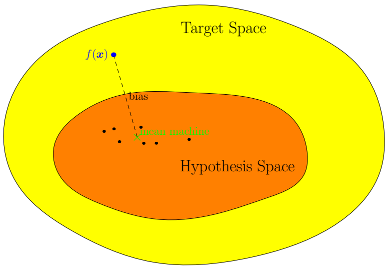
# Advanced Machine Learning

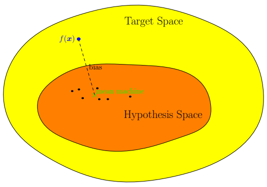
## *When Machine Learning Works*



*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 $\boldsymbol{x}$
- We construct a learning machine that makes a prediction $\hat{f}(\boldsymbol{x}|\boldsymbol{\theta})$
- We typically choose the machine to minimise a *training loss*

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

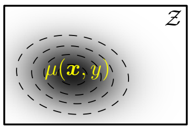
  where $\mathcal{D} = \{(\boldsymbol{x}_i, y_i)\}_{i=1}^m$ is a set of size $m$, sampled from a probability distribution $\mu(\boldsymbol{x}, y)$

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

# Generalisation Error

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

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

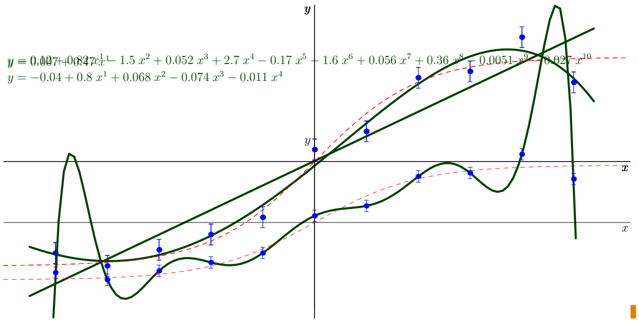


  (we can estimate this if we have some labelled examples $(\boldsymbol{x}_i, y_i)$ which we have not trained on)

- 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?*

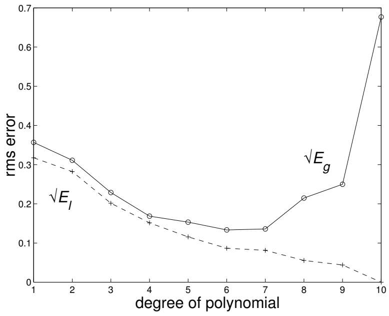
# Too Simple or Too Complex?

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



# Measuring Generalisation Error for Regression

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



# Outline

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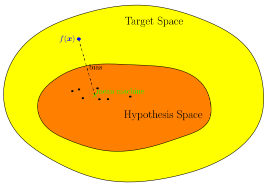
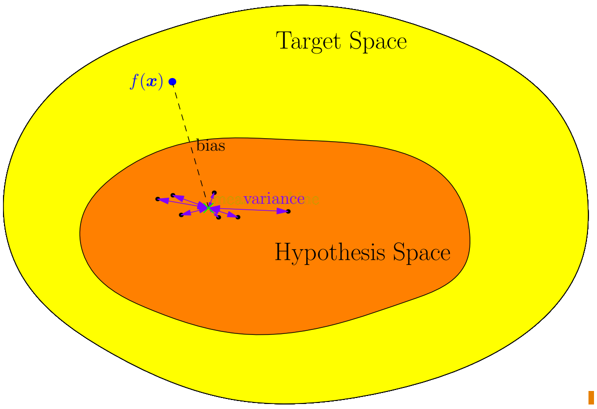


# Expected Generalisation Performance

- 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 $\mu(\boldsymbol{x}, y)$
- For each data set, $\mathcal{D}$, we would learn a different approximator $\hat{f}(\boldsymbol{x}|\boldsymbol{\theta}_\mathcal{D})$
- 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

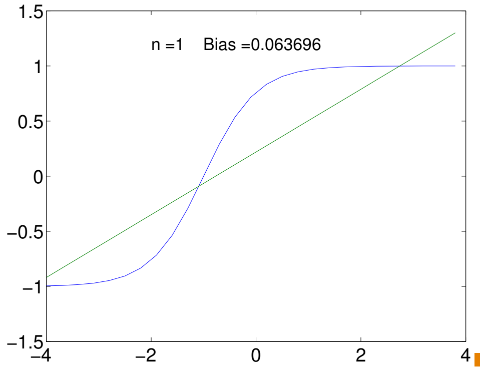
- To help understand generalisation we can consider the mean prediction with respect to machines trained with all data sets of size $m$

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

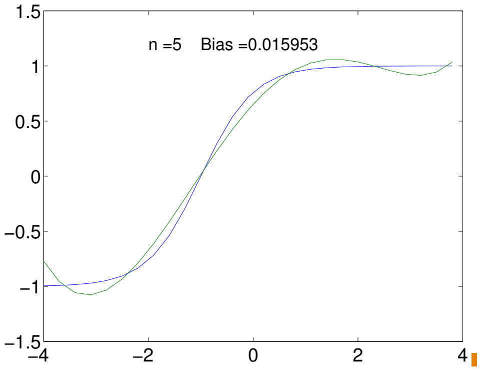
- We can define the **bias** to be generalisation performance of the mean machine

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

# Regression Example $n = 1$



# Regression Example $n = 5$



# Bias and Variance

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

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

# Cross Term

- The cross term vanishes

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

- Thus

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

## Bias and Variance

- We can write the expected generalisation loss as

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

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

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

## 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

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

- 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)