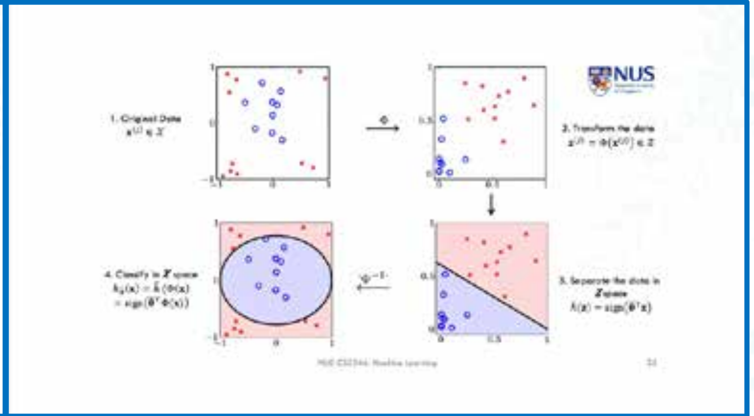
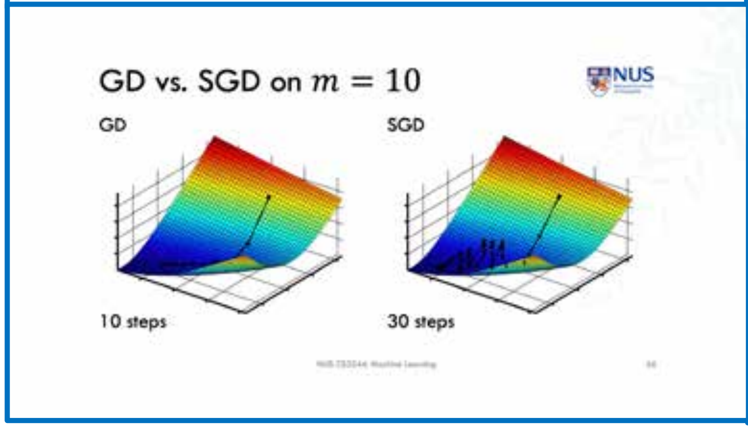
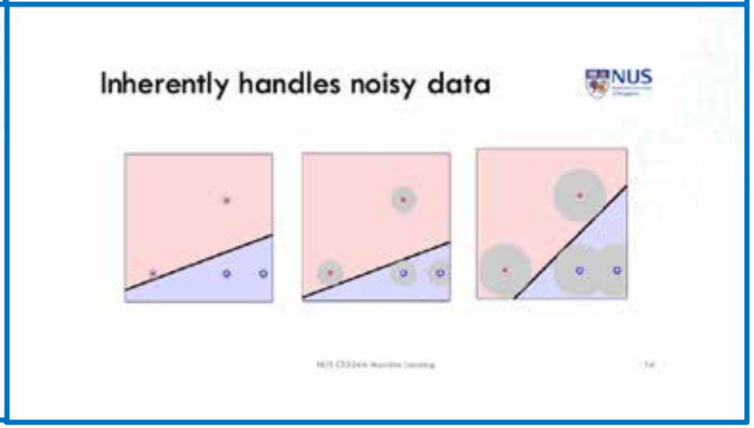
Recap from Week 04









Forecast for Week 05

Learning Outcomes for this week:

- Understand the bias–variance tradeoff
- Understand why overfitting occurs: the role of model complexity and the sampled dataset
- Apply bias and variance decomposition in simple scenarios

Bias and Variance, Illustrated

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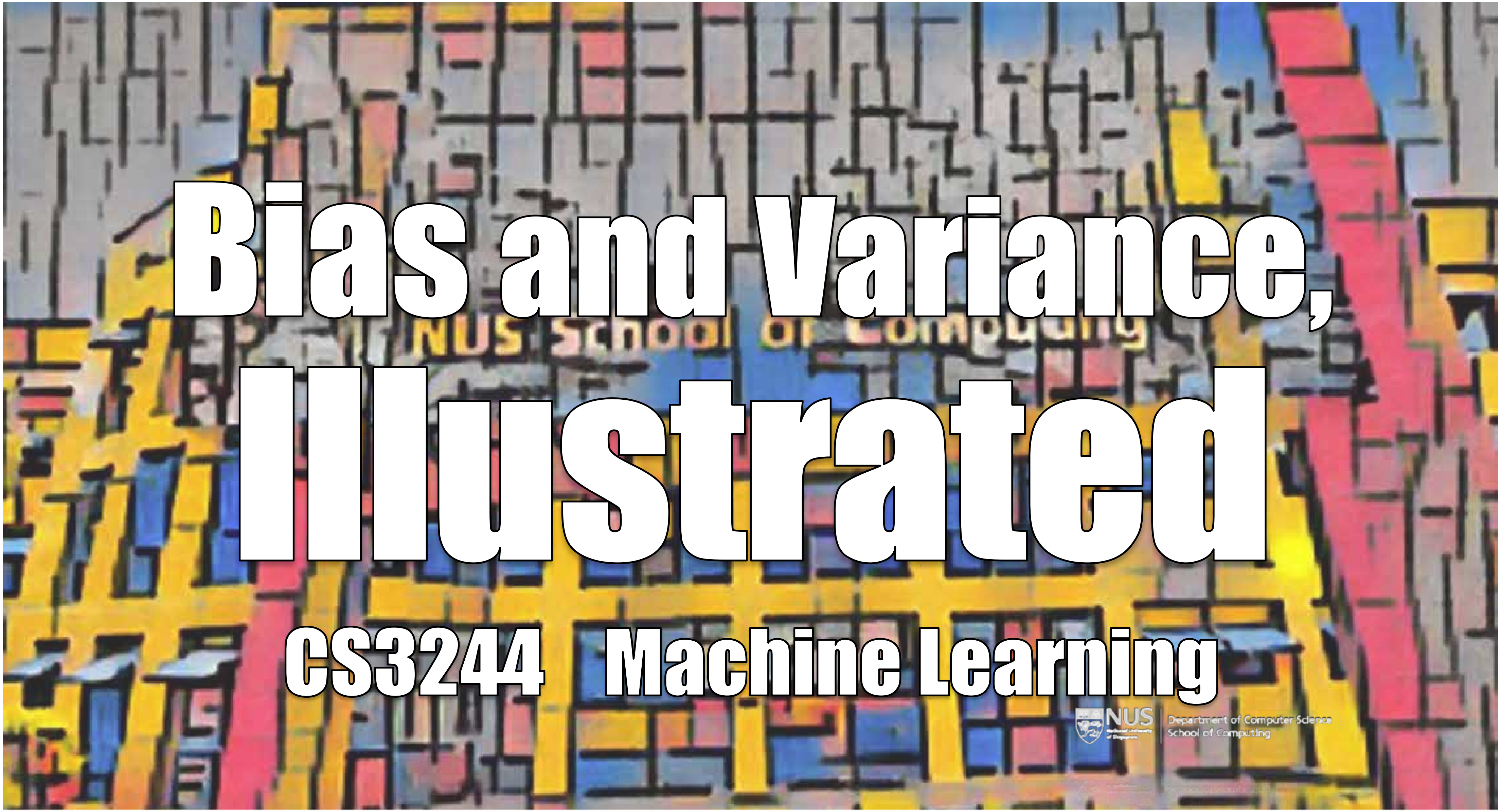
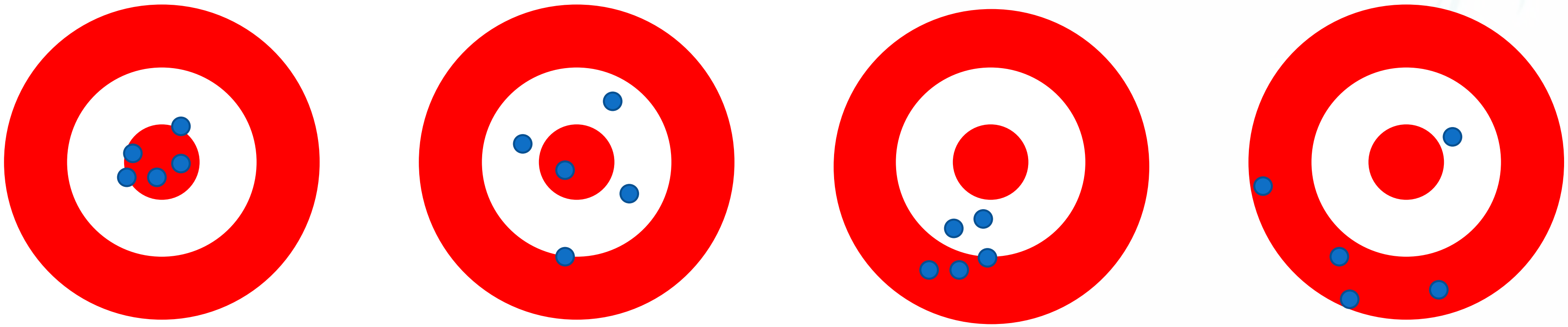


Bias

The difference between the average prediction and the true value.

Variance

The variability of the model prediction, for given data. Tells us spread of our data.



Regressing the sine function

$f: [-1,1] \to \mathbb{R}$

$f(x) = \sin(\pi x)$

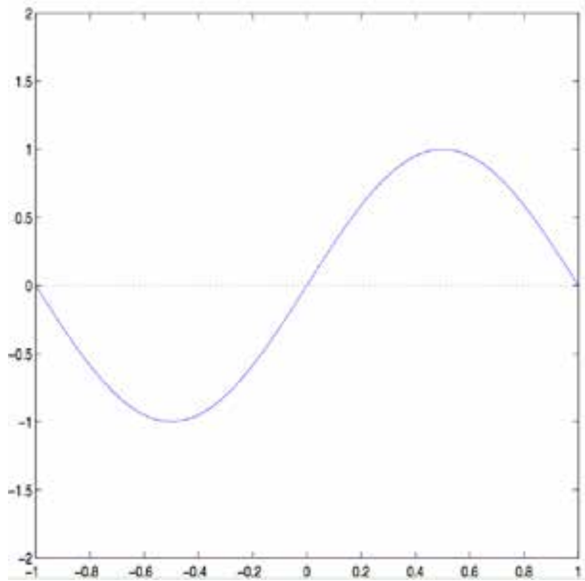
Only two training examples! $m = 2$

Two models used for learning:

🥇 $\mathcal{H}_1: h(x) = \theta_1 x + \theta_0$

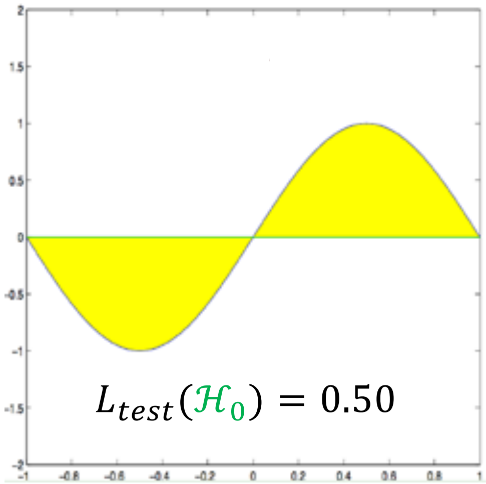
🥈 $\mathcal{H}_0: h(x) = \theta_0$

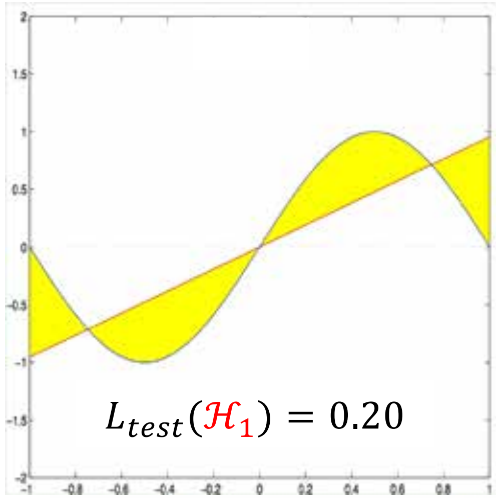
Your turn Q1: Which is better, $\mathcal{H}_0$ or $\mathcal{H}_1$?



