Week 4b:

Model selection

G6061: Fundamentals of Machine Learning [23/24]

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Recap: Regularised linear regression

$$\underset{\mathbf{w}}{\text{minimise}} \quad \left\{ \mathcal{L}(y, \hat{f}(x; \mathbf{w})) + \frac{\lambda}{2} \mathbf{w}^\top \mathbf{w} \right\}$$

- **Larger** λ, higher regularisation:
  too large, we will not capture any useful trends in the data

- **Smaller** λ, lower regularisation:
  too small, our function will likely be too complex

More regularization tends to cause less overfitting.

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Outline

At the end of this session, you should be able to:

- Understand what model selection is and why it is an essential part of machine learning
- Understand the decomposition of an error into bias and variance terms, and how model complexity can trade-off between them.
- Be able to explain how validation data can be used for model selection, and to choose regularisation hyper-parameters.

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Model selection

- Model selection is the process of choosing an appropriate model, in terms of complexity and hyper-parameters,.
- For simple problems, like most we've considered so far, we can choose an appropriate level of complexity just by visual inspection.
- For high-dimensional regression problems, such as predicting variables associated with climate change, it can be less obvious.
- Can you think of a good guiding principle for model selection?

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Occam's razor

Entities should not be multiplied without necessity.
The simplest explanation is usually the best one.

- This is a fundamental principle that is often followed in science, extra complexity needs to be *justifiable*.
- Simple models are easier to test, understand and in the case of ML, fit the parameters.
- Bayesian inference provides a principled solution to reducing model complexity, through regularisation.
- Today we'll talk about methods for interpreting model fitting issues and overcoming them.

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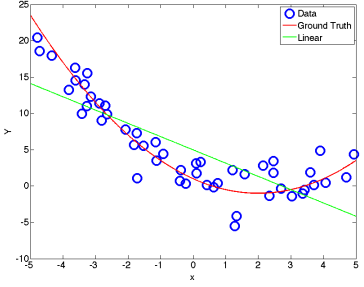
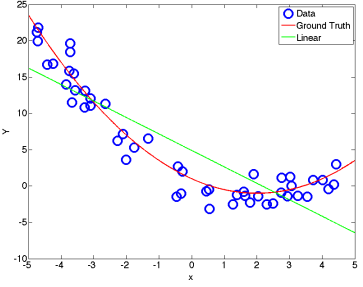
Model complexity

- The simplest models? Functions that return a constant number or a straight line.
- These models are likely to have a large degree of error!
  - Model too "simple" $\rightarrow$ does not fit the data well

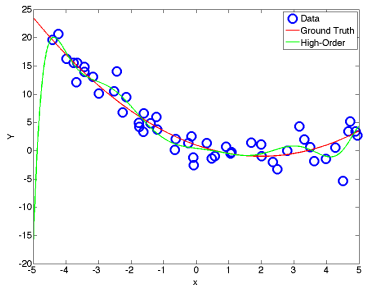


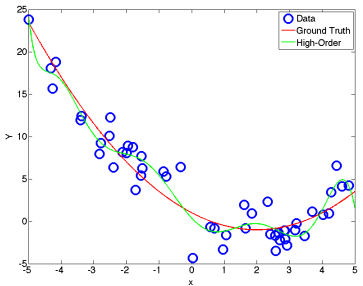


- However, the parameters will be *reliable* to estimate from different subsets of data.
- These models are referred to as *biased*.

Model complexity

- A more complex model will fit the training samples much better.
- However, if the model is too "complex" $\rightarrow$ small changes in the training data lead to large differences in the trained model.





- Because of the variability in model fitting with different training samples, these models are said to have high *variance*.

