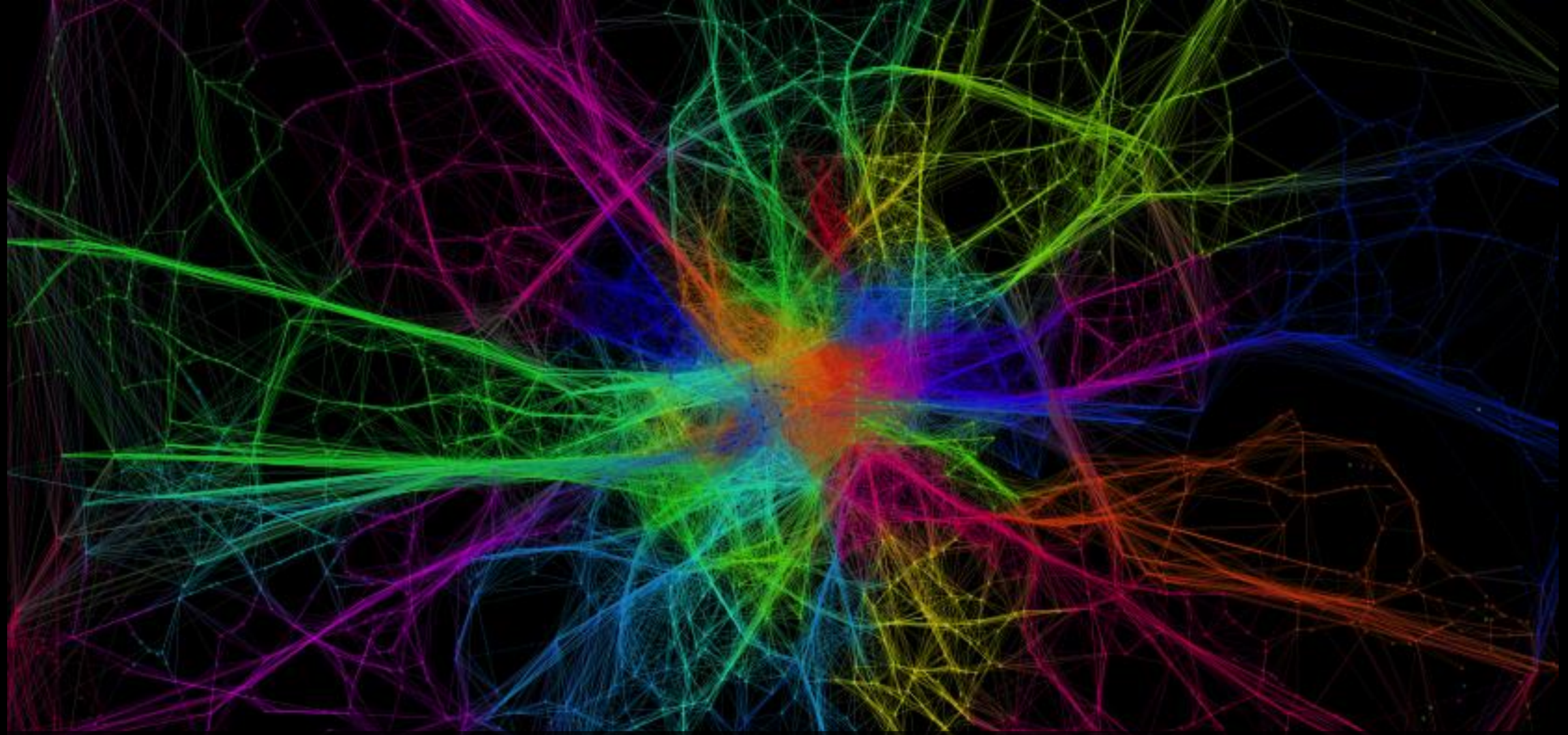


Analysis Workflow

CASA0006: Data Science for Spatial Systems

Huanfa Chen

CASA0006

1. Introduction to Module
2. Supervised Machine Learning
3. Tree-based Methods
4. Artificial Neural Networks
5. Analysis Workflow
6. Spatial Clustering
7. Panel Regression
8. Difference in Difference
9. Regression Discontinuity
10. Dimensionality Reduction

Objectives

- Be able to understand and conduct basic error analysis (*'is my model overfitting on the training data'*)
- Be able to improve machine learning models using strategies (*'how to tackle overfitting or underfitting'*)
- Be able to detect and prevent data leakage

Note: the theory of bias and variance may be a bit hard to follow. You don't need to understand everything of this part. The key point is model diagnosis based on training and testing error.