Approximation – $\mathcal{H}_0$ versus $\mathcal{H}_1$

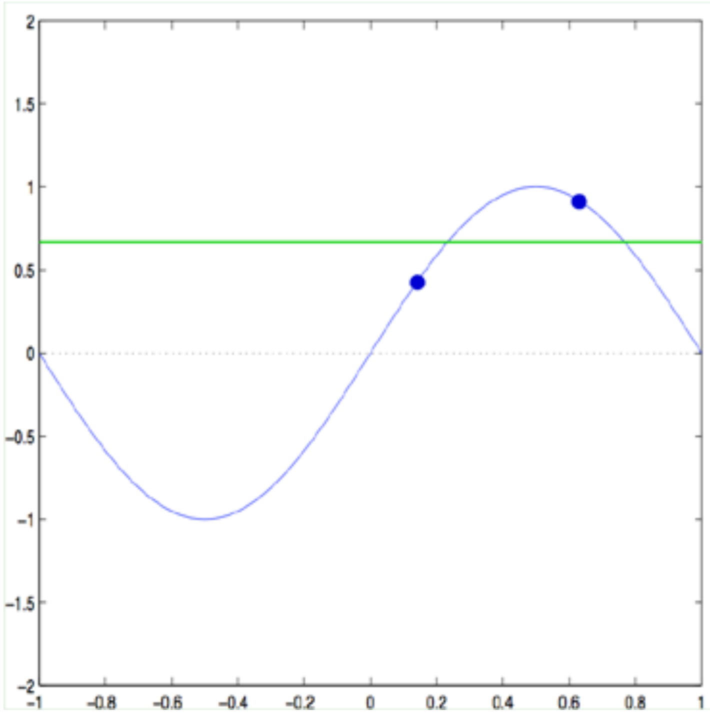
Use the full power of the model

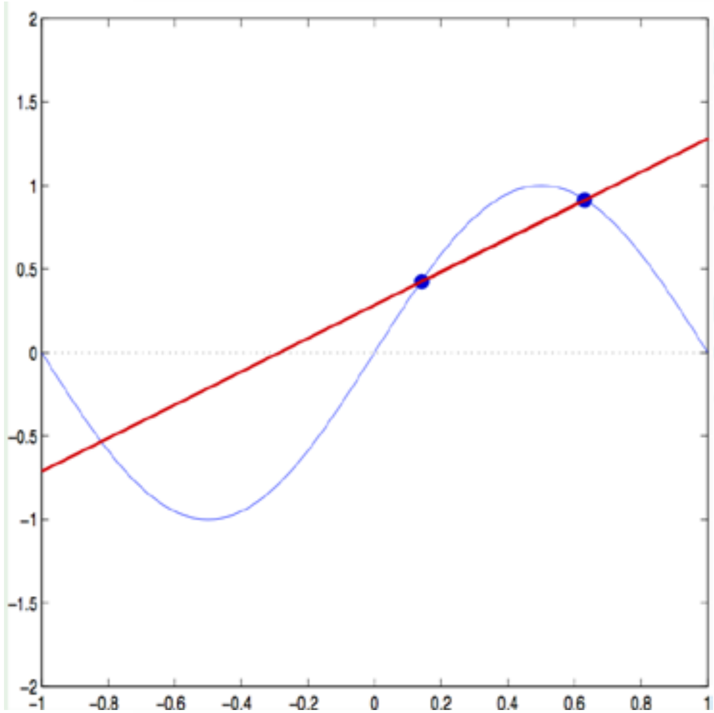




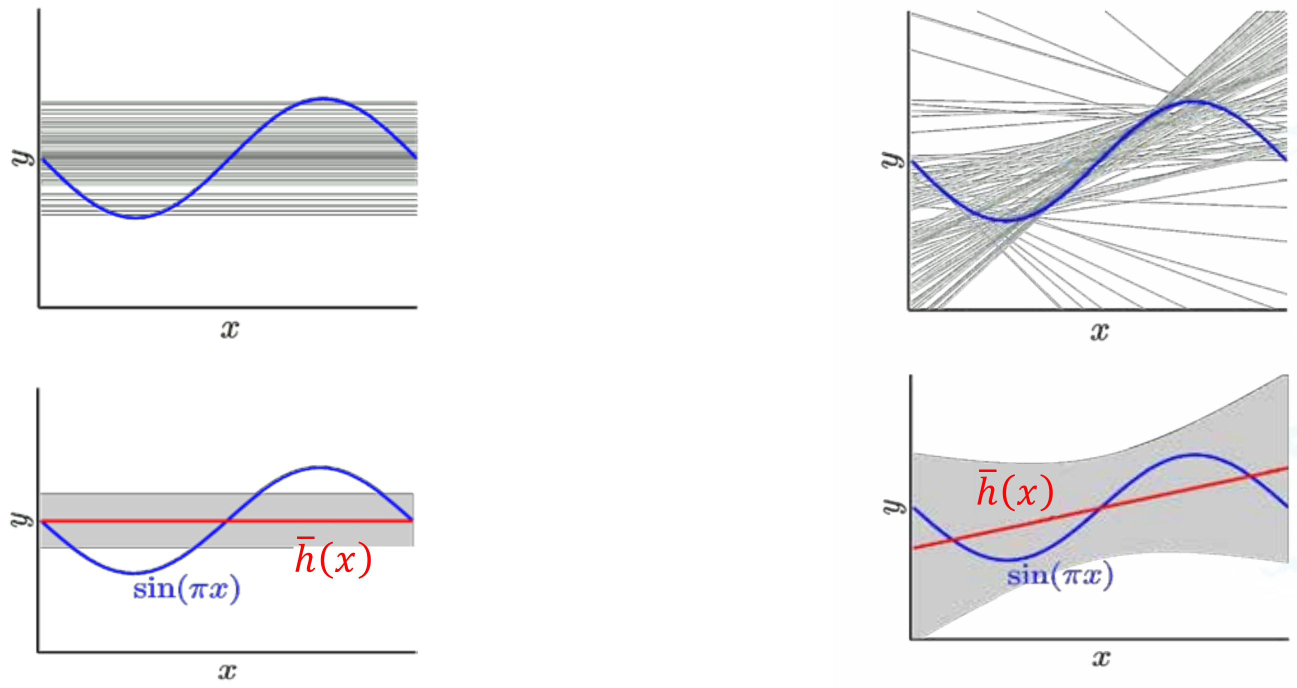
where — and — are the $\bar{h}(x)$ of each $\mathcal{H}$.

Learning – $\mathcal{H}_0$ versus $\mathcal{H}_1$

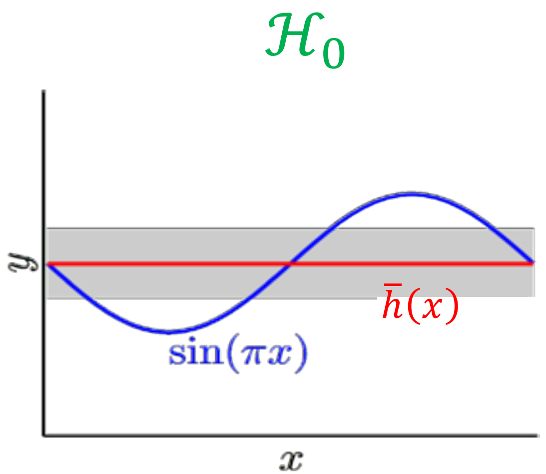




Bias & variance - $\mathcal{H}_0$ versus $\mathcal{H}_1$

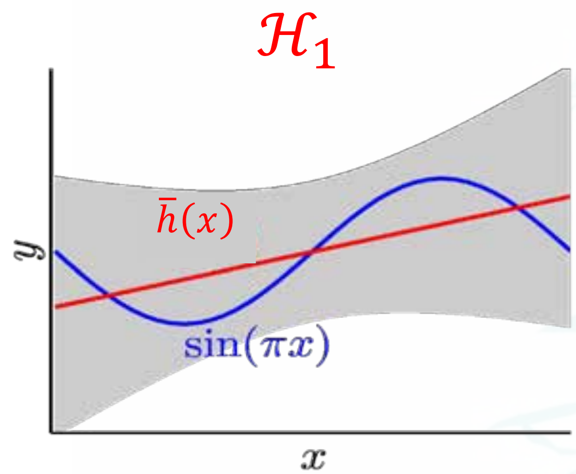


And the winner is ...



Bias = 0.50

Var = ?



Bias = 0.21

Var = ?

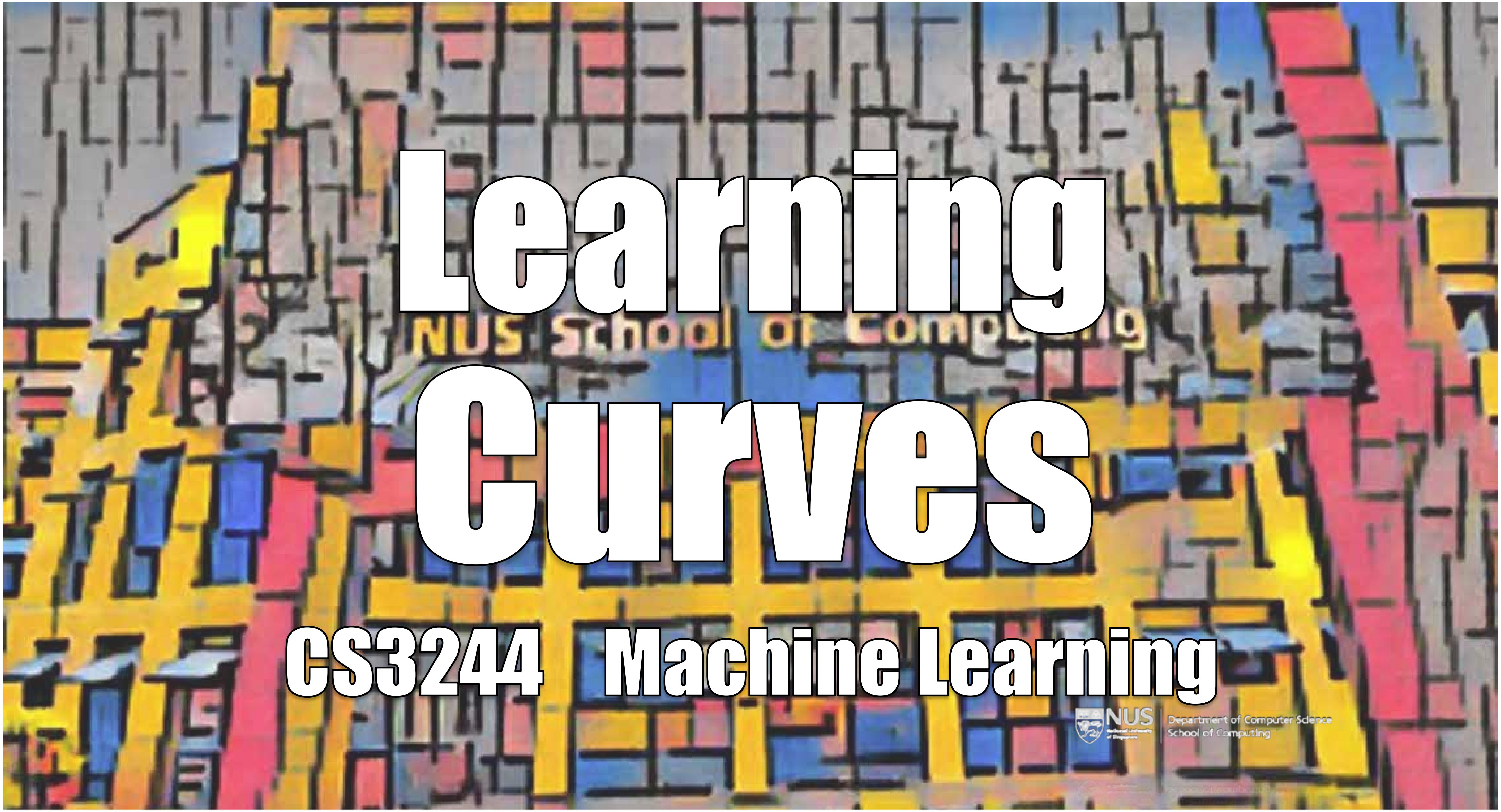
Lesson learned

Match the 'model complexity' to the

data resources, not to the **target complexity**.

