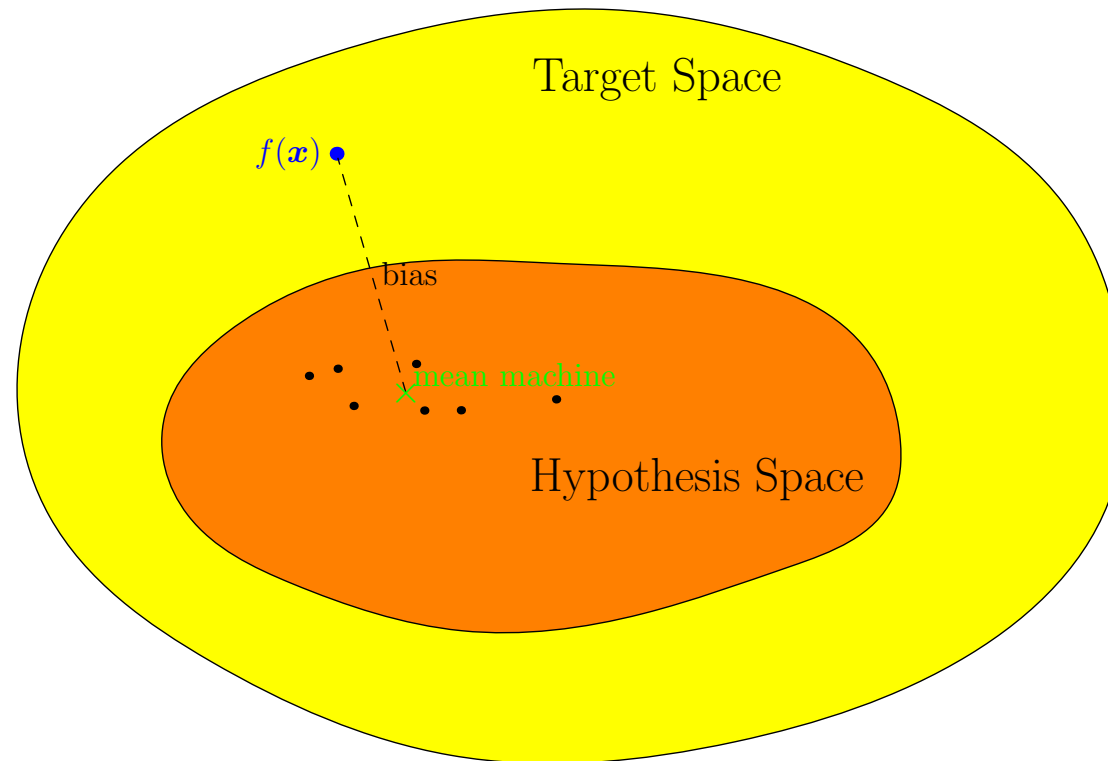


Advanced Machine Learning

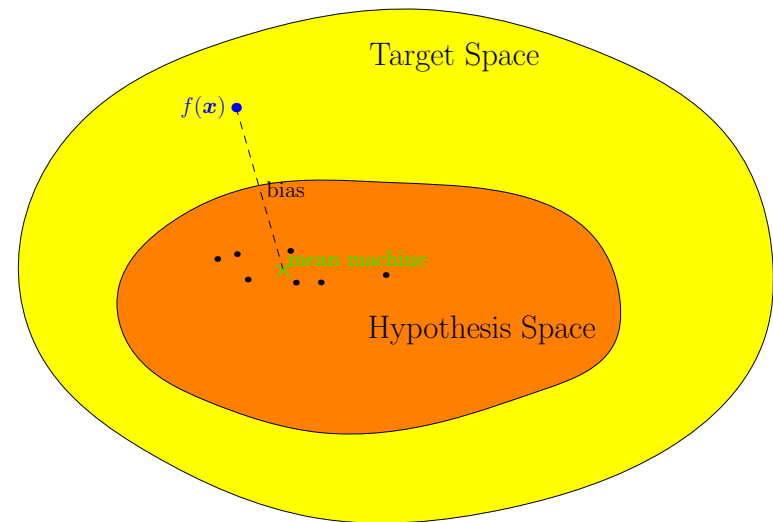
When Machine Learning Works



When ML Works, Bias Variance

Outline

1. **What Makes a Good Learning Machine?**
2. Bias-Variance Dilemma



What Makes a Good Learning Machine?