Outline

1. Basic error analysis
2. Machine learning strategy
3. Data leakage

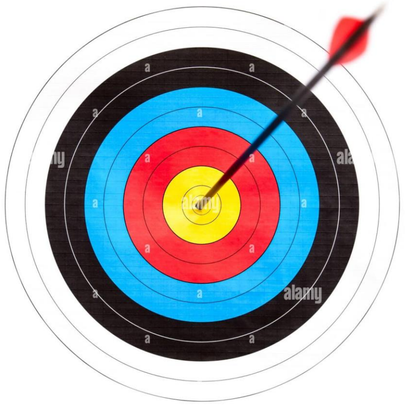

Basic error analysis
St. George's
Bermuda
Imagery ©2014 CNES / Astrium, DigitalGlobe

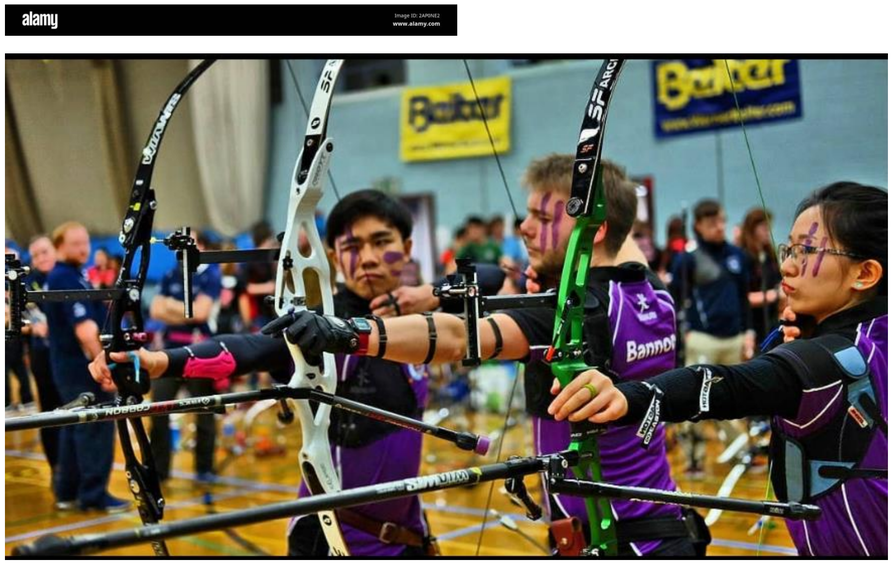
Basic error analysis

- When we discuss supervised learning models, prediction errors can be decomposed into two main subcomponents
  - Error due to bias
  - Error due to variance
- There is a tradeoff between a model's ability to minimise bias and variance (called bias-variance tradeoff)
- Why important? These two errors are linked to over- and under-fitting. Understanding these two types of error can help us diagnose model results and mitigate over- or under-fitting.
- Three ways to understand bias & variance: graphically, conceptually, mathematically

Bias-variance in archery

- Archery is as cool as machine learning.
- Archery: supervised learning
- Archer: prediction algorithm (like, neural network)
- Task: hit the ‘Gold’ or ‘bull’s eye’ (Centre of the target, often in yellow).
- To know your performance: you shoot many times and then summarise the **mean** and **variance** of scores.
- **Bias** = full score - mean score
- **Variance** = variance of the scores



