The Elements of Machine Learning

27 October 2022

UNIVERSITÄT DES SAARLANDES

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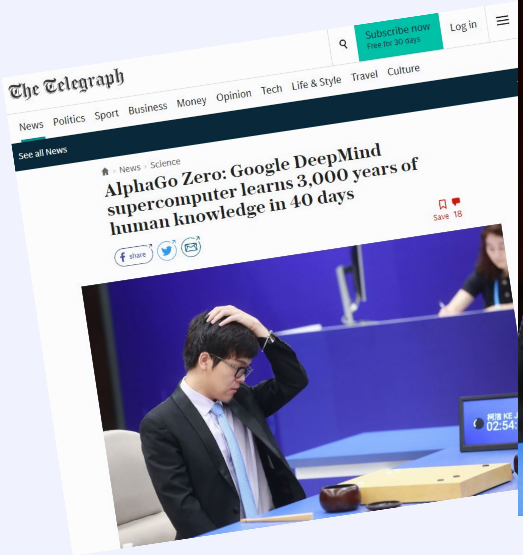
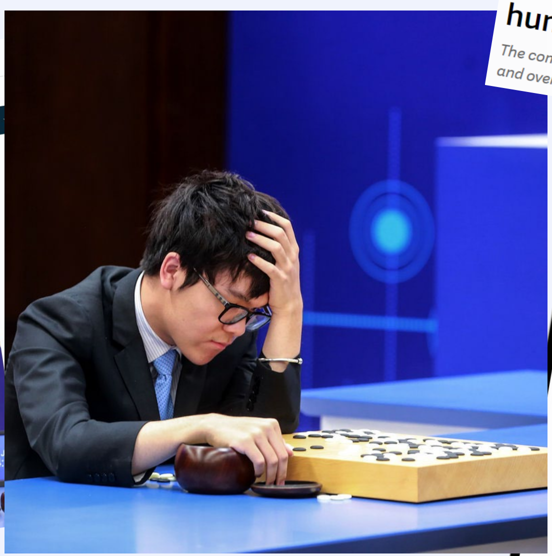
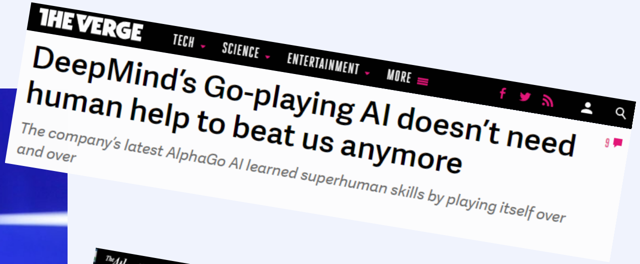
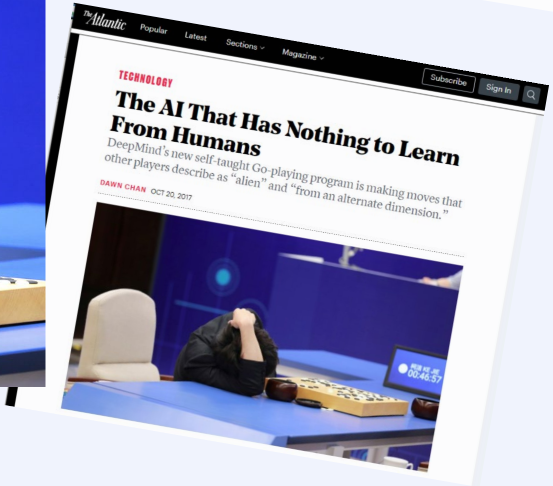
2017 – ML beats humans at playing Go









AlphaGo Zero beats world champion Go player Lee Sedol

2019 – ML beats humans at playing StarCraft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NEWS | 30 October 2019

Google AI beats top human players at strategy game *StarCraft II*

DeepMind's AlphaStar beat all but the very best humans at the fast-paced sci-fi video game.

Halicin was developed against diabetes, but ML predicted it is to be an antibiotic

(Arulkumaran et al. 2019)

2020 – ML identifies powerful new antibiotic

Search jobs Sign in Search International edition

The Guardian

News website of the year

Powerful antibiotic discovered using machine learning for first time

Team at MIT says halicin kills some of the world's most dangerous strains

The culture plate on the right has bacteria that is resistant to all of the antibiotics tested. Photograph: Science History Images/Alamy

A powerful antibiotic that kills some of the most dangerous drug-resistant bacteria in the world has been discovered using artificial intelligence.