- We want to understand why some machine learning techniques work well and other don't
- To understand why these works we need to understand what makes a good learning machine
- For this we have to get conceptual and think about **generalisation** performance

generalisation: how well do we do on unseen data as opposed to the training data

What Makes Machine Learning Hard?

- Typically we work in high dimensions (i.e. have many features)■
- The problem can be over-constrained (i.e. we have conflicting data to deal with)■—solve by minimising an error function■
- The problem can be under-constrained (i.e. there are many possible solutions that are consistent with the data)■—need to choose a plausible solution■
- Typically in machine learning the data will be over-constrained in some dimensions and under-constrained in others■
- We can't visualise the data to know what is going on■

Least Squared Errors

- Suppose we want to learn some output y for a feature vector \mathbf{x} ■
- We construct a learning machine that makes a prediction $\hat{f}(\mathbf{x}|\boldsymbol{\theta})$ ■
- We typically choose the machine to minimise a *training loss*

$$L_T(\mathcal{D}) = \sum_{(\mathbf{x}, y) \in \mathcal{D}} \left(\hat{f}(\mathbf{x}|\boldsymbol{\theta}) - y \right)^2 \quad \blacksquare = \sum_{i=1}^m \left(\hat{f}(\mathbf{x}_i|\boldsymbol{\theta}) - y_i \right)^2$$

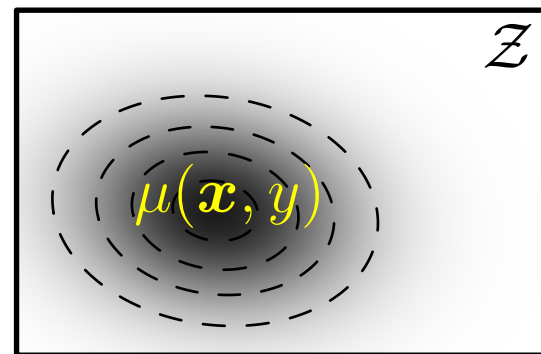
where $\mathcal{D} = \{(\mathbf{x}_i, y_i)\}_{i=1}^m$ is a set of size m , sampled from a probability distribution $\mu(\mathbf{x}, y)$ ■

- We call this machine $\hat{f}(\mathbf{x}|\boldsymbol{\theta}_{\mathcal{D}})$ ■

Generalisation Error

- We want to minimise the *generalisation loss* which in this case is

$$L_G(\boldsymbol{\theta}_{\mathcal{D}}) = \sum_{(\mathbf{x}, y) \in \mathcal{Z}} \mu(\mathbf{x}, y) \left(\hat{f}(\mathbf{x} | \boldsymbol{\theta}_{\mathcal{D}}) - y \right)^2 \blacksquare$$