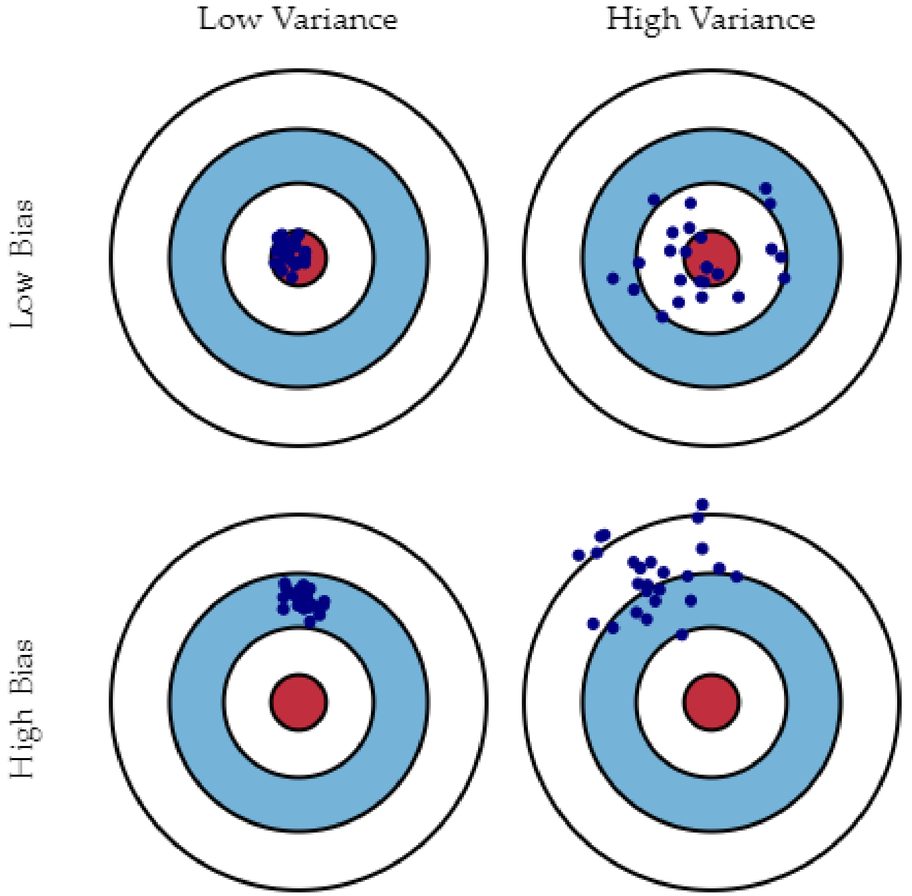


https://clubs-societies.london.ac.uk/organisation/archery/

Bias-variance in archery

- Four combinations of bias and variance (two levels each)

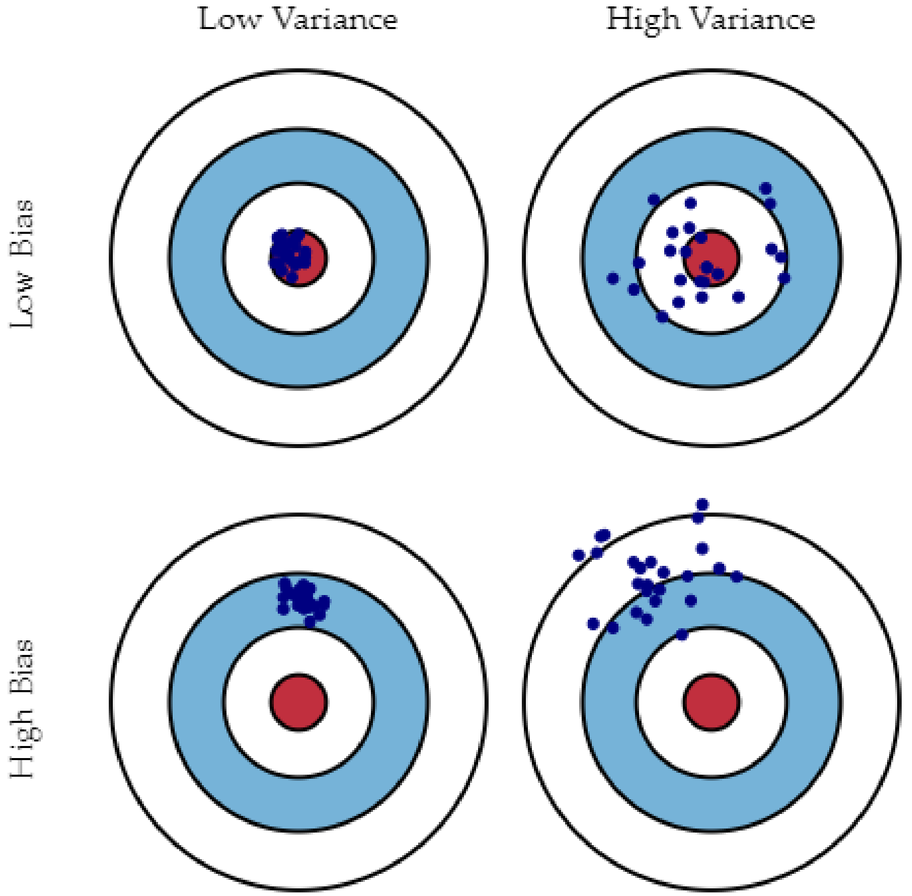
Bias \ Variance	Low	High
Low	Great!	High-variance, not consistent
High	Low accuracy, need more training	*Improvement needed*



Conceptual definition

- **Error due to Bias**: the difference between the expected (or average) prediction of our model and the correct value which we are trying to predict
- **Error due to Variance**: the variability of a model prediction for a given data point

- Note: to measure bias or variance, multiple runs of models are necessary, which is similar to estimate the mean or variance of a variable.