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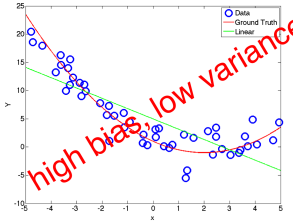
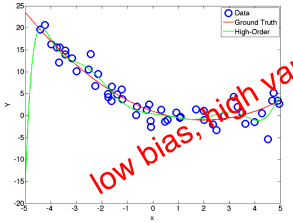
Bias-variance trade-off

- Choice of hypothesis class and hyper-parameters affects bias
  - More complex hypothesis class → less bias
  - More complex hypothesis class → more variance



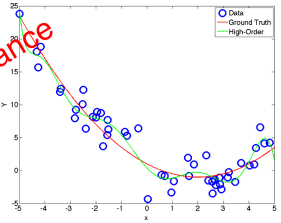
1st degree of polynomial

...



10th degree of polynomial

low bias, low variance
(ideal case)



10th degree of polynomial

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Bias-variance example

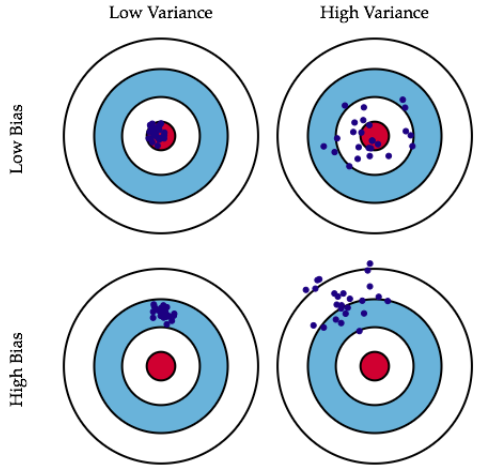

figure is from S. Fortmann-Roe

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(Squared) bias of predictor

- Given dataset $\mathcal{D}$ with N examples, we would like to learn function $\hat{f}_{\mathcal{D}}(x)$
- Learning a different dataset $\mathcal{D}'$ also with N examples, results in a different $\hat{f}_{\mathcal{D}'}(x)$
- **Expected hypothesis**: $\text{Expectation}_{\mathcal{D}}[\hat{f}_{\mathcal{D}}(x)] := \hat{f}_{\text{ave}}(x)$

- **Bias**:
  difference between what you expect to learn $\hat{f}_{\text{ave}}(x)$ and the ground truth $f(x)$
  - Measures how well you expect to represent true solution
  - Decreases with more **complex** model
  - Bias^2 at a single data point x: $(f(x) - \hat{f}_{\text{ave}}(x))^2$
  - Average Bias^2: $\text{Expectation}_x[(f(x) - \hat{f}_{\text{ave}}(x))^2]$

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Variance of predictor

- Given dataset $\mathcal{D}$ with N examples, we would like to learn function $\hat{f}_{\mathcal{D}}(x)$
- Learning a different dataset $\mathcal{D}'$ also with N examples, results in a different $\hat{f}_{\mathcal{D}'}(x)$
- **Expected hypothesis**: $\text{Expectation}_{\mathcal{D}}[\hat{f}_{\mathcal{D}}(x)] := \hat{f}_{\text{ave}}(x)$

- **Variance**:
  difference between what you expect to learn $\hat{f}_{\text{ave}}(x)$ and what you learn from a particular dataset $\hat{f}_{\mathcal{D}}(x)$
  - Measures how sensitive predictor is to specific dataset
  - Decreases with **simpler** model
  - Variance at a single data point x: $\text{Expectation}_{\mathcal{D}}[(\hat{f}_{\mathcal{D}}(x) - \hat{f}_{\text{ave}}(x))^2]$
    Note: $\text{Var}(x) = \text{Expectation}_x[(x - \mu)^2]$
  - Average Variance: $\text{Expectation}_x[\text{Expectation}_{\mathcal{D}}[(\hat{f}_{\mathcal{D}}(x) - \hat{f}_{\text{ave}}(x))^2]]$

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Bias-variance decomposition of squared error

$$\begin{aligned}&\text{Expectation}_{\mathcal{D}}[(\hat{f}_{\mathcal{D}}(x) - f(x))^2] \\ &= \underbrace{\text{Expectation}_{\mathcal{D}}[(\hat{f}_{\mathcal{D}}(x) - \hat{f}_{\text{ave}}(x))^2]}_{\text{variance}(x)} + \underbrace{(\hat{f}_{\text{ave}}(x) - f(x))^2}_{\text{bias}^2(x)}\end{aligned}$$