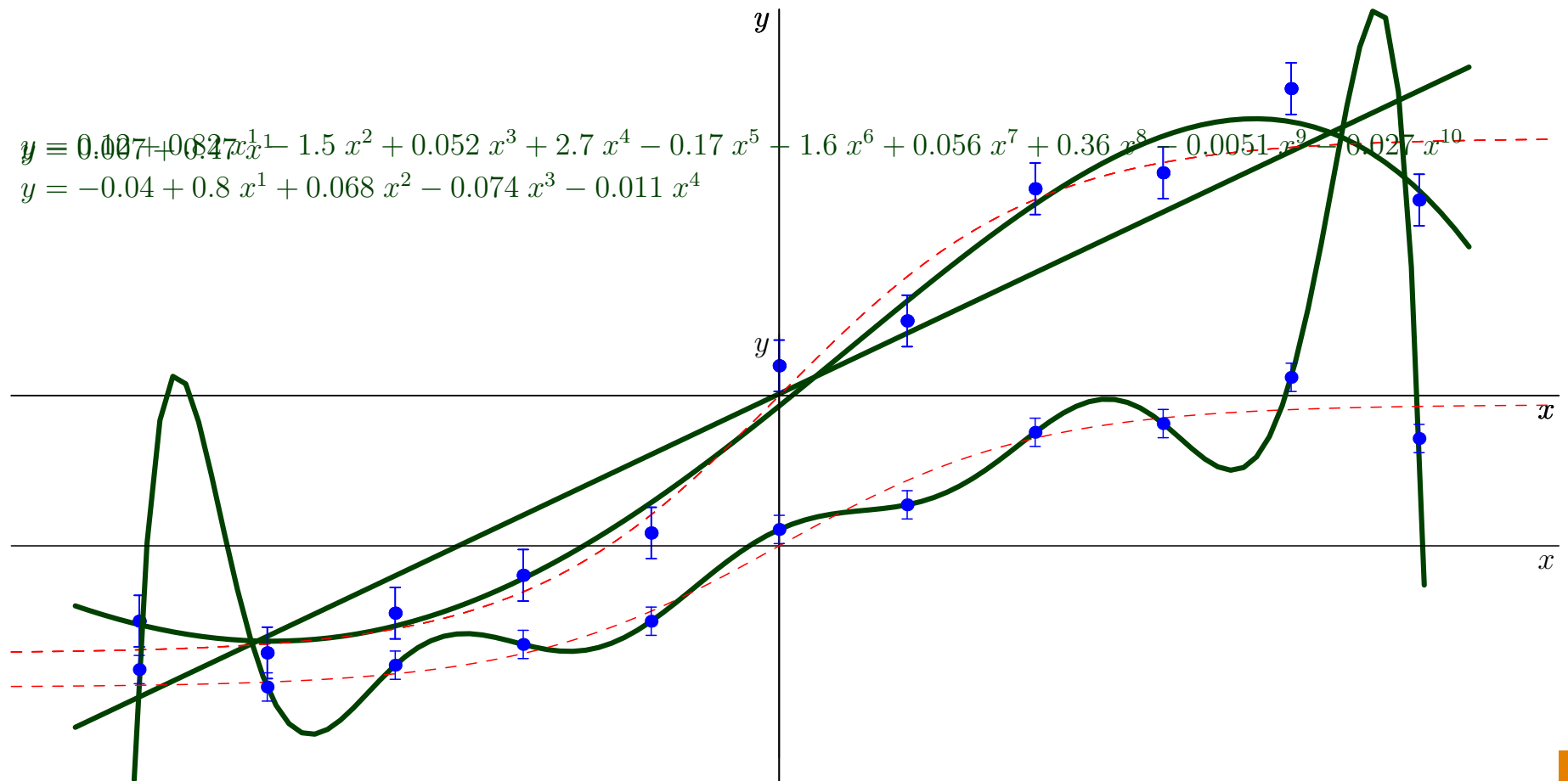


(we can estimate this if we have some labelled examples (\mathbf{x}_i, y_i) which we have not trained on) \blacksquare

- We want to minimise $L_G(\boldsymbol{\theta}_{\mathcal{D}})$ but in practice we are minimising $L_T(\mathcal{D})$, *what could possibly go wrong?* \blacksquare

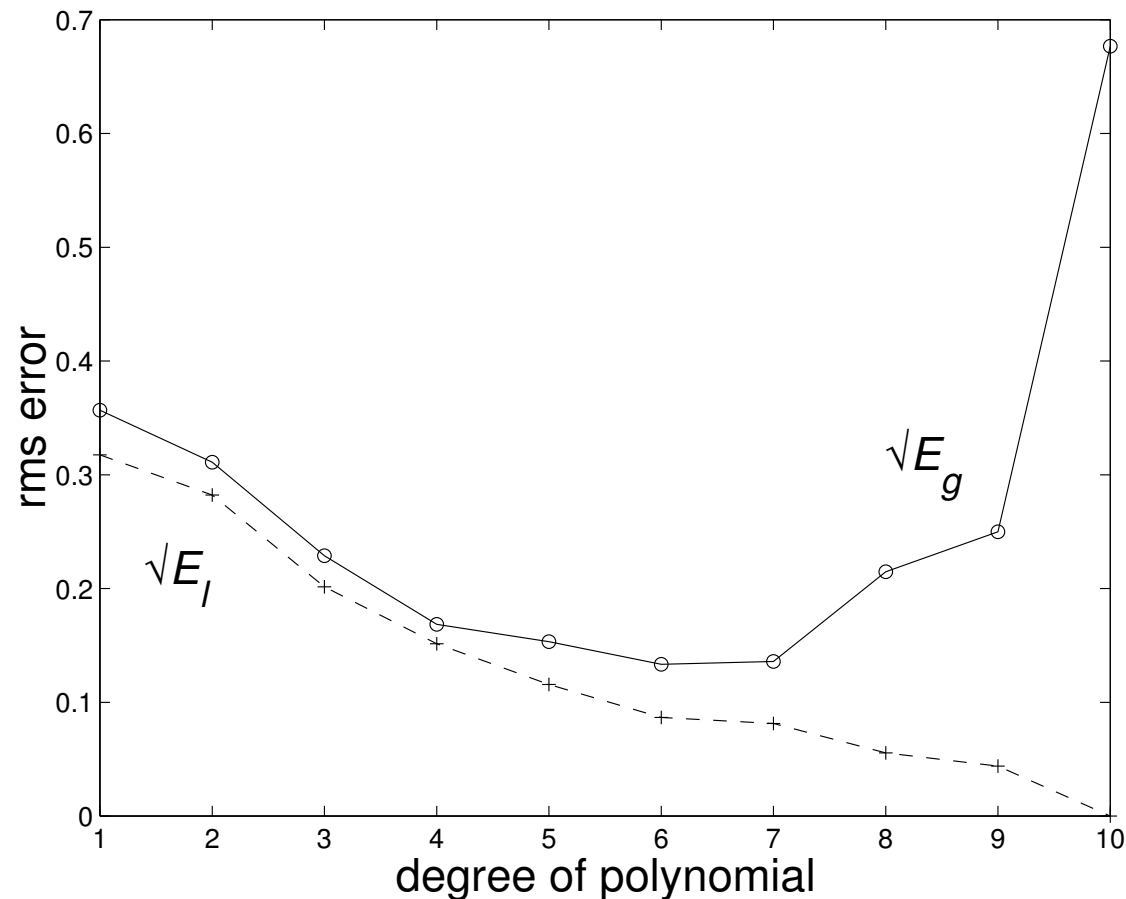
Too Simple or Too Complex?