Mathematical definition

- If we denote the target variable as Y and covariates as X, we assume that there is a relationship: $Y = f(X) + \in$
- We build a model to estimate $f(X)$, which leads to $\hat{f}(x)$.
- The expected square error at a data point x is

$$Err(x) = \mathrm{E}[\left(\mathrm{Y} - \hat{f}(x)\right)^2]$$

- This error can be decomposed into three components:

$$Err(x) = Bias^2 + Variance + Irreducible\ Error$$

- Irreducible Error: the noise term, which can't be reduced by any model

Bias-variance in machine learning

In the context of ML models

- **Bias**: how close the model can get to the true relationship between the predictors and the outcome

- Normally, a linear regression model has a higher bias than decision trees or neural networks, as it has strong assumptions regarding linear relationship between y and x and would fail to fit when the actual relationship is non-linear.

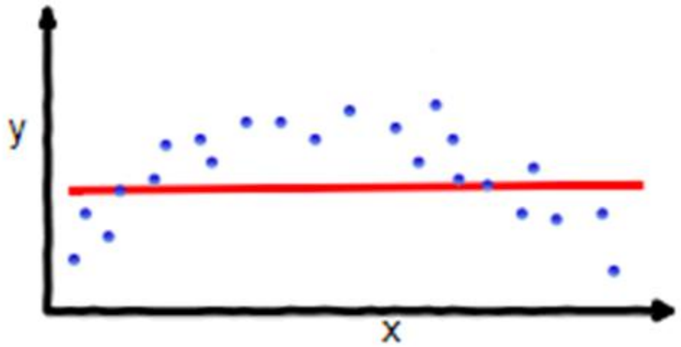
Bias-variance in machine learning

- **Variance**: the amount by which the model would change if we estimated it using a different training data set
- A high-variance model will change a lot with small changes to training dataset
- Given an algorithm, the higher complexity, the higher variance. (Link with model hyperparameters)
- Decision tree (DT): variance ↑ when max_depth ↑ or min_samples_leaf ↓
- Neural networks (NN): variance ↑ when n_layer ↑ or n_neurons ↑
- Note: we can't directly compare variance of a CART and NN

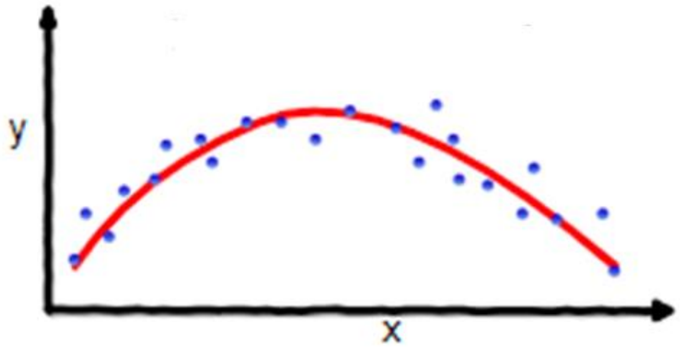
Bias-variance in machine learning

- Example of curve fitting (1-dimensional x)

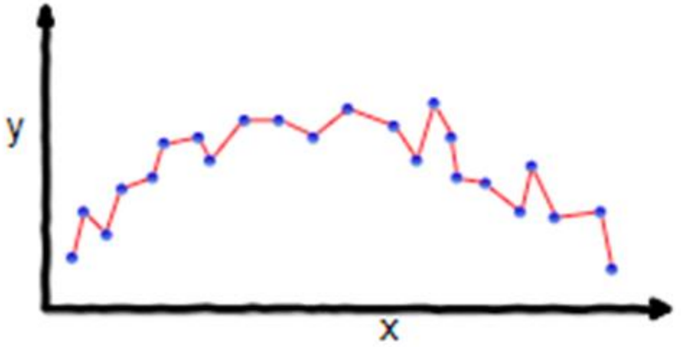
Y = ax+b



Y = ax^2+bx+c



Y = $\sum_{i=0}^{N} a_i x_i$



Model complexity & variance: low -> high

Bias-variance trade-off

- Ideally, we want a model with low bias and low variance, but this is very challenging in practice. In fact, this could be described as the goal of applied machine learning for a given predictive problem.
- The bias-variance trade-off
  - Reducing the bias can easily be achieved by increasing the variance.
  - Reducing the variance can easily be achieved by increasing the bias.
- This is a good conceptual framework for thinking how to choose models and model configuration (or hyperparameters).