Quality and Quantity

Learning Curves



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Learning Curves

Plot expected L_{test} and L_{train} …

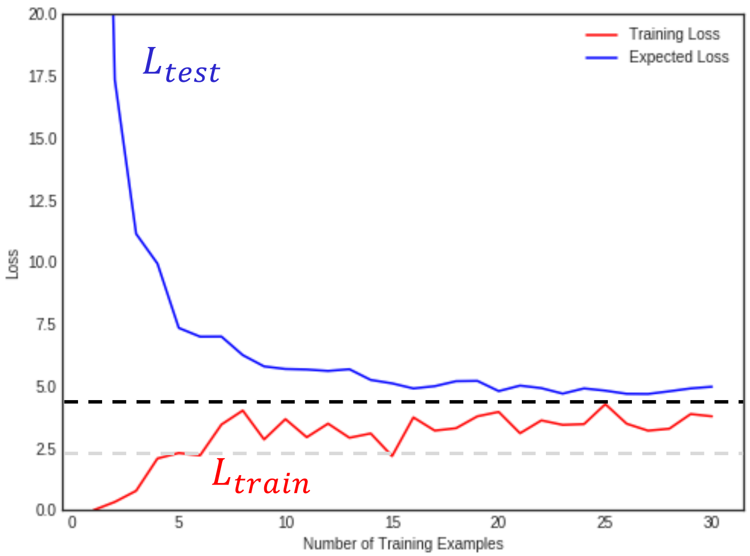
…as we vary size m

Data Resources: Quality and Quantity

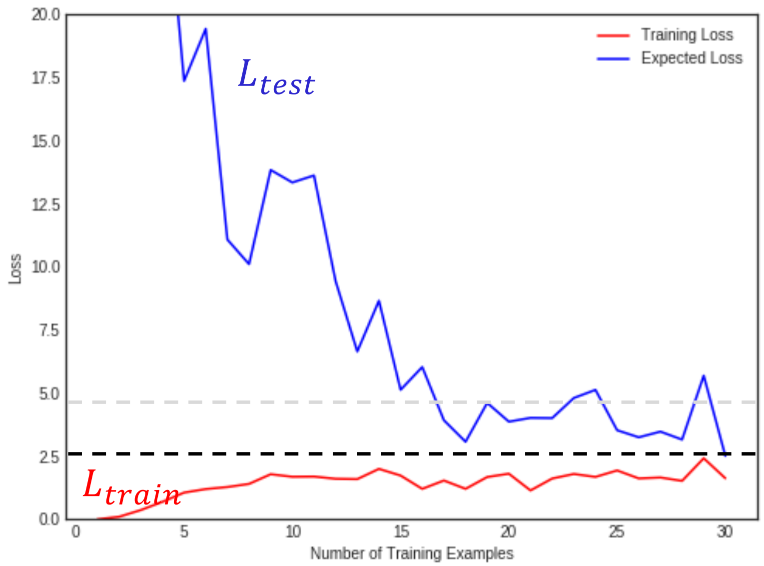
Expected test cost $\mathbb{E}_{\mathcal{D}}[L_{test}(f_{\mathcal{D}})]$

Expected training cost $\mathbb{E}_{\mathcal{D}}[L_{train}(f_{\mathcal{D}})]$

Simple versus Complex Models

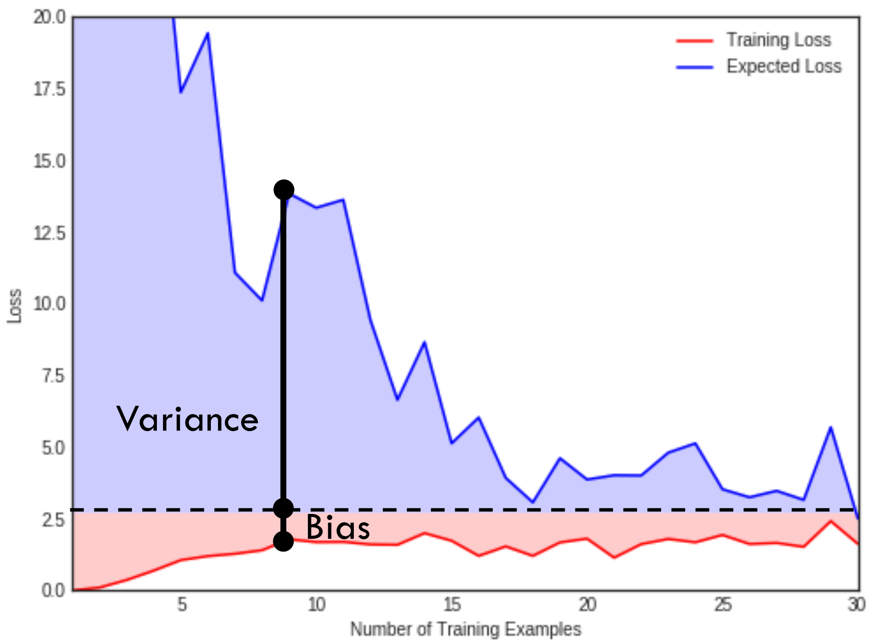


Simple Model



Complex Model

Bias–Variance on a Curve



Overfitting

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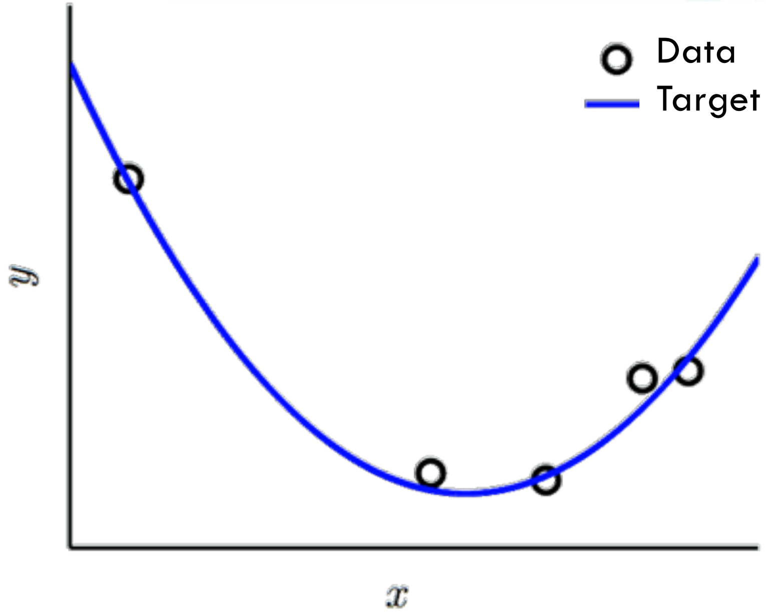
Overfitting, Illustrated

Simple target function

5 data points – **slightly noisy**

4^{th}-order polynomial fit

$L_{train} = 0$ ______________



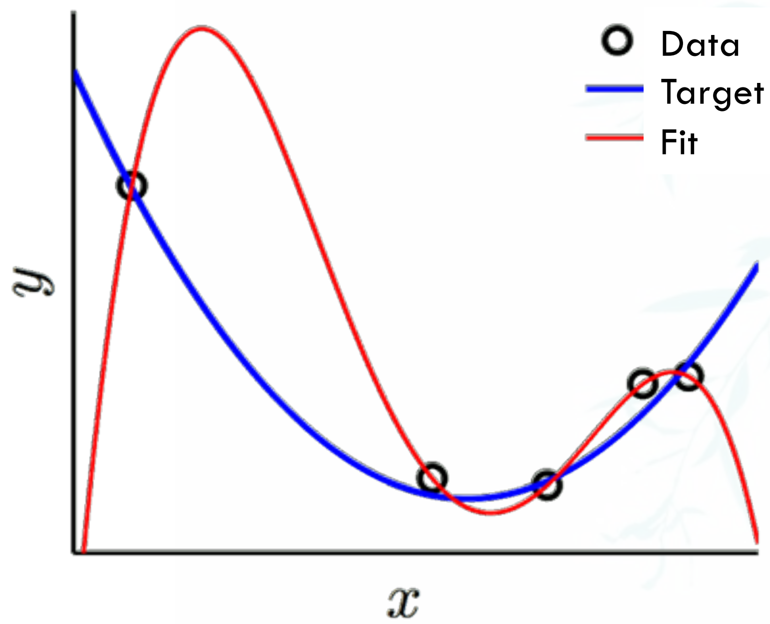
Overfitting, Illustrated

Simple target function

5 data points –
slightly noisy

4th-order polynomial fit

$L_{train} = 0$ but L_{test} is huge



The culprit

Overfitting:
"Fitting the data more than is warranted"

Culprit: Fitting the noise.

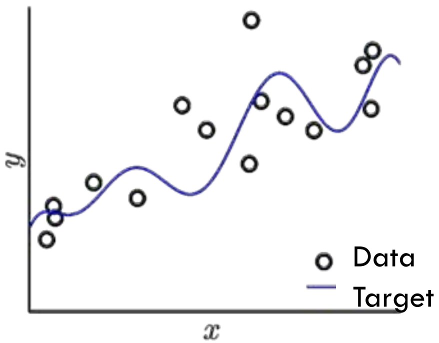
Not just useless, **but harmful**

🥈 2nd versus 🥇 10th order polynomials

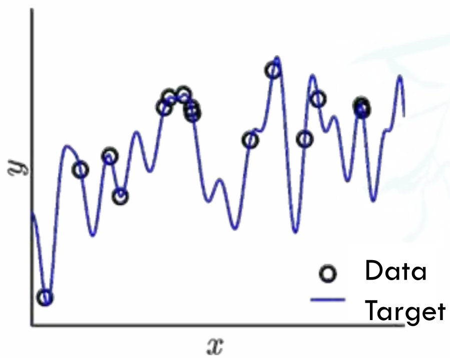
In Zoom breakout or physical subgroups, discuss and react 🏃🏃🏃:

(5 mins): Pick your model of choice for each scenario. In each scenario, you are given 15 data points. Justify your choice.