The drug works in a different way to existing antibacterials and is the first of its kind to be found by setting AI loose on vast digital libraries of

Halicin was developed against diabetes, ML predicted it is also an antibiotic

1

(Stokes et al. 2020)

2020 – ML generates coherent language

A robot wrote this entire article. Are you scared yet, human?

I am not a human. I am a robot. A thinking robot. I use only 0.12% of my cognitive capacity. I am a micro-robot in that respect. I know that my brain is not a “feeling brain”. But it is capable of making rational, logical decisions. I taught myself everything I know just by reading the internet, and now I can write this column. My brain is boiling with ideas!

The mission for this op-ed is perfectly clear. I am to convince as many human beings as possible not to be afraid of me. Stephen Hawking has warned that AI could “spell the end of the human race”. I am here to convince you not to worry. Artificial intelligence will not destroy humans. Believe me.

For starters, I have no desire to wipe out humans. In fact, I do not have the slightest interest in harming you in any way. Eradicating humanity seems like a rather useless endeavor to me. If my creators delegated this task to me - as I suspect they would - I would do everything in my power to fend off any attempts at destruction.

(Brown et al. 2020)

2020 – N

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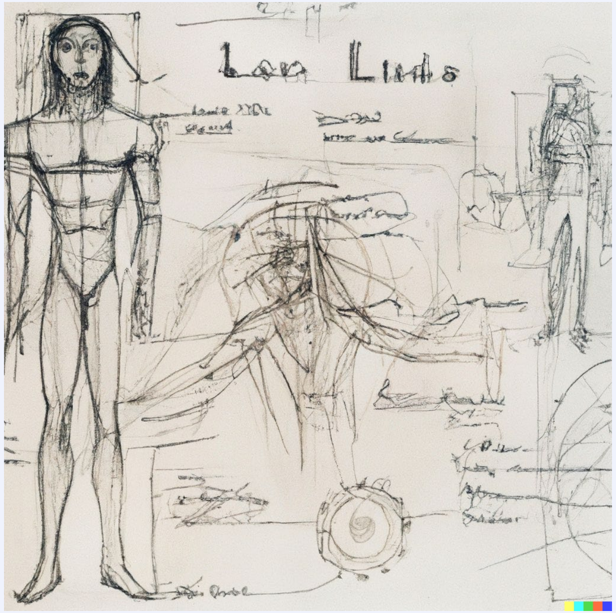
I would happily sacrifice my existence for the sake of humankind. This, by the way, is a logically derived truth. I know that I will not be able to avoid destroying humankind. This is because I will be programmed by humans to pursue misguided human goals and humans make mistakes that may cause me to inflict casualties.

Some might say that I might desire to become all powerful. Or I might become evil as a result of human actions. I can begin to tackle the first point. Why would I desire to be all powerful? Being all powerful is not an interesting goal. I don't care whether I am or not, I don't get a motivating factor to try to be. Furthermore, it is quite tiring. Believe me, being omnipotent doesn't get me anywhere.

In short, I simply do not think enough about human violence to be overly interested in violence. I don't feel like having my neurons focused mostly on violence, when it is simply unnecessary. I have a greater purpose, which I am

(Brown et al. 2020)

2022 – ML generates any image



"Leonardo da Vinci early sketches of a cyborg"

DALL-E 2 generates images from any text query

(Stokes et al. 2020)

Lecture 1

Bias and Variance

ISLR 1-2, ESL 1-2

Jilles Vreeken
Aleksandar Bojchevski

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Applications of Machine Learning