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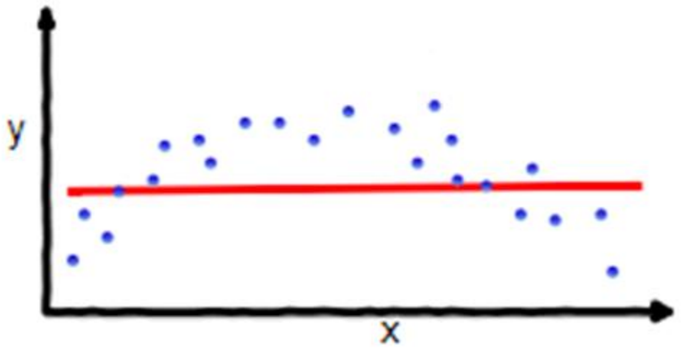
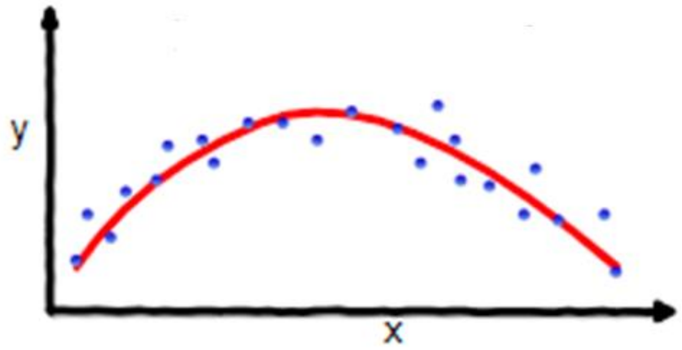
Bias-variance trade-off

- How to choose the N hyperparameter for curve fitting?