- **Bias**:
  difference between what you expect to learn $\hat{f}_{\text{ave}}(x)$ and the ground truth $f(x)$
  - More complex hypothesis class $\rightarrow$ less bias
- **Variance**:
  difference between what you expect to learn $\hat{f}_{\text{ave}}(x)$ and what you learn from a particular dataset $\hat{f}_{\mathcal{D}}(x)$
  - More complex hypothesis class $\rightarrow$ more variance

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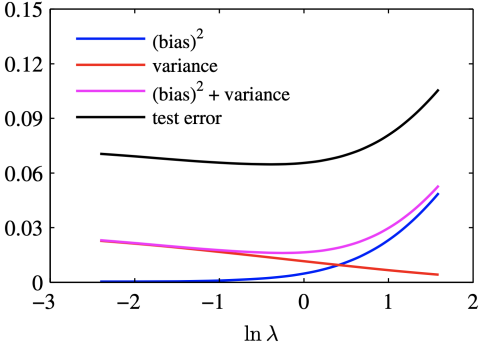
Bias-variance decomposition - demonstration

- This approach of understanding model error gives us some insight into the appropriateness of our model complexity.
- For example, you wanted some more intuition into the performance of a regression model, rather than just looking at the squared error.



[1] from Bishop, Pattern Recognition and Machine Learning

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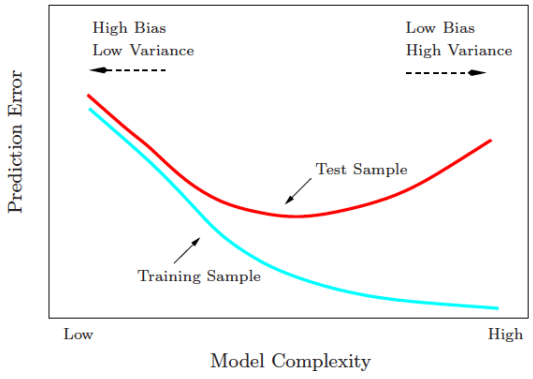
Training and test error as a function of model complexity

For example, the higher the degree of a polynomial, the more complex.



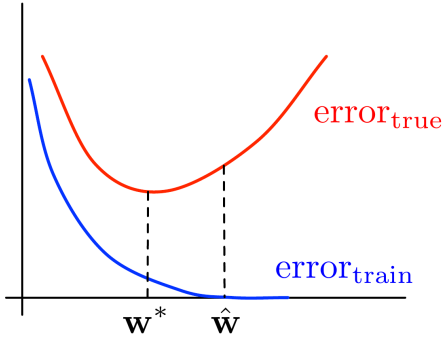
The Elements of Statistical Learning

Extreme case of bias vs. variance

- **Over-fitting**: a learning algorithm overfits the training data if it outputs a solution $\hat{\mathbf{w}}$ when there exists another solution $\mathbf{w}^*$ such that

$$\text{error}_{\text{train}}(\hat{\mathbf{w}}) < \text{error}_{\text{train}}(\mathbf{w}^*) \wedge \text{error}_{\text{true}}(\mathbf{w}^*) < \text{error}_{\text{true}}(\hat{\mathbf{w}})$$

where $\text{error}_{\text{true}}$ is the error at test set and $\text{error}_{\text{train}}$ is the error at training set.



- Low (near zero) bias but very high variance is over-fitting

Analysing machine learning models

- Imagine you're training a model, but it's not going well.
- Common approach: try improving the algorithm in different ways:
  - Try a smaller set of features
  - Try a larger set of features
  - Use a different value for regularisation parameter
  - Try using different machine learning models: naïve Bayes, logistic regression, decision tree, k-Nearest Neighbour, linear perceptron, random forest, etc.
- The approach above might work, but it is very time consuming, and largely a matter of luck whether you end up fixing what the problem really is.