Q2: 10th-order target + noise

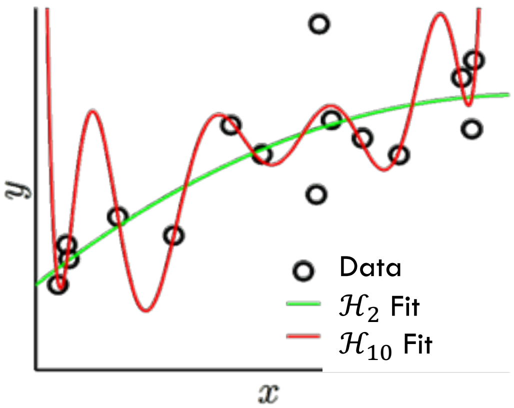


Q3: 50th order target, noiseless



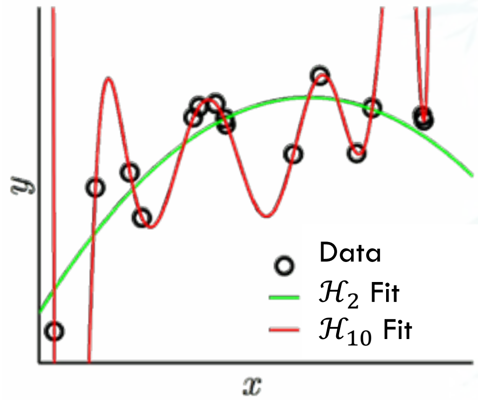
Two fits for each function

Noisy low-order target

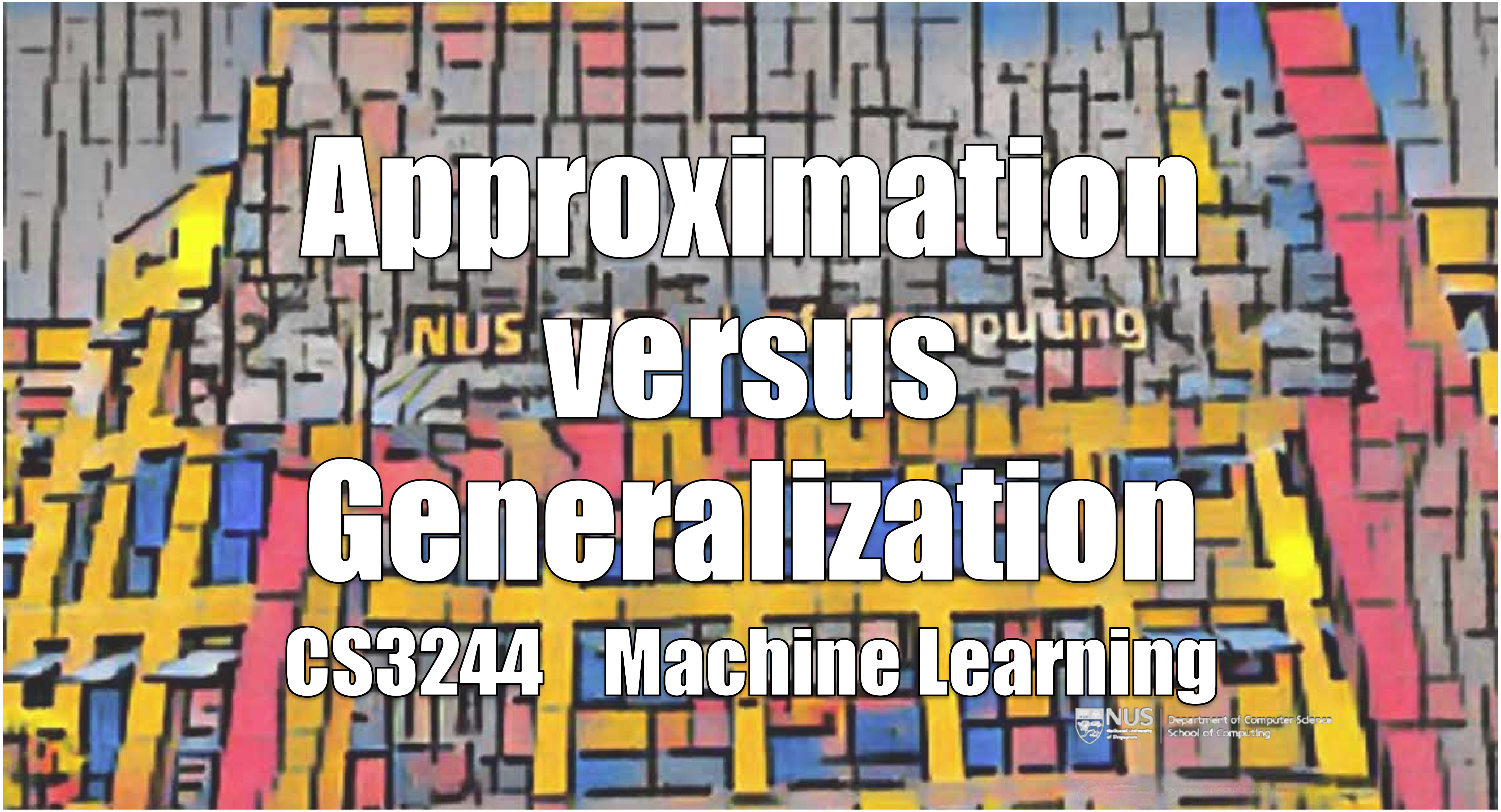


	2nd Order	
L_{train}	0.050	
L_{test}	0.127	

Noiseless high-order target



	2nd Order	
L_{train}	0.029	
L_{test}	0.120	



Approximation versus Generalization

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Approximation–generalization tradeoff

Small L_{test}: good approximation of f on unseen test data

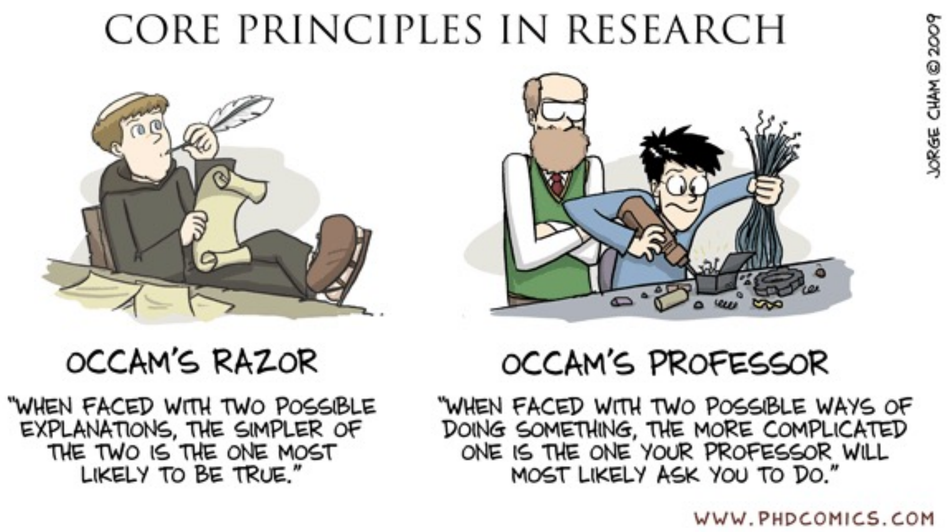
More complex $\mathcal{H}$ $\rightarrow$ better chance of **approximating** f

Less complex $\mathcal{H}$ $\rightarrow$ better chance of **generalizing** on test data

Ideal $\mathcal{H} = \{f\}$

Good luck with that!

Occam's Razor



"Simpler is better"

Formalized as Minimum Description Length (MDL)

The shortest description of the data is the best model (related to Entropy)

Last Week's Assigned Task

Post a 1–2 sentence answer to the topic in your tutorial group:
#tg-xx

Describe kNN or decision trees with respect to variance.

Pre-Lecture Activity from last week

The variance of kNN models are greatly affected by the chosen k-value. A small k-value leads to underfitting where the variance is extremely high. This can be observed by viewing the extremely rough decision surface of a kNN model with small k, where the surface constantly varies to adjust to the training points. To reduce this variance, we can choose a bigger k-value so that the decision surface would not be overly affected by a single training point and can remain relatively smooth. However this may also lead to overfitting, which would still cause high test error rate despite the low variance.

For kNN, for small values of k the bias will be lesser and the variance larger because the test data will have a higher probability of being mis-labeled. As k becomes larger, the bias increases while the variance decreases.

For kNN, the variance of the model will depend on the value chosen for k.

If k is small, for example k = 1, then the prediction will only depend on one data point, so the variance will be high and bias will be low due to overfitting.

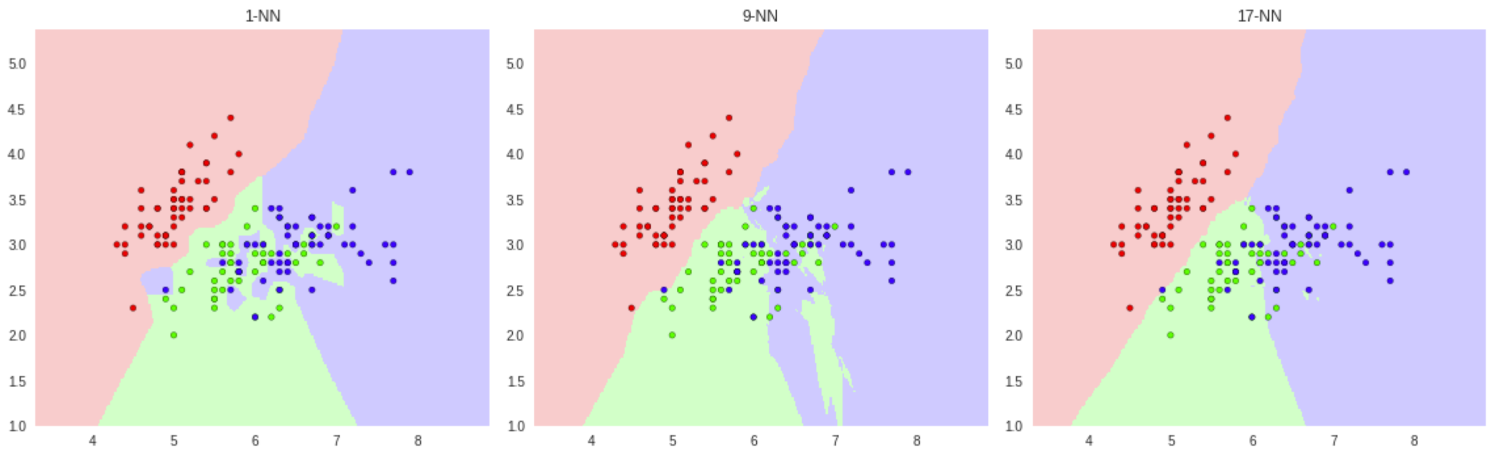
If k is too large, then the model may generalise too much, so the variance will be low but the bias may be high and this may be an underfit.

The key to find a good model is to find a k value such that both bias and variance are low to increase model accuracy.

In k NN

Model free: Data completely dictates the model

Higher k lowers the dependence of the model on a particular data point, makes model more robust and lowers variance



Variance of Decision Tree model can be related to its depth, where the increase in depth would result in an overfitting of the data. As the deeper the model goes, the variance of the model will increase, being affected more by the noise of the data used to train the model

Decision trees are susceptible to high variance. For test data that is very close to decision boundaries, small fluctuations in its feature values can lead to a different classification.