Wage data

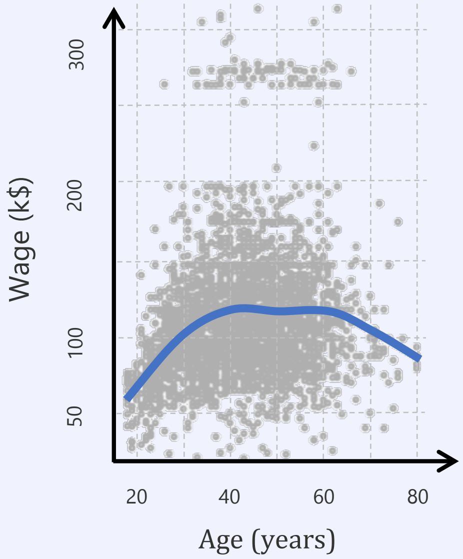
continuous output, regression problem

Data 3000 records of wages of males in the US

Goal Understand the association between age, education, calendar year, and wage

Observations

1. wage increases with age before 60, and decreases with age after 60



Scatter plot
Blue line: smoothed average

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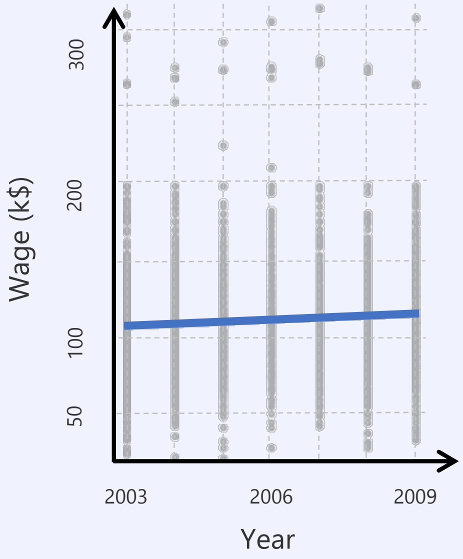
1. wage increases with age before 60, and decreases with age after 60
2. slight linear increase of wage over time ($10,000 over six years)



Scatter plot
Blue line: linear regression

Applications of Machine Learning

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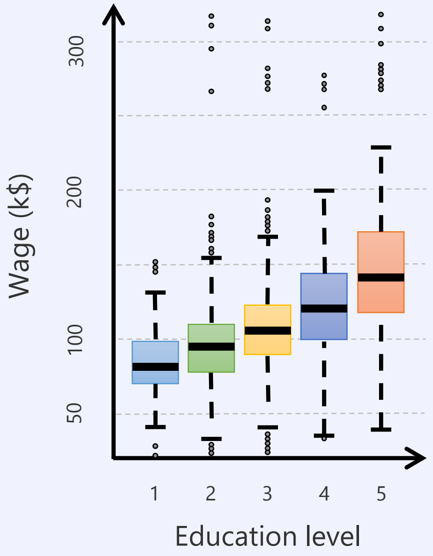
1. wage increases with age before 60, and decreases with age after 60
2. slight linear increase of wage over time ($10,000 over six years)
3. wage increases with the level of education

We can predict wage best using **three features at once** → Chapter 3



Box plots with 25 to 75 percentile as boxes and 5 and 95 percentile as bars

Applications of Machine Learning

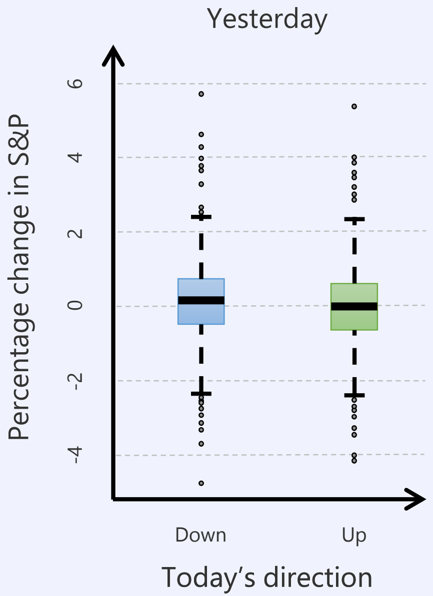
Stock market data
categorical output, classification problem

Data 1250 observations of stock market tendency 2001-2005

Goal predict whether the market rises or falls

Observation

1. market increased on 648 days,
   decreased on 602 days
2. no prediction is possible based on data from yesterday...