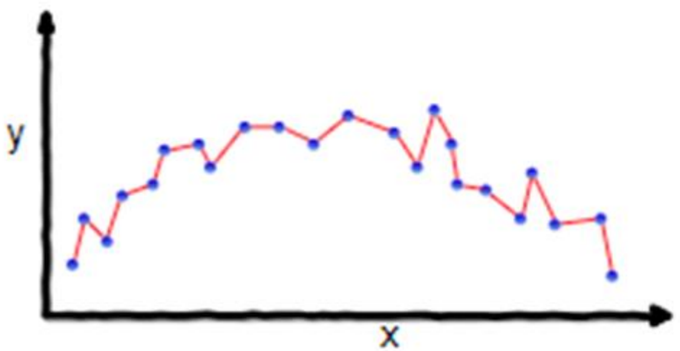
Y = ax+b



Y = ax^2+bx+c



Y = $\sum_{i=0}^{N} a_i x_i$



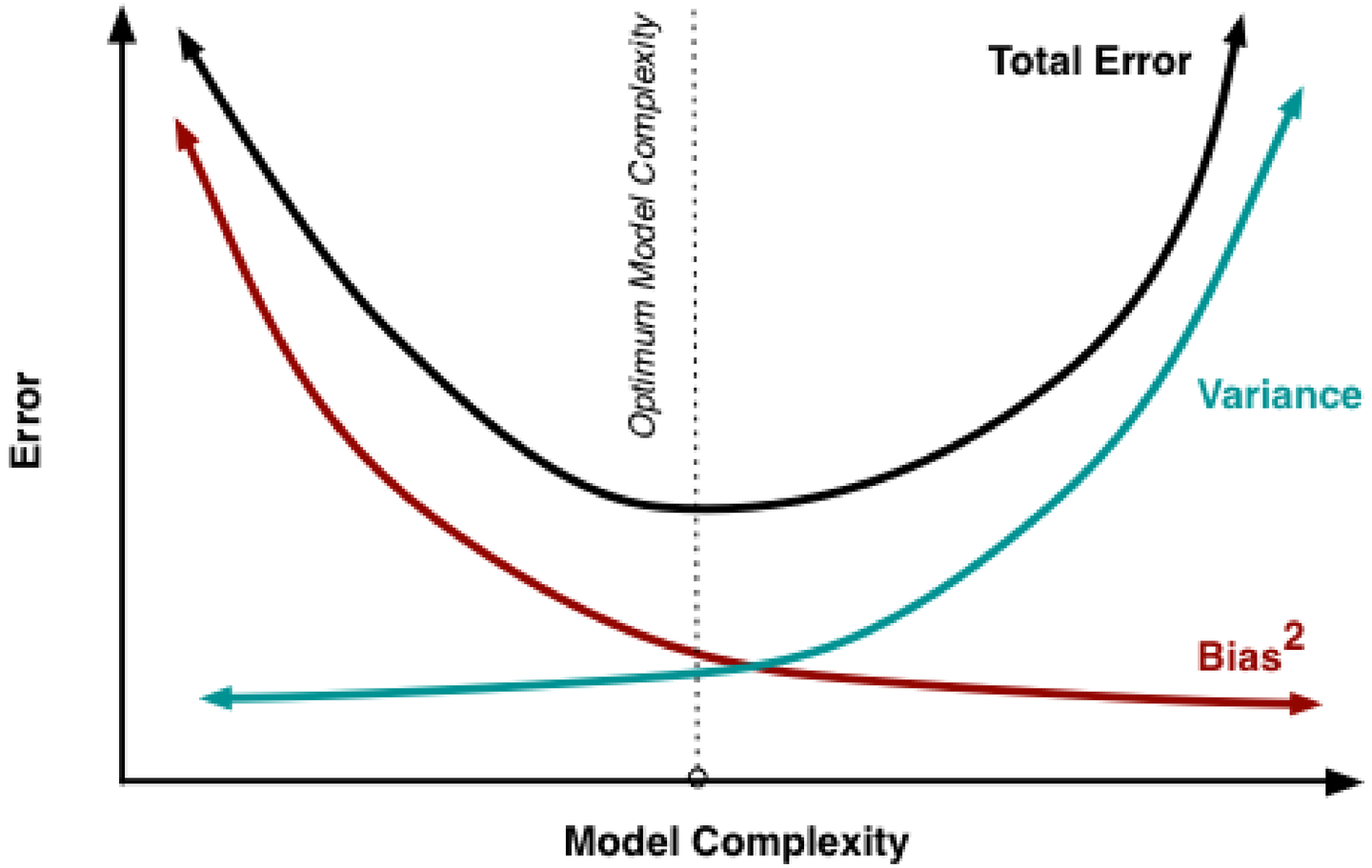
Variance

low → **high**

Bias

high → **low**

Bias-variance trade-off



When the model becomes more complex, the model bias decreases, and variance increases, and the total error firstly decreases and then increases.

The challenge is to find the optimum model complexity.

Bias-variance trade-off

In practice, can we compute bias and variance of a model?

- We can estimate the bias and variance of a model. The Python library of ‘mlxtend’ provide this function. (We will use this library in the workshop, although this computation is optional)

Bias-variance trade-off

Do people directly use bias and variance?

- In practice, people don’t directly use bias and variance. Rather, they often use the training error and testing error to diagnose the model (overfitting or underfitting)

Model diagnosis: comparing training and testing error

Training error: the error on the training data.
Testing error: the error on the testing data.
Error diff = testing error – training error

Training error	Error difference	
	Low	High
Low	Low-bias & low-variance Good balance	Low-bias & high-variance Overfitting
High	High-bias & low-variance Underfitting	*Improvement needed*

Model diagnosis: comparing training and testing error

It is INCORRECT to say: training error is an estimate of bias; the error difference is an estimate of variance

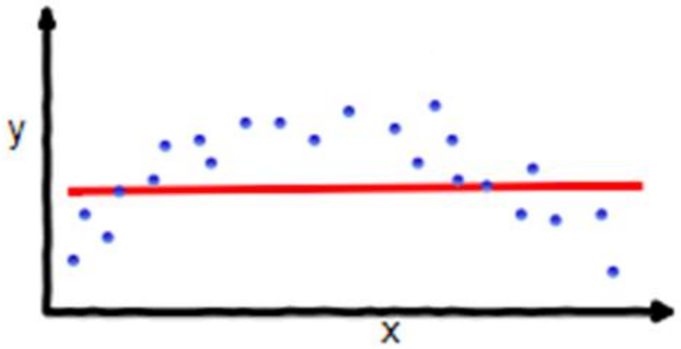
These are roughly of the same direction: when training error is high, the model bias is high; when testing error is high, the model variance is high.