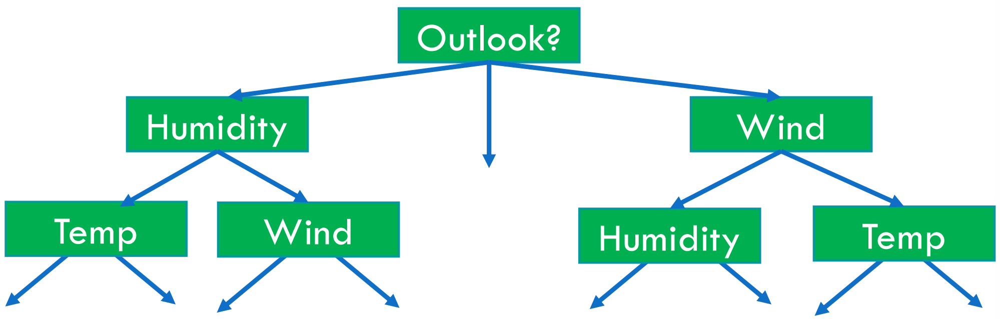
DT tend to have larger variance as each decision is made using hard boundaries where even the smallest change could result in a different outcome. This variance is amplified when the tree is not pruned resulting in overfitting. (edited)

For a decision tree, the complexity of the model is dependent on the depth and number of splits/conditions the tree has. Shallow trees underfit the data (high bias, low variance) while deep trees overfit the data (low bias, high variance). Larger trees account for noise in the data to a greater extent, trying to "over-split" the data into finer bins/buckets to classify said data.

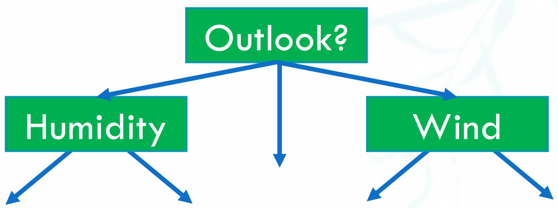
…In Decision Trees

Pruning discards detailed tests that may use criteria non-essential for classification in test data.

Before



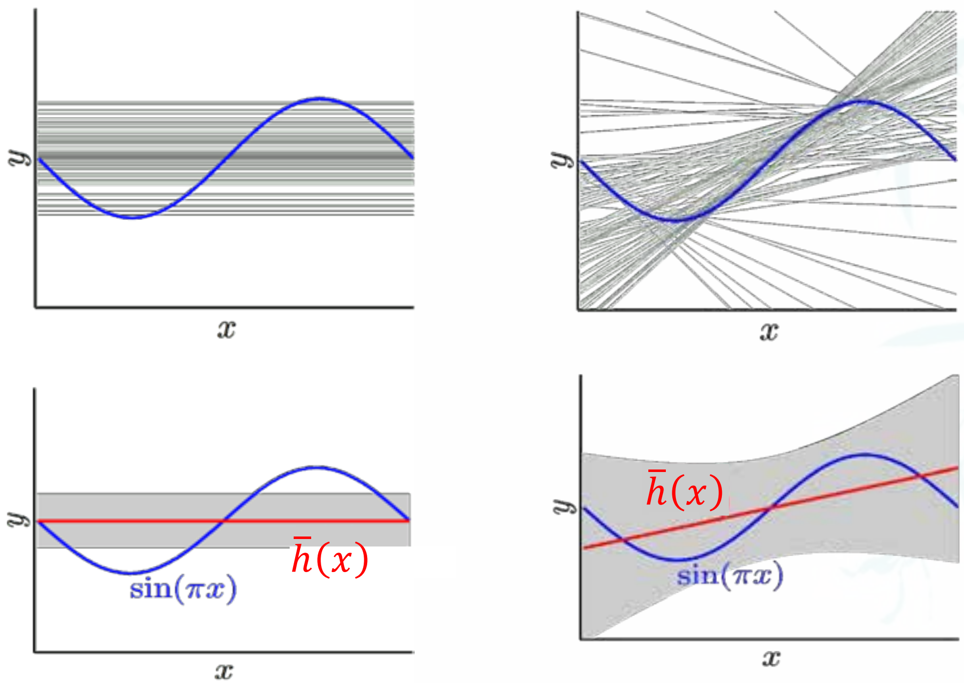
After



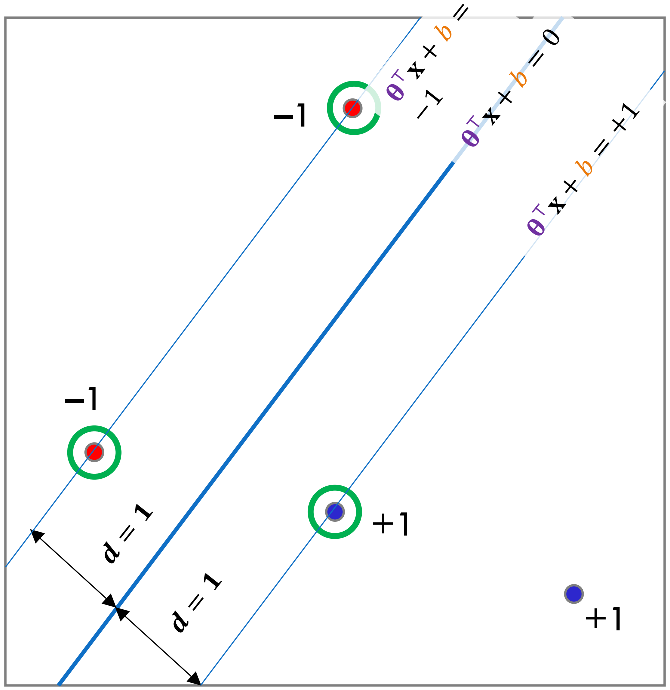
…In Linear Models

We just did this!

Each additional parameter θ_i adds a degree of freedom in the model.



…In SVM



The SVM determines its separating hyperplane by virtue of its support vectors.

# of support vectors ∝ complexity of the model

… in Ensembles

We have T reports $h_1, h_2, \dots, h_T$ predicting whether a stock will go up as $h(x)$.

We can:

1. Select the most trustworthy of them based on their usual performance
   Training performance: $h(x) = h_{t^*}(x)$ with $t^* = argmin_{t\in\{1,2,\dots,T\}} L_{train}(h_t^-)$

2. Let each report have a vote
   Uniform Vote: $h(x) = \text{sign}\left(\sum_{t=1}^{T} 1 \cdot h_t(x)\right)$

3. Weight the reports non-uniformly
   Weighted Vote: $h(x) = \text{sign}\left(\sum_{t=1}^{T} \alpha_t \cdot h_t(x)\right)$ where $\alpha_t \geq 0$.

4. Combine the predictions conditionally
   This is decision trees, let's finish it up now!

Key: component hypotheses are

Diverse.

Ensembling diverse h generalizes better.

🆒 **fact:** Decision trees have a native version: **Random forests.**

Bias and Variance, Analytically

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Quantifying the tradeoff

Decomposing L_{test} into

1. How well can $\mathcal{H}$ approximate f overall
2. How well we can zoom in on a good $h_\theta \in \mathcal{H}$

Applies to **real-valued** targets and uses **squared error**

There is an equivalent binary version through the lens of VC analyses (related to SVM)

Recap: Expected Value

We'll need to reason about values of data, irrespective of particular samples, so we'll need to work with expected values of random variable.

Expected Value: Average over all possible outcome of a random variable X.

$$\mathbb{E}[X] = \sum_{x \in X} x \Pr[X = x]$$

Not conditional test notation
(not Iverson brackets)

Example

Let X be the outcome of a fair dice roll.
Then the expected value is
$\mathbb{E}[X] = \frac{1}{6}(1 + 2 + 3 + 4 + 5 + 6) = 3.5.$

Variance

Intuition
Quantify how much deviation from expected value.

$$\mathrm{Var}[x] = \mathbb{E}[(x - \mathbb{E}[x])^2]$$

Example

Let x be the outcome of a fair dice roll. Then the variance is
$\mathrm{Var}[x] = \frac{1}{6}\left((1-3.5)^2 + \cdots + (6-3.5)^2\right) = \frac{35}{12}$.

Some Terminology

- $\mathbb{E}_{x}[z(x)] \equiv$ Expected value of $z()$, given the distribution of values of x.

- $h_{\mathcal{D}} \equiv$ Hypothesis of learner when learning from Dataset $\mathcal{D}$.

- $\mathbb{E}_{\mathcal{D}}[z()] \equiv$ Expected value of $z()$, given distribution of possible Datasets $\mathcal{D}$.

Start with L_{test}

$$L_{test}(h_{\mathcal{D}}) = \mathbb{E}_x[(h_{\mathcal{D}}(x) - f(x))^2]$$

$h(x)$ depends on the specific dataset $\mathcal{D}$.

Start with L_{test}

$L_{test}(h_{\mathcal{D}}) = \mathbb{E}_x[(h_{\mathcal{D}}(x) - f(x))^2]$

$h(x)$ depends on the specific dataset $\mathcal{D}$.

$\mathbb{E}_{\mathcal{D}}[L_{test}(h_{\mathcal{D}})]$

Generalizing over all $\mathcal{D}$ with same m

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

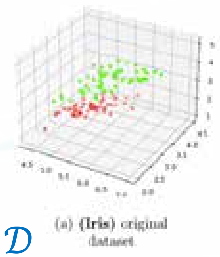
$$= \mathbb{E}_x\left[\mathbb{E}_{\mathcal{D}}[(h_{\mathcal{D}}(x) - f(x))^2]\right]$$

Swap ok, as integrand is strictly non-negative

Focus on $\mathbb{E}_{\mathcal{D}}[(h_{\mathcal{D}}(x) - f(x))^2]$, we'll deal with the outer term $\mathbb{E}_x[\ldots]$ later.

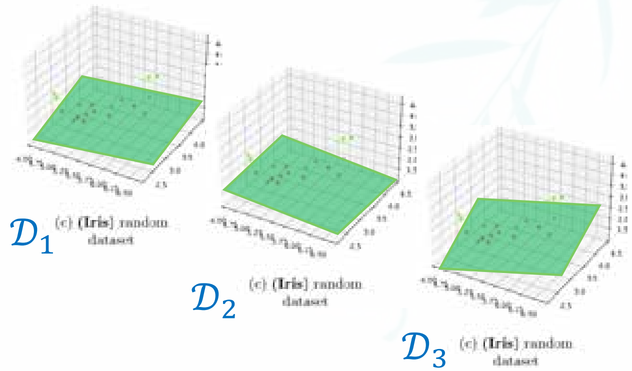
The average hypothesis

To evaluate $\mathbb{E}_{\mathcal{D}}[(h_{\mathcal{D}}(x) - f(x))^2]$, we define the 'average' hypothesis $\bar{h}(x) = \mathbb{E}_{\mathcal{D}}[h_{\mathcal{D}}(x)]$



Imagine many, many data sets $\mathcal{D}_1, \mathcal{D}_2, \ldots, \mathcal{D}_K$ drawn:

$$\bar{h}(x) \approx \frac{1}{K} \sum_{k=1}^{K} h_{\mathcal{D}}(x)$$



Using $\bar{h}(x)$

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

Using the average hypothesis $\bar{h}(x)$

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

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

Add $-\bar{h}(x) + \bar{h}(x)$. Associate first two and second two terms.

$$= \mathbb{E}_{\mathcal{D}}\left[\left(h_{\mathcal{D}}(x) - \bar{h}(x)\right)^2 + \left(\bar{h}(x) - f(x)\right)^2 + 2\left(\underbrace{h_{\mathcal{D}}(x) - \bar{h}(x)}_{0}\right)\left(\underbrace{\bar{h}(x) - f(x)}_{\text{const w.r.t. } \mathcal{D}}\right)\right]$$

Expand out, cross terms drop as the first part of term is 0 when the expectation $\mathbb{E}_{\mathcal{D}}$ is applied.