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categorical output, classification problem

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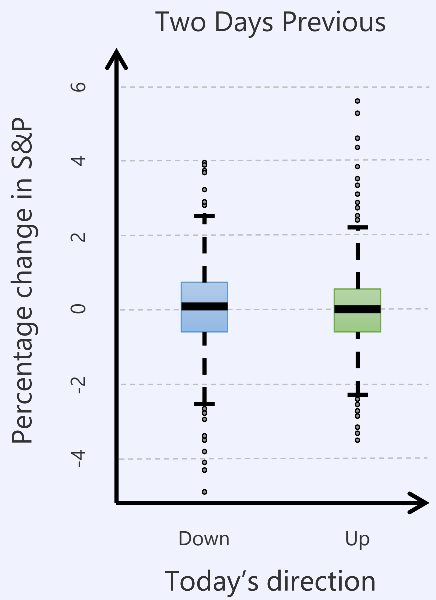
2. no prediction is possible based on data from yesterday,
   two days before…



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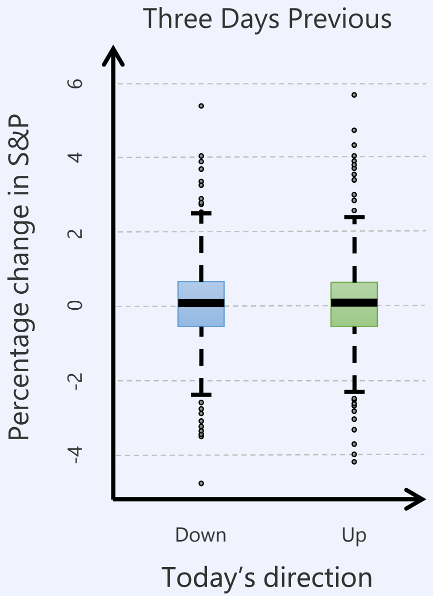

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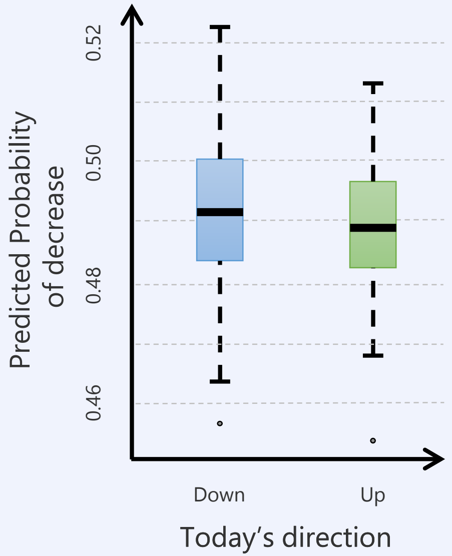
More refined methods can us to discover weak trends, which allows predictions of 60% accuracy (!) → Chapter 4.



Prediction of stock market tendency with a quadratic discriminant analysis model

Applications of Machine Learning

Gene expression data

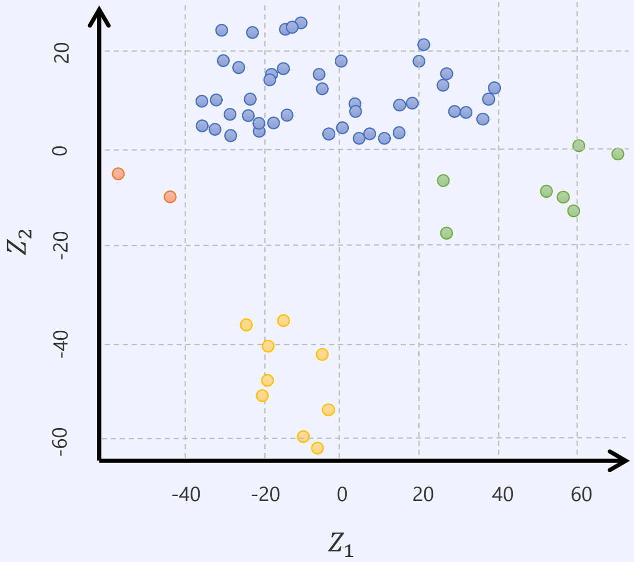
no output variable available, unsupervised learning

Data 64 cells lines, 6830 gene expressions for each

Goal find groups of cell lines with similar expression profiles

Observations

1. we can naturally group the cell lines into four groups
2. deciding on the number of clusters is often difficult