- Fit $\hat{f}(x|\theta_{\mathcal{D}})$ to data



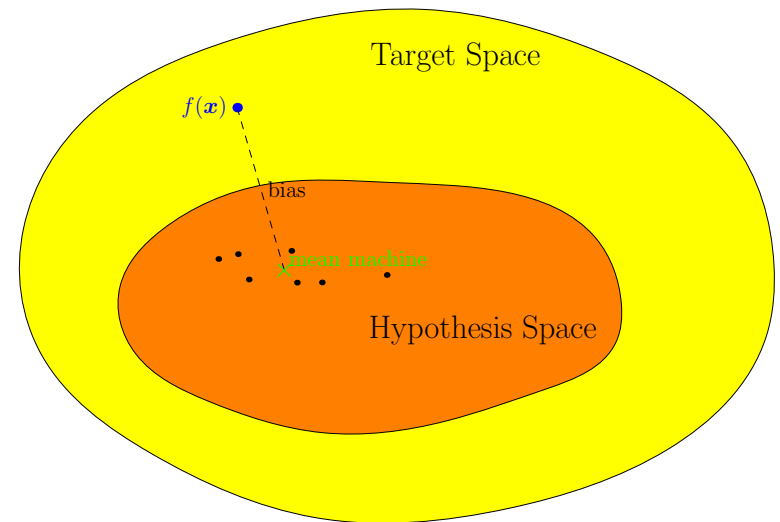
Measuring Generalisation Error for Regression