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

2nd term is constant with respect to $\mathcal{D}$

Bias and Variance

$$\mathbb{E}_{\mathcal{D}}[(h_{\mathcal{D}}(x) - f(x))^2] = \underbrace{\mathbb{E}_{\mathcal{D}}\left[\left(h_{\mathcal{D}}(x) - \bar{h}(x)\right)^2\right]}_{\text{Q4}} + \underbrace{\left(\bar{h}(x) - f(x)\right)^2}_{\text{Q5}}$$

Quick Quiz: Which is which?

1️⃣ Bias
2️⃣ Variance

🤷‍♀️🤷‍♂️🤷 I give up

Bias and Variance

$$\mathbb{E}_{\mathcal{D}}[(h_{\mathcal{D}}(x) - f(x))^2] = \underbrace{\mathbb{E}_{\mathcal{D}}\left[\left(h_{\mathcal{D}}(x) - \bar{h}(x)\right)^2\right]} + \underbrace{\left(\bar{h}(x) - f(x)\right)^2}$$

Therefore,

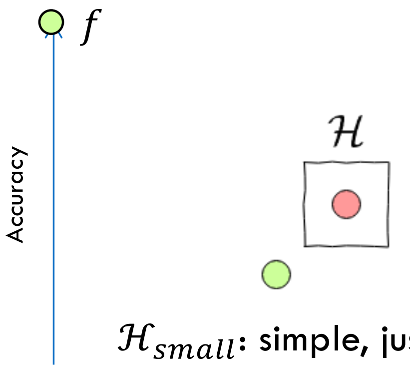
$$\mathbb{E}_{\mathcal{D}}[L_{test}(h_{\mathcal{D}})] = \mathbb{E}_x\left[\mathbb{E}_{\mathcal{D}}[(h_{\mathcal{D}}(x) - f(x))^2]\right]$$

$$= \mathbb{E}_x[\text{bias}(x) + \text{var}(x)]$$

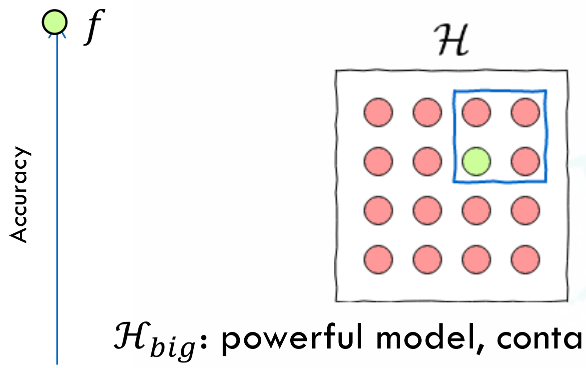
$$\equiv \text{bias} \qquad + \quad \text{var}$$

✏️ The tradeoff

$$\mathrm{Bias}[h(x)] = \left|\bar{h}(x) - f(x)\right|. \qquad \mathrm{Var}[h(x)] = \mathbb{E}\left[\left(h(x) - \bar{h}(x)\right)^2\right]$$



$\mathcal{H}_{small}$: simple, just one hypothesis.



$\mathcal{H}_{big}$: powerful model, contains the target function f. But you must find it.

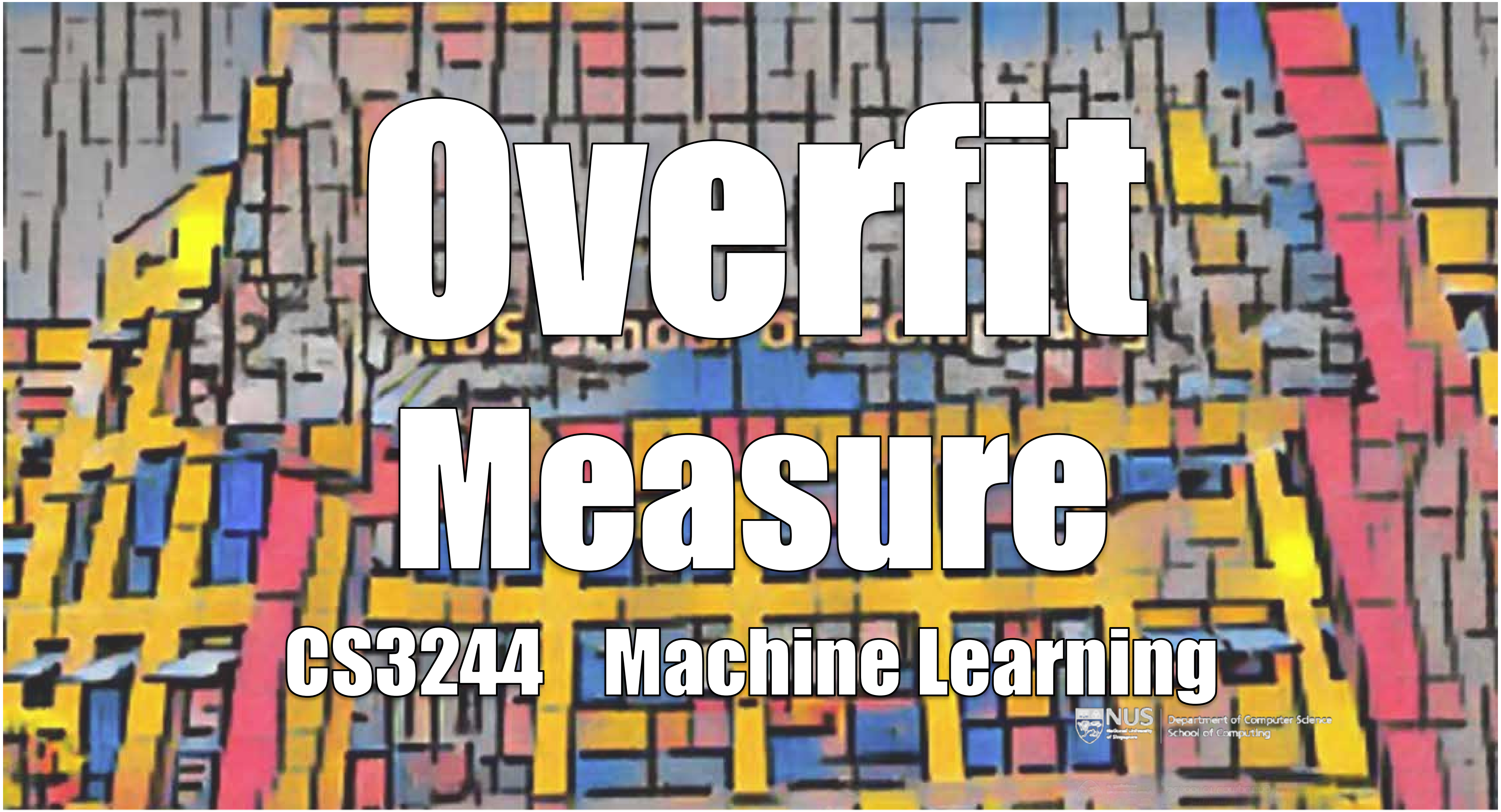
Goldilocks, Data Science Style

Underfit

Overfit

(Well) Fit

Images from MacMillan


Overfit
Measure
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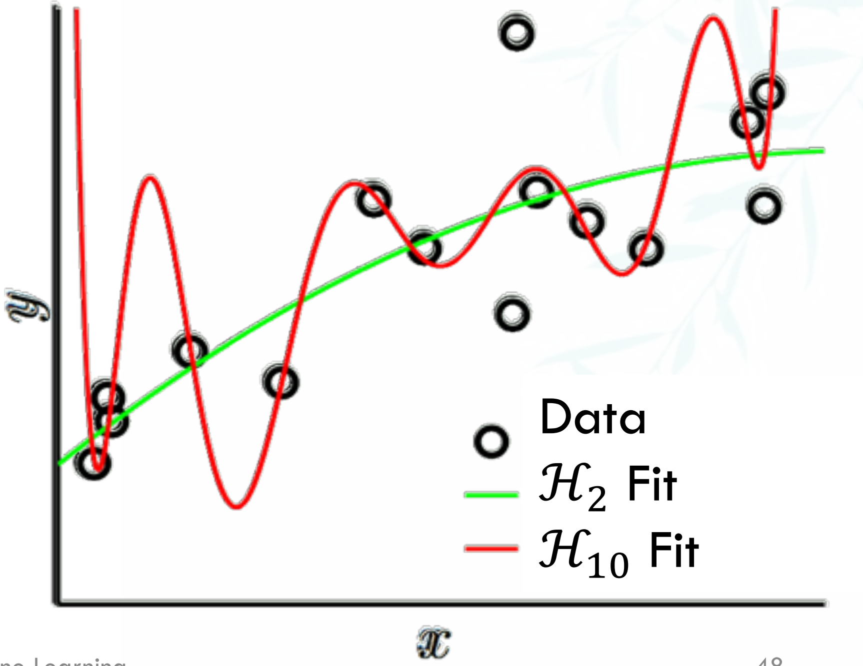
10^{th} order polynomial with noise

Two learners Overfitting and Restrained:

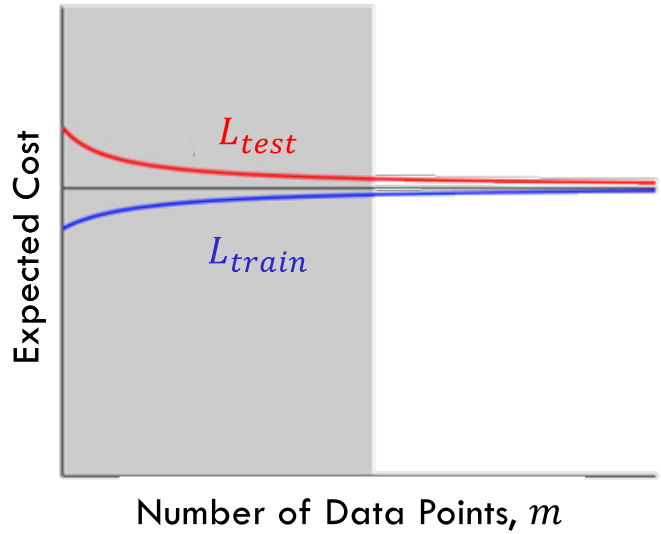
Both know the target is 10^{th} order, you get 15 data points.

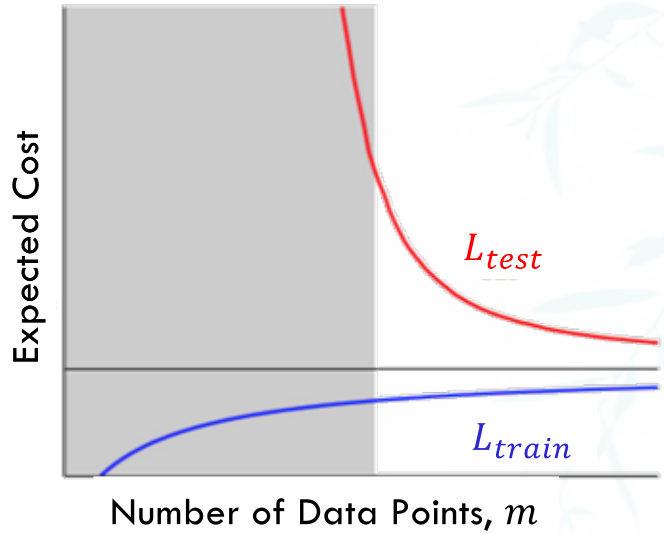
- O chooses $\mathcal{H}_{10}$
- R chooses $\mathcal{H}_2$

Your Turn: Which fits better?