Training error	Error difference	
	Low	High
Low	Low-bias & low-variance Good balance	Low-bias & high-variance Overfitting
High	High-bias & low-variance Underfitting	*Improvement needed*

Model diagnosis

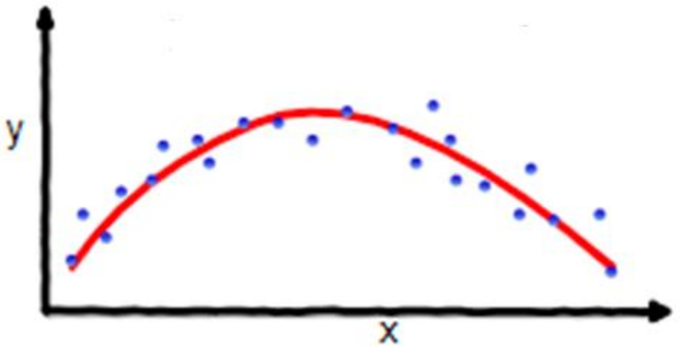
A

$Y = ax+b$



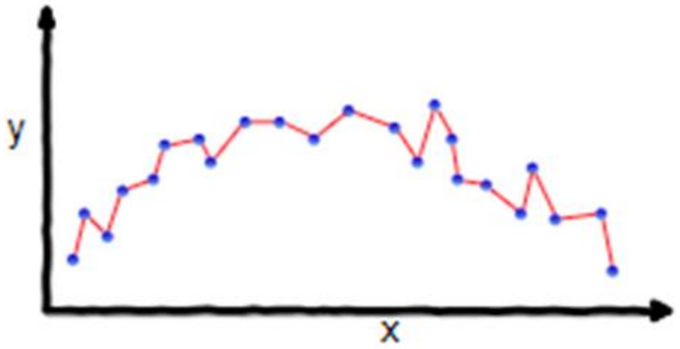
B

$Y = ax^2+bx+c$



C

$Y = \sum_{i=0}^{N} a_i x_i$



	A	B	C
Bias	High	Intermediate	Low
Variance	Low	Intermediate	High
Model diagnosis	Underfitting	Good balance	Overfitting

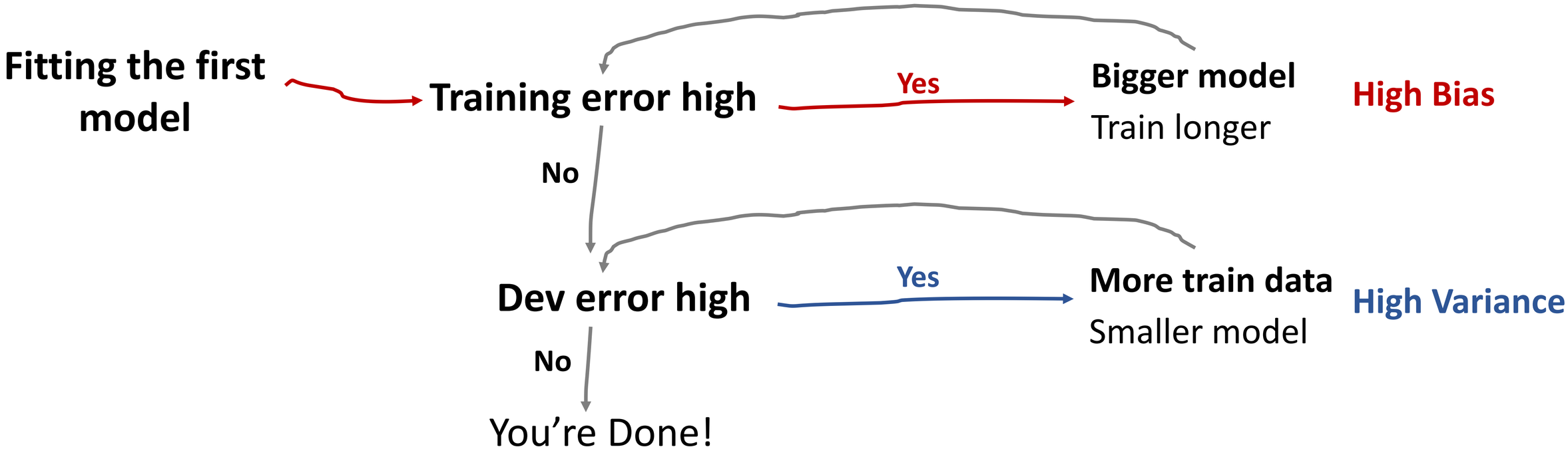
Model diagnosis – cat classification tasks

Example: Building an app to detect cats from photos

Training error	1%	15%	15%	0.5%
Test error	11%	16%	30%	1%
	High Variance	**High Bias**	**High Bias** **High Variance**	**You're done!**

Machine learning strategy

Machine Learning Workflow



Using the bias-variance conceptual framework as tools

Techniques for reducing bias

Increase model complexity

- Replace a simple linear regression model with a more flexible model, such as random forest or deep learning.
- Add more neurons or layers in a deep learning model.