- Consider the regression example. The root mean squared error is



Outline

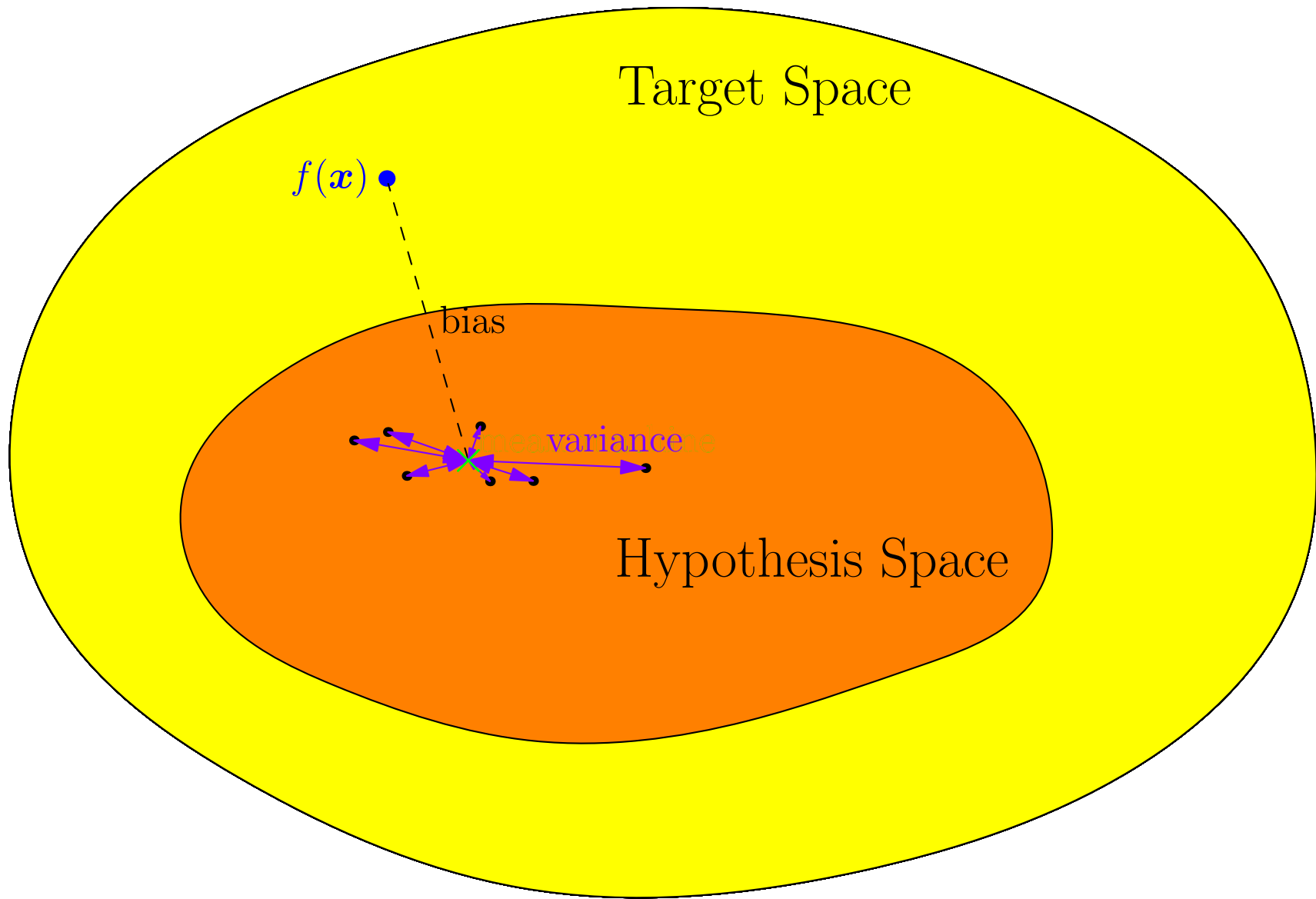
1. What Makes a Good Learning Machine?
2. **Bias-Variance Dilemma**



Expected Generalisation Performance

- Our generalisation performance will depend on our training set, \mathcal{D} ■
- To reason about generalisation we can ask what is the *expected generalisation loss*, when we average over all different data sets of size m drawn independently from $\mu(\mathbf{x}, y)$ ■
- For each data set, \mathcal{D} , we would learn a different approximator $\hat{f}(\mathbf{x}|\boldsymbol{\theta}_{\mathcal{D}})$ ■
- Note that in practice we only get one data set. We might be lucky and do better than the expected generalisation or we might be unlucky and do worse■