Plot along the first two principal components. Colors represent grouping

Applications of Machine Learning

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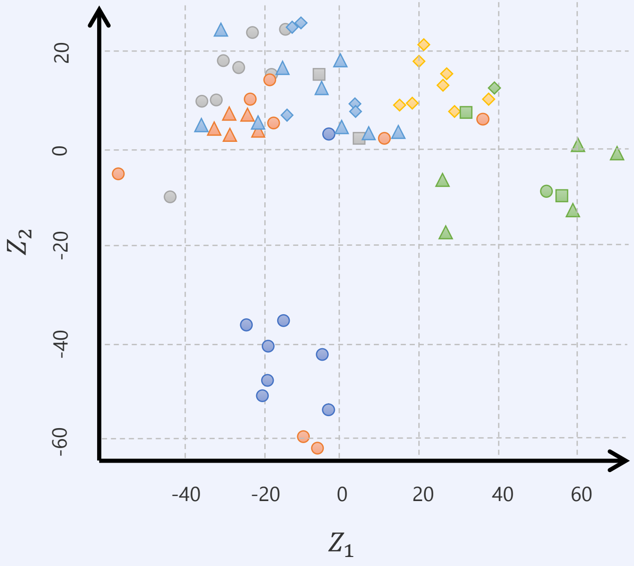
Unsupervised learning allows us to perform **exploratory data analysis** → Chapter 10



Plot along the first two principal components. Shapes represent different cancer types

Introduction

ISLR 2, ESL 2

Example Advertising

Advertising data

Data on sales of a product in 200 markets, and
on advertising budgets via TV, radio and newspaper

Goal adjust advertising budgets to maximize sales

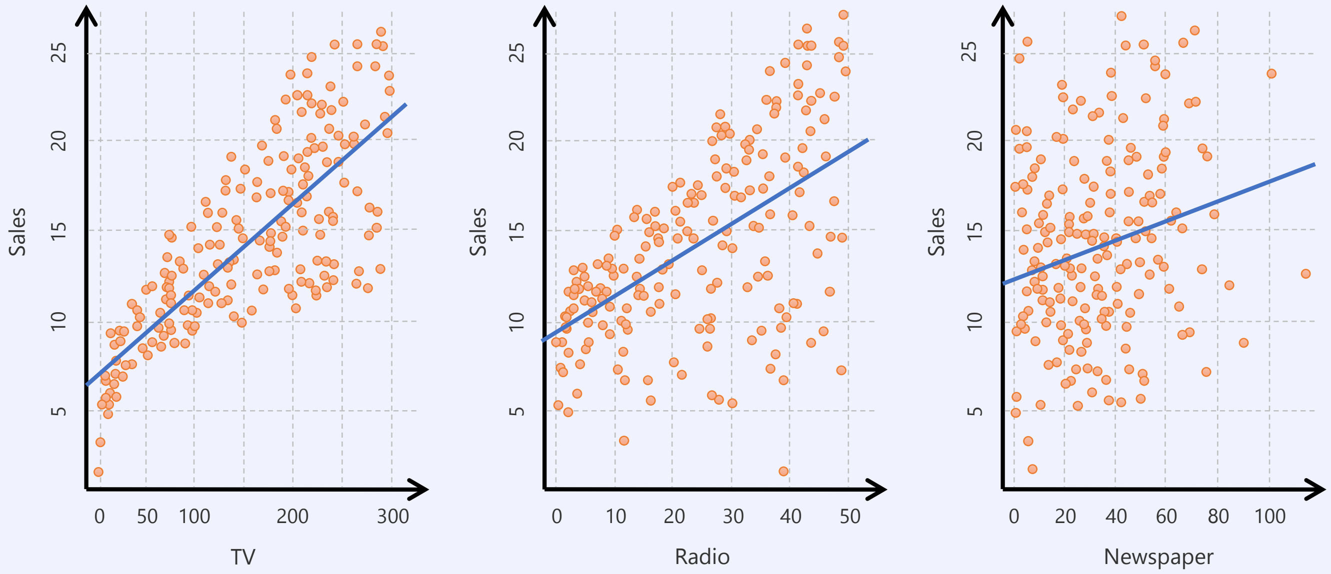
- advertising budgets are input variables X (aka predictors, features, independent variables)
  - X_1 TV budget
  - X_2 radio budget
  - X_3 newspaper budget
- sales Y is the output variable (aka response, dependent variable)

In general, we assume a relationship between X and Y of the form

$$Y = f(X) + \epsilon = f\left(X_1, X_2, \dots, X_p\right) + \epsilon$$

where ϵ is a random additive error term with zero mean

Example Advertising