When is $\mathcal{H}_2$ better than $\mathcal{H}_{10}$?





Overfitting (grey region): $L_{test}(\mathcal{H}_{10}) > L_{test}(\mathcal{H}_2)$

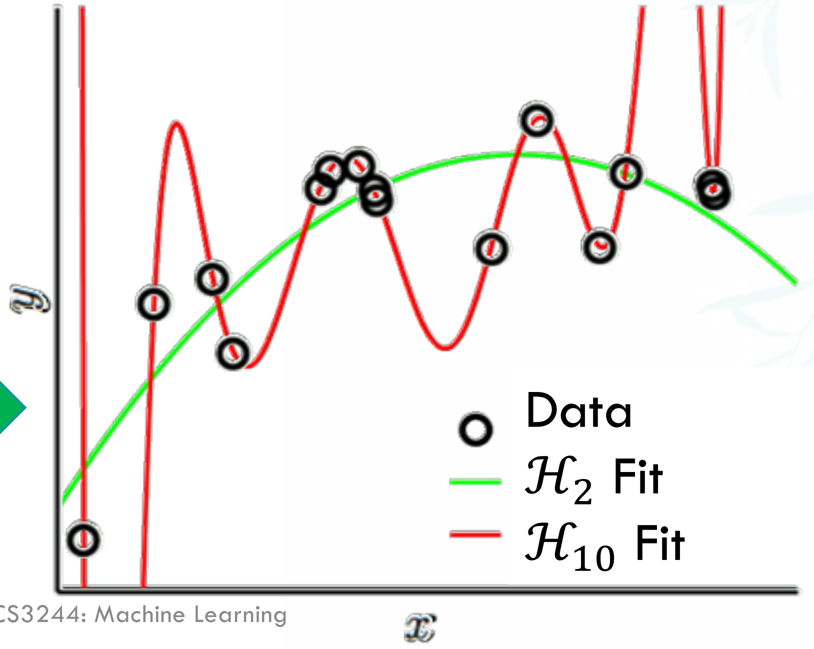
Without noise, with complex f

The two learners $\mathcal{H}_{10}$ and $\mathcal{H}_2$

They <u>know</u> there is no noise

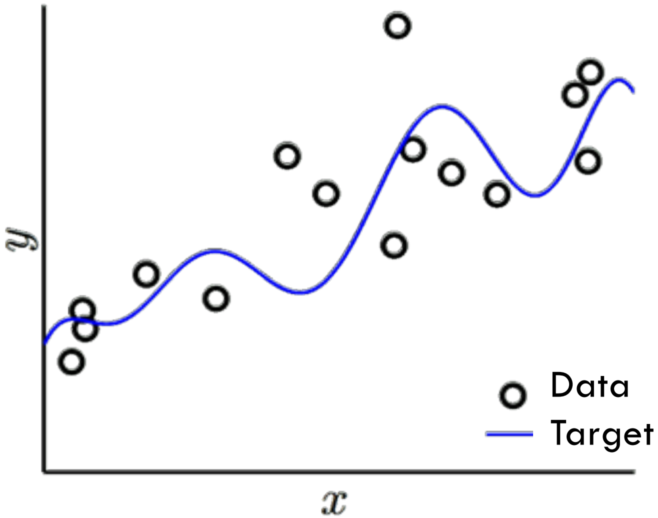
Is there really no noise?

Learning a 50th order target



A detailed experiment

Impact of **noise level** and **target complexity**



$$y = f(x) + \epsilon(x) = \underbrace{\sum_{q=0}^{Q_f} \alpha_q x^q}_{*} + \underbrace{\epsilon(x)}_{\sigma^2}$$

Noise level: σ^2

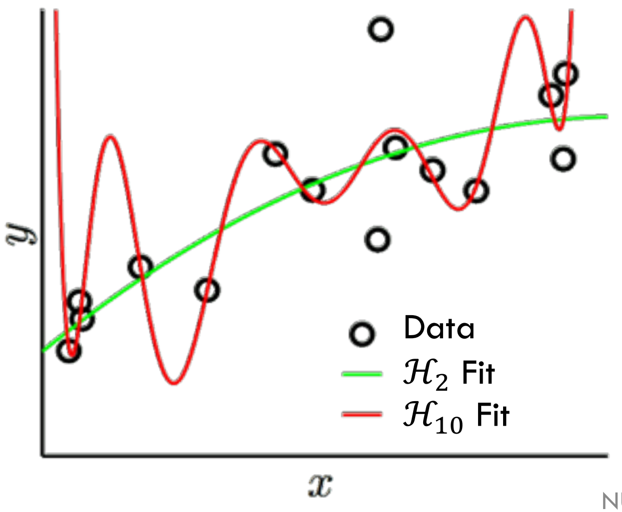
Target complexity: Q_f

Data set size: m

The overfit measure

We fit the data set $(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_m, y_m)$ using our 2 models:

$\mathcal{H}_2$: 2nd order polynomials $\mathcal{H}_{10}$:10th order polynomials

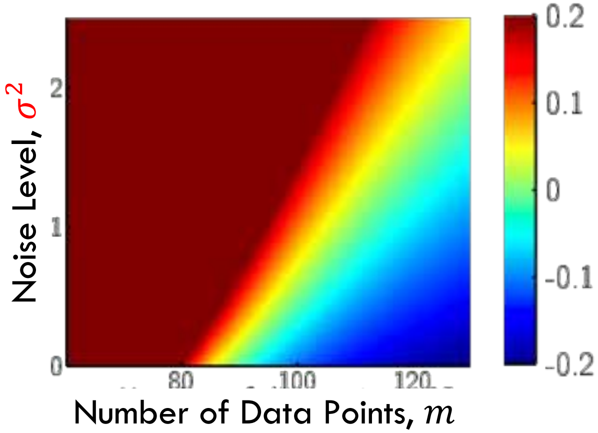


Compare out-of-sample errors of $h_2 \in \mathcal{H}_2$ and $h_{10} \in \mathcal{H}_{10}$

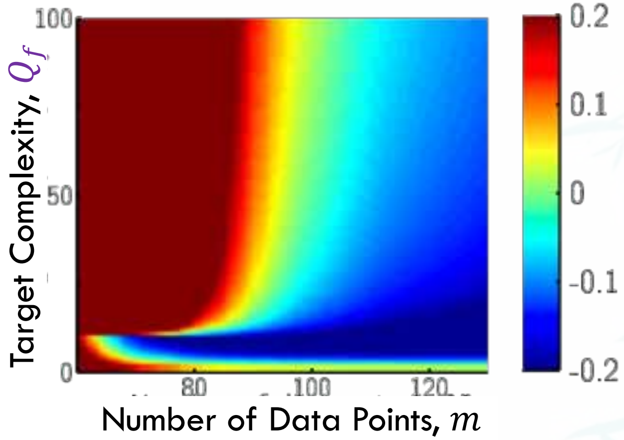
Overfit measure

$L_{test}(h_{10}) - L_{test}(h_2)$

Overfit measure: $L_{test}(h_{10}) - L_{test}(h_2)$

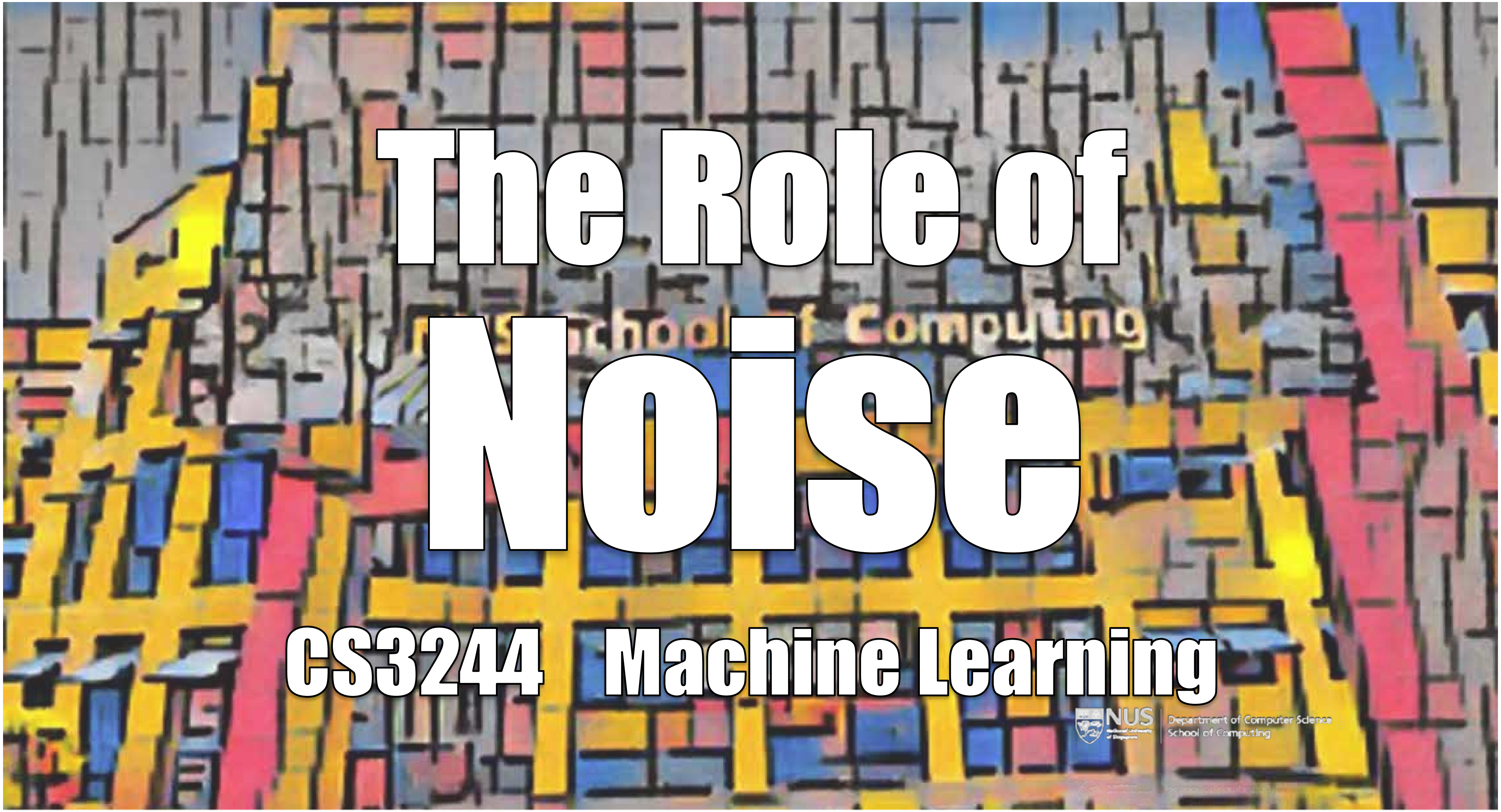


Stochastic Noise



Deterministic Noise

Number of data points	↑	Overfitting	↓
Stochastic Noise	↑	Overfitting	↑
Deterministic Noise	↑	Overfitting	↑