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Diagnostic for bias vs. variance

- Better approach:
  - Run diagnostics to figure out what the problem is
  - Fix whatever the problem is
- Suppose you suspect the problem is either:
  - Over-fitting (high variance)
  - Too few features to differentiate positive class from negative class (high bias)
- Diagnostic:
  - High variance: training error will be much lower than test error
  - High bias: training error will also be high

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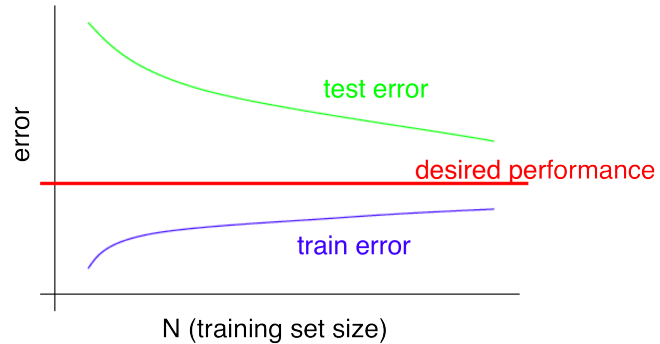
More on bias vs. variance

Typical learning curve for **high variance** (at fixed model complexity):

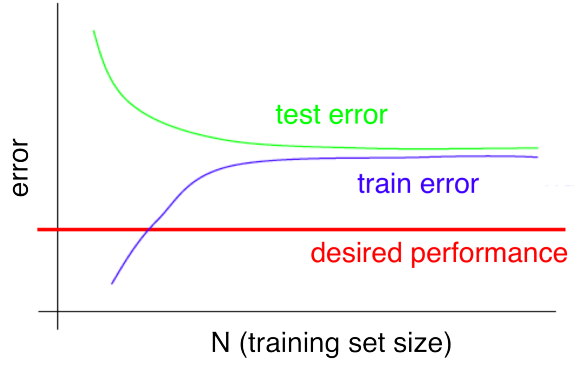


- Validation error still decreasing as N increases.
- Large gap between training and validation error.

figure is from Andrew Ng

More on bias vs. variance

Typical learning curve for **high bias** (at fixed model complexity):



- Even training error is unacceptably high
- Small gap between training and validation error

figure is from Andrew Ng

Diagnostics tell you how to proceed

- Fixes to try:
  - Try a smaller set of features (feature selection) or introduce more regularisation

    Fixes high variance
  - Try a larger set of features (non-linear mapping on features / kernel methods) or reduce regularisation

    Fixes high bias

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How to choose our hyper-parameters?

- How do we pick the regularisation constant λ
  - and all other constants or parameters in machine learning models: one thing machine learning does not lack is constants to tune!

Training/validation split

- What we really care about is whether the classifier has learned to *generalise*.
- This can be evaluated by assessing the classification accuracy on a **validation set**.
  - This is a set of labelled data that *was not* used during training.
  - It is assumed that this data is randomly chosen from a set of images that share common characteristics.
  - this is often referred to as "independently and identically distributed" or iid.
  - If the validation set is unusual in some way, it will give us a poor measure of how good our classifier is.
- Penalises the model *overfitting*, i.e., just understanding the training set really well.

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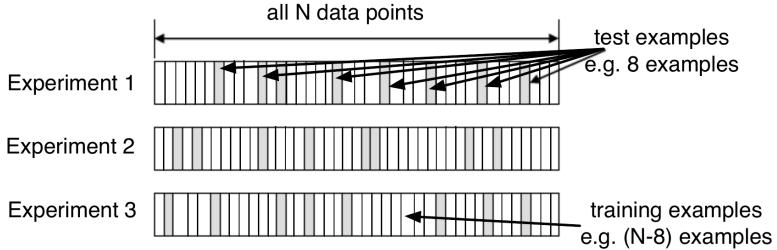
Random subsampling