Approximation and Estimation Errors



Mean Machine

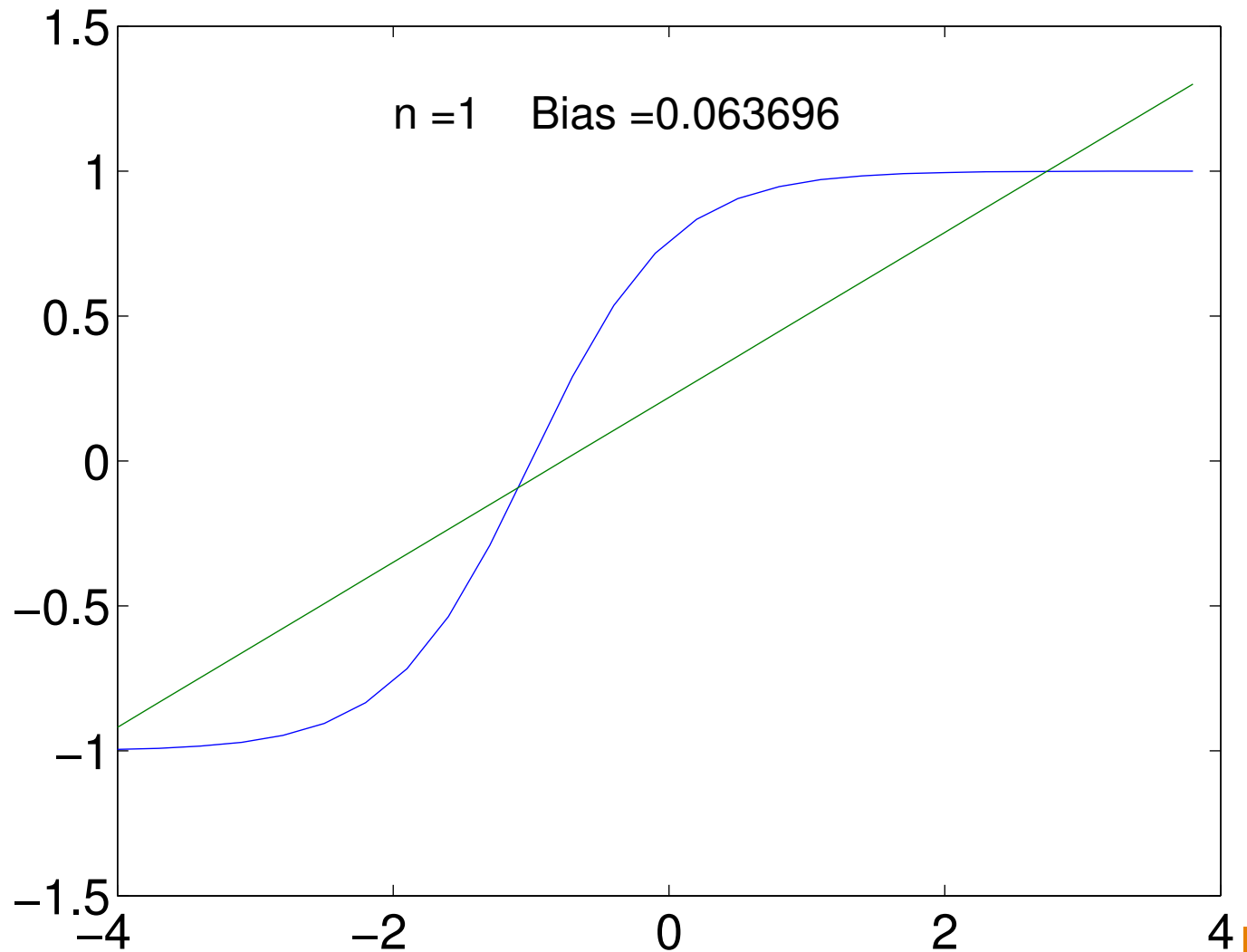
- To help understand generalisation we can consider the mean prediction with respect to machines trained with all data sets of size m

$$\hat{f}_m(\mathbf{x}) = \mathbb{E}_{\mathcal{D}} \left[\hat{f}(\mathbf{x} | \boldsymbol{\theta}_{\mathcal{D}}) \right] \blacksquare$$