Modify input features

- Inspect your training data to understand which examples your model is not doing well on.
- See if you can modify data features to eliminate these errors.

Techniques for reducing variance

Add more training data

- This is the simplest and the most reliable way to address variance, so long as you have access to significantly more data.

Reduce model size/complexity

- Replace a large neural network with a random forest.
- Add regularization to your neural network.
- Decrease neural network size.

Feature selection to decrease number/type of input features

- This technique might help with variance problems, but it might also increase bias.
- In deep learning, there has been a shift away from feature selection, and we are now more likely to give all the data to the algorithm and let the algorithm sort out which ones to use.


Data leakage
St. George's
Bermuda
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Data leakage in machine learning

- The goal of machine learning is to develop a model that generalizes well to new data
- Principle: We need to estimate the model performance on unseen data, which can’t be used in any stage of model training
- When this principle is broken, data leakage occurs: it leads to invalid predictive models, or overly optimistic models.
- Definition: data leakage is when the data you are using to train a machine learning algorithm happens to have the information you are trying to predict. This invalidate the estimated performance of the model

Examples of data leakage

- Data leakage occurs if we use the same data for training and testing, i.e. no train-test split
- In this case: training accuracy = testing accuracy

- Tip: when you achieve performance that seems too good to be true, this is a potential sign of data leakage. But the reverse is NOT true – “when there is a data leakage, the accuracy is always very high”.

More examples of data leakage

1. We randomly split the original data (OD) into two subsets: A (70%) and B (30%).
2. We use the A dataset to train a model (M).
3. We again randomly split OD into two subset: C (70%) and D (30%)
4. Then we apply M on D, getting an accuracy of 80% and report 80% is the finalised model performance.

Is this a case of data leakage? **Yes, as there can be overlap between A and D.**

More examples of data leakage

1. This is a task of predicting house price in London, using data from two companies, Rightmove and Zoopla.
2. We use the data from Rightmove to train a neural network model (M), getting an accuracy of 90%.
3. Then, we use model M to the housing data from Zoopla, getting an accuracy of 60%.

Is this a case of data leakage?

Yes, many properties are on both Rightmove and Zoopla.

More examples of data leakage

1. You are working to predict house price in London, using data from two companies, Rightmove and Zoopla.
2. This time, you combine all data from the two companies and get dataset D. You randomly split D into two subset, A (70%) and B (30%).
3. You train the model using A and evaluate the model performance using B.

Is this a case of data leakage? **Yes, as many properties are on both Rightmove and Zoopla**

More examples of data leakage

1. You are working to predict house price in London, using data from Zoopla.
2. You have removed all duplicate items from the data.
3. You normalise the house price using the average value of the whole dataset. Then, you split the data into A (70%) and B (30%).
4. You train the model using A and evaluate the model performance using B.

Is this a case of data leakage? **Yes. In the data preparation (including normalisation), you use the information of the testing data. In data normalisation, the parameters (e.g. mean, standard deviation) should come from the training data only.**

Time series datasets – predicting ‘future’

1. You are working on predicting future house price in London, using three-year data (2019/20/21) from Zoopla.
2. This time, there are two ways to do train-test split
    1. Shuffle the data and split it into A (70%) and B(30%);
    2. Use 2019/2020 data as training data and the 2021 data as testing data.

Which split is more reasonable? Why?

#2 of split is more reasonable, as the purpose is to predict the future house price. It’s better to train the model using 19/20 data and report model performance using 2021 data.

#1 of split does not train a model for predicting ‘future’ house price.

Techniques to minimise data leakage

1. **Hold back a testing dataset** for final sanity check of your developed models
2. **Perform data preparation without using testing dataset**. If you are using cross validation, perform data preparation within your cross validation folds
3. **Add Noise**. Add random noise to input data to try and smooth out the effects of possibly leaking variables.
4. **Use Pipelines**. Heavily use pipeline architectures that allow a sequence of data preparation steps to be performed within cross validation folds, such as the caret package in R and Pipelines in scikit-learn. (note: pipeline is not about parallel computing; it is a way of combining multiple steps in data analysis)

Summary

- Basic error analysis
- Machine learning strategy
- Data leakage

Workshop

- Weekly quiz on Moodle: please finish them before the workshop and we will discuss the quiz in the workshop
- Python notebooks for workshop: will be ready by 5pm Thursday.
- See you in the workshop on Friday 1-3pm