Random subsampling performs K data splits of the entire dataset

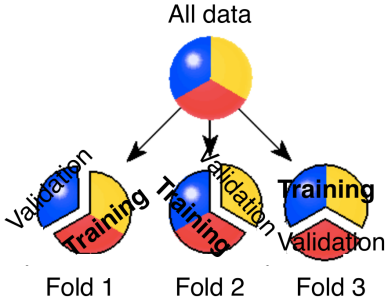
- Each data split randomly selects a fixed number of examples without replacement as test examples
- For each data split we retrain the classifier from scratch with the training examples and then estimate error rate for split i, e_i, with the test examples



- The true error estimate is obtained as the average of the separate estimates e_i

$$e = \frac{1}{K}\sum_{i=1}^{K} e_i$$

K-fold cross-validation



- The dataset is split into K sections, in this case K=3.
- In each run, one fold of data instances is removed from the training set and used to validate or test the model.
- Expected accuracy calculate by averaging over splits:

$$e = \frac{1}{K} \sum_{i=1}^{K} e_i$$

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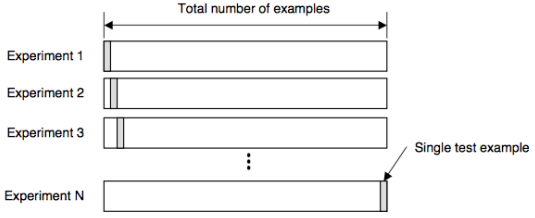
Leave-One-Out (LOO) cross-validation

Leave-one-out is the degenerate case of K-fold cross-validation, where K is chosen as the total number of examples

- For a dataset with N examples, perform N experiments
- For each experiment use N-1 examples for training and the remaining example for testing



- As before, the true error is estimated as the average error rate on test examples

$$e = \frac{1}{N}\sum_{i=1}^{N} e_i$$

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Peeking and maintaining a test set

- Having validation sets is all well and good, but it still leaves a problem: as we may make choices based on validation set performance.
- For this reason we might want to keep a separate test set, to evaluate our final performance.
- We *never* look at the test set, until right at the end.
- This is useful if we build a real-life system and need to say how accurate we think it will be.
- If we ever mix our training/validation/testing datasets, this is called peeking. It results in over-inflating our ideas of how well our model will perform.
- Always choose your train/test/split randomly, otherwise you might introduce some odd differences, e.g., the first half of the dataset might only contain cats.

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Case study

- Model: linear classifier?

$$\mathcal{L}' = \mathcal{L}_{\text{mse}} + \frac{\lambda}{2}\mathbf{w}^\top\mathbf{w}$$

- We search λ in the λ-parameter space over $\{10^{-4}, 10^{-3}, 10^{-2}, 10^{-1}, 1\}$
- We will use 10-fold stratified cross-validation for each λ and compute accuracy
- Accuracy rate$\pm$ STD result: 10-fold cross-validation table for varying the parameter λ

results are example only!

$\lambda = 10^{-4}$	10^{-3}	10^{-2}	10^{-1}	1
63.15 ± 2.7	66.47 ± 1.8	67.79 ± 1.5	67.27 ± 1.9	63.11 ± 2.5

- Based on the cross-validation results, I will choose $\lambda = 10^{-2}$
- Re-train the classifier with $\lambda = 10^{-2}$ using the whole training dataset and predict the labels for test set where the labels are *unknown*.

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Case study – more generally

- Magic parameters are everywhere in machine learning models, for example,
  - number of trees, minimum number of instances required to split an internal node, choice of impurity measure in random forest
  - choice of kernel function, value of kernel coefficients, and regularisation parameter in support vector machine
  - choice of regularisation parameter in logistic regression
  - choice of parameter k in k nearest neighbour (kNN) classifier
  - ...
- The more parameters to find, the more computational cost to do cross-validation
  - Suppose we want to find out the best number of trees and minimum samples at leaf nodes in random forest

number of trees \ minimum samples	1	5	10	50
500	?	?	?	?
1,000	?	?	?	?
5,000	?	?	?	?
10,000	?	?	?	?

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Summary and outlook

- Today we've discussed some of the principles behind model selection: Occam's razor, model complexity, bias-variance trade-off
- We've talked about how to diagnose model training issues, and choose your hyper-parameters:
  training/validation split

Next lecture:

- Neural networks I

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