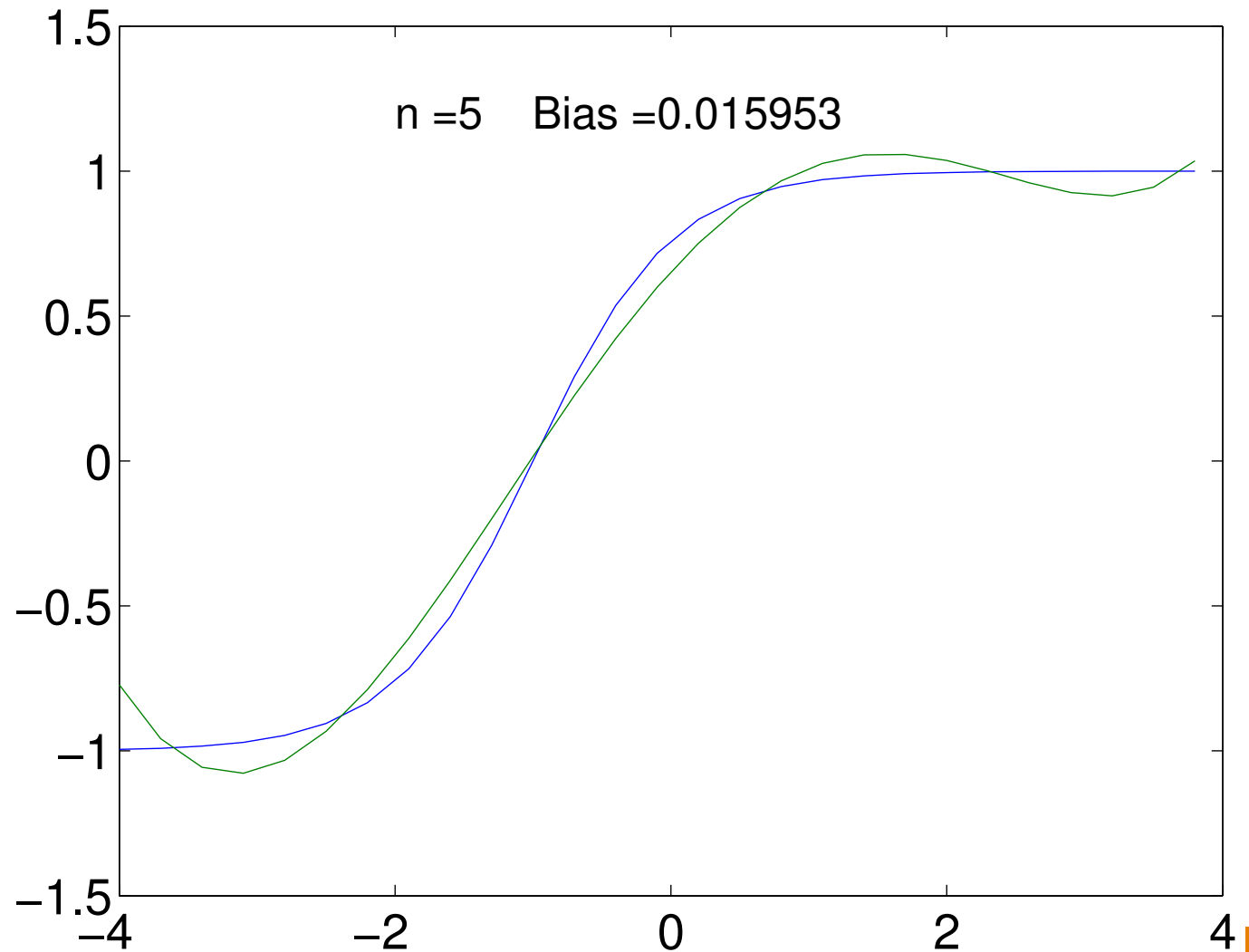
- We can define the **bias** to be generalisation performance of the mean machine

$$B = \sum_{\mathbf{x} \in \mathcal{X}} \mu(\mathbf{x}, y) \left(\hat{f}_m(\mathbf{x}) - y \right)^2 \blacksquare$$

Regression Example $n = 1$



Regression Example $n = 5$



Bias and Variance

Consider the expected generalisation for data sets of size $|\mathcal{D}| = m$

$$\begin{aligned}\bar{L}_G &= \mathbb{E}_{\mathcal{D}}[L_G(\boldsymbol{\theta}_{\mathcal{D}})] = \mathbb{E}_{\mathcal{D}} \left[\sum_{\mathbf{x} \in \mathcal{X}} \mu(\mathbf{x}, y) \left(\hat{f}(\mathbf{x} | \boldsymbol{\theta}_{\mathcal{D}}) - y \right)^2 \right] \\&= \sum_{\mathbf{x} \in \mathcal{X}} \mu(\mathbf{x}, y) \mathbb{E}_{\mathcal{D}} \left[\left(\hat{f}(\mathbf{x} | \boldsymbol{\theta}_{\mathcal{D}}) - y \right)^2 \right] \\&= \sum_{\mathbf{x} \in \mathcal{X}} \mu(\mathbf{x}, y) \mathbb{E}_{\mathcal{D}} \left[\left(\left(\hat{f}(\mathbf{x} | \boldsymbol{\theta}_{\mathcal{D}}) - \hat{f}_m(\mathbf{x}) \right) + \left(\hat{f}_m(\mathbf{x}) - y \right) \right)^2 \right] \\&= \sum_{\mathbf{x} \in \mathcal{X}} \mu(\mathbf{x}, y) \left(\mathbb{E}_{\mathcal{D}} \left[\left(\hat{f}(\mathbf{x} | \boldsymbol{\theta}_{\mathcal{D}}) - \hat{f}_m(\mathbf{x}) \right)^2 \right] + \left(\hat{f}_m(\mathbf{x}) - y \right)^2 \right. \\&\quad \left. + 2 \mathbb{E}_{\mathcal{D}} \left[\left(\hat{f}(\mathbf{x} | \boldsymbol{\theta}_{\mathcal{D}}) - \hat{f}_m(\mathbf{x}) \right) \left(\hat{f}_m(\mathbf{x}) - y \right) \right] \right)\end{aligned}$$