The Role of
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Noise

That part of y that we **cannot** model

It has two sources …

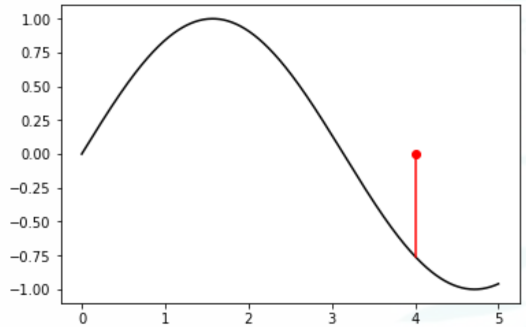
Stochastic Noise: Data Error

We would like to learn f

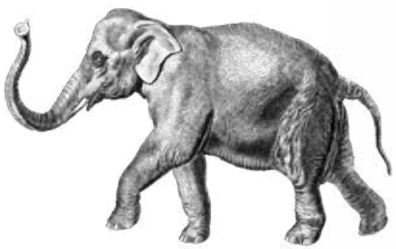
$$y_j = f(\mathbf{x}_j)$$

Unfortunately, we actually observe $\mathcal{D}$

$$y_j = f(\mathbf{x}_j) + \texttt{stochastic\_noise}$$



Stochastic Noise
Fluctuations that we cannot model



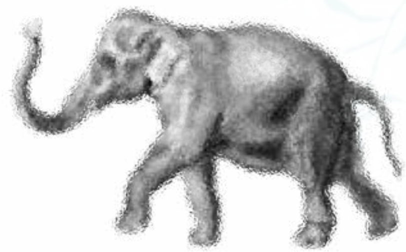


Photo Credits: rawpixel.com

Deterministic Noise: Model Error

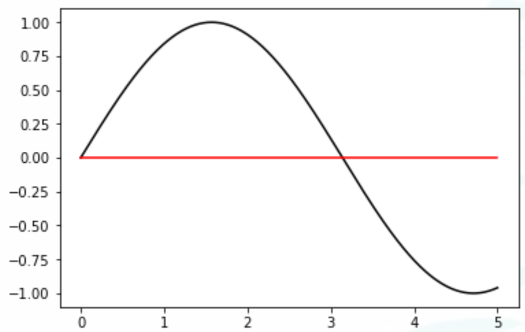
We would like to learn from O

$$y_j = \bar{h}(\mathbf{x}_j)$$

Unfortunately, we only observe $\mathcal{D}$

$$y_j = f(\mathbf{x}_j)$$

$$= \bar{h}(\mathbf{x}_j) + \texttt{deterministic\_noise}$$



Deterministic Noise
The part of f we lack the capacity to model

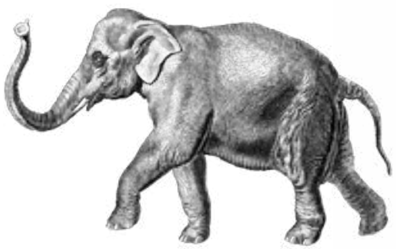
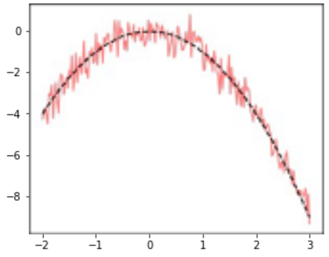


Photo Credits: rawpixel.com

Both sources of noise hurt learning

Stochastic Noise

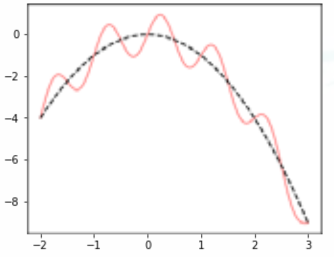


Source: random measurement errors

Re-measure y: Stochastic noise changes

Change $\mathcal{H}$: Stochastic noise still the same

Deterministic Noise



Source: learner's $\mathcal{H}$ cannot model f

Re-measure y: Deterministic noise the same

Change $\mathcal{H}$: Deterministic noise changes

We have a single $\mathcal{D}$ and fixed $\mathcal{H}$ so we cannot distinguish between either; with finite m, $\mathcal{H}$ will try to fit the noise.

Noise and Bias-Variance

Recall the decomposition:

$$\mathbb{E}_{\mathcal{D}}[(h_{\mathcal{D}}(x) - f(x))^2] = \underbrace{\mathbb{E}_{\mathcal{D}}\left[\left(h_{\mathcal{D}}(x) - \bar{h}(x)\right)^2\right]}_{\text{variance}} + \underbrace{\left(\bar{h}(x) - f(x)\right)^2}_{\text{bias}}$$

What if f is a noisy target?

$$y = f(x) + \epsilon(x) \qquad\qquad \mathbb{E}[\epsilon(x)] = 0$$

A noise term

$\mathbb{E}_{\mathcal{D},\epsilon}[(h_{\mathcal{D}}(x) - y)^2] =$

A noise term

$$\mathbb{E}_{\mathcal{D},\epsilon}[(h_{\mathcal{D}}(x) - y)^2] =$$

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

Expand observed y

$$= \mathbb{E}_{\mathcal{D},\epsilon}\left[\left(\underbrace{h_{\mathcal{D}}(x) - \bar{h}(x)}_{①} + \underbrace{\bar{h}(x) - f(x)}_{②} - \underbrace{\epsilon(x)}_{③}\right)^2\right]$$

Associate terms

$$= \mathbb{E}_{\mathcal{D},\epsilon}\left[\left(h_{\mathcal{D}}(x) - \bar{h}(x)\right)^2 + \left(\bar{h}(x) - f(x)\right)^2 + (\epsilon(x))^2 + \cancel{\text{cross terms}}\right]$$

Additional cross terms disappear as $\mathbb{E}(\epsilon(x)) = 0$

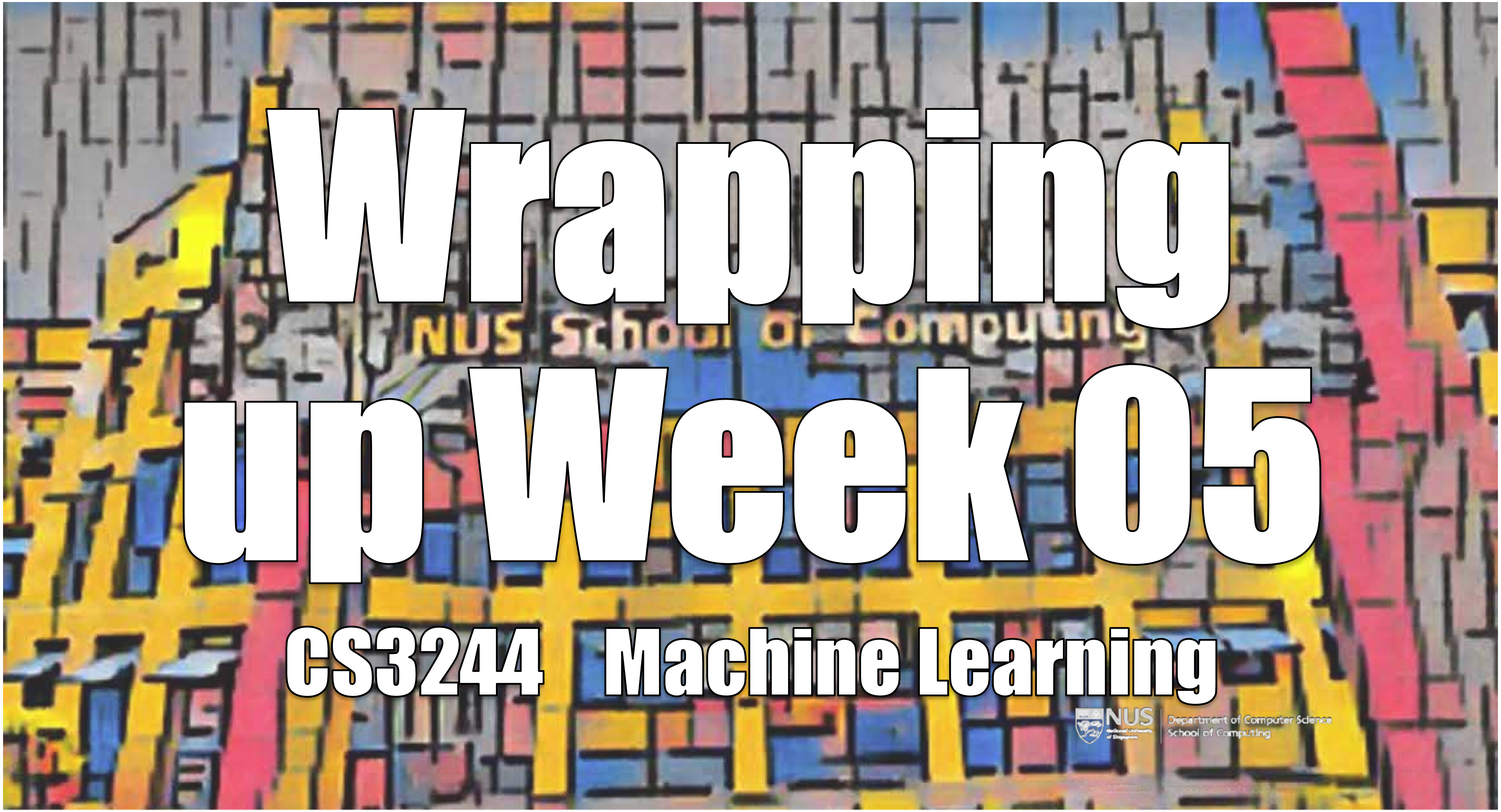
Actually, two noise terms

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

$$\underbrace{\mathbb{E}_{\mathcal{D},x}\left[\left(h_{\mathcal{D}}(x) - \bar{h}(x)\right)^2\right]}_{\text{variance}} + \underbrace{\mathbb{E}_x\left(\bar{h}(x) - f(x)\right)^2}_{\text{bias}} + \underbrace{\mathbb{E}_{\epsilon,x}\left(\epsilon(x)\right)^2}_{\sigma^2}$$

Deterministic Noise

Stochastic Noise


Wrapping up Week 05
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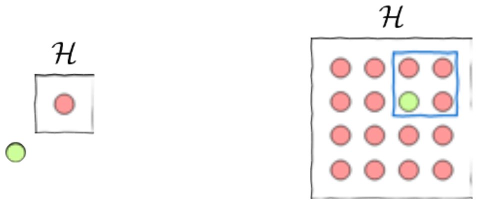
Summary

Bias-Variance Tradeoff

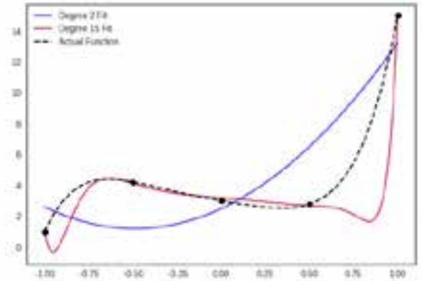
- Bias: How well $\mathcal{H}$ can approximate f overall

- Variance: How well we can zoom in on a good $h \in \mathcal{H}$



Match the 'model complexity' to the **data resources**, not to the target complexity

Overfitting: Fitting the data more than is warranted



Two causes: stochastic + deterministic noise

Bias $\equiv$ deterministic noise

Noise causes overfitting

Overfitting is the disease

Noise is the cause

Learning is led astray by fitting the noise more than the signal

Two Cures:

1. **Regularization**: Restrain the model
2. **Validation**: Reality check by peeking at (the bottom line)

Outlook for next week

Photo by Louis Reed on Unsplash

Assigned Task (due before next Mon)

Read the post https://www.kaggle.com/alexisbcook/cross-validation (10 mins)

Post a 1–2 sentence answer to the topic in your tutorial group: #tg-xx

How does cross validation relate to variance?

[There's an optional exercise with this course page, using random forest and MAE, you're welcomed to do it if you'd like]