Cross Term

- The cross term vanishes

$$\begin{aligned} C &= \mathbb{E}_{\mathcal{D}} \left[\left(\hat{f}(\mathbf{x}|\boldsymbol{\theta}_{\mathcal{D}}) - \hat{f}_m(\mathbf{x}) \right) \left(\hat{f}_m(\mathbf{x}) - y \right) \right] \\ &= \mathbb{E}_{\mathcal{D}} \left[\left(\hat{f}(\mathbf{x}|\boldsymbol{\theta}_{\mathcal{D}}) - \hat{f}_m(\mathbf{x}) \right) \right] \left(\hat{f}_m(\mathbf{x}) - y \right) \\ &= \left(\mathbb{E}_{\mathcal{D}} \left[\hat{f}(\mathbf{x}|\boldsymbol{\theta}_{\mathcal{D}}) \right] - \hat{f}_m(\mathbf{x}) \right) \left(\hat{f}_m(\mathbf{x}) - y \right) \\ &= \left(\hat{f}_m(\mathbf{x}) - \hat{f}_m(\mathbf{x}) \right) \left(\hat{f}_m(\mathbf{x}) - y \right) = 0 \end{aligned}$$

- Thus

$$\bar{L}_G = \sum_{\mathbf{x} \in \mathcal{X}} \mu(\mathbf{x}, y) \mathbb{E}_{\mathcal{D}} \left[\left(\hat{f}(\mathbf{x}|\boldsymbol{\theta}_{\mathcal{D}}) - \hat{f}_m(\mathbf{x}) \right)^2 + \left(\hat{f}_m(\mathbf{x}) - y \right)^2 \right]$$

Bias and Variance

- We can write the expected generalisation loss as

$$\begin{aligned}\mathbb{E}_{\mathcal{D}}[L_G(\boldsymbol{\theta}_{\mathcal{D}})] &= \sum_{\mathbf{x} \in \mathcal{X}} \mu(\mathbf{x}, y) \mathbb{E}_{\mathcal{D}} \left[\left(\hat{f}(\mathbf{x} | \boldsymbol{\theta}_{\mathcal{D}}) - \hat{f}_m(\mathbf{x}) \right)^2 \right] \\ &\quad + \sum_{\mathbf{x} \in \mathcal{X}} \mu(\mathbf{x}, y) \left(\hat{f}_m(\mathbf{x}) - y \right)^2 = V + B\end{aligned}$$

- Where B is the bias and V is the variance defined by

$$V = \sum_{\mathbf{x} \in \mathcal{X}} \mu(\mathbf{x}, y) \mathbb{E}_{\mathcal{D}} \left[\left(\hat{f}(\mathbf{x} | \boldsymbol{\theta}_{\mathcal{D}}) - \hat{f}_m(\mathbf{x}) \right)^2 \right]$$

Bias-Variance Dilemma

- The bias measure the generalisation performance of the *mean machine* and is large if the machine is too simple to capture the changes in the function we want to learn■
- The variance measures the variation in the prediction of the machines as we change the data set we train on

$$V = \sum_{\mathbf{x} \in \mathcal{X}} \mu(\mathbf{x}, y) \mathbb{E}_{\mathcal{D}} \left[\left(\hat{f}(\mathbf{x} | \boldsymbol{\theta}_{\mathcal{D}}) - \hat{f}_m(\mathbf{x}) \right)^2 \right] \blacksquare$$

- The variance is usually large if we have a complex machine■
- Striking the right balance is often the key to getting good results■

Balancing Bias and Variance

- We want to choose a learning machine that is complex enough to capture the underlying function we are trying to learn, but otherwise as simple as possible■
- There are a number of tricks to achieve this balance■
- Some require us to preprocess the data to reduce the number of inputs■
- Some machines cleverly adjust their own complexity■
- This course looks at machines that achieve this balance■

Lessons

- This course is about understanding machine learning techniques that work well■
- Which one to use will depend on the data set■
- One of the most useful intuitions about what works is the bias-variance framework■
- The bias is high for simple machines that can't capture the data■
- The variance is high for complex machines that are sensitive to the training set■
- Good machines are powerful enough to capture complex data sets, but they can control their own capacity (ability to (over-)fit the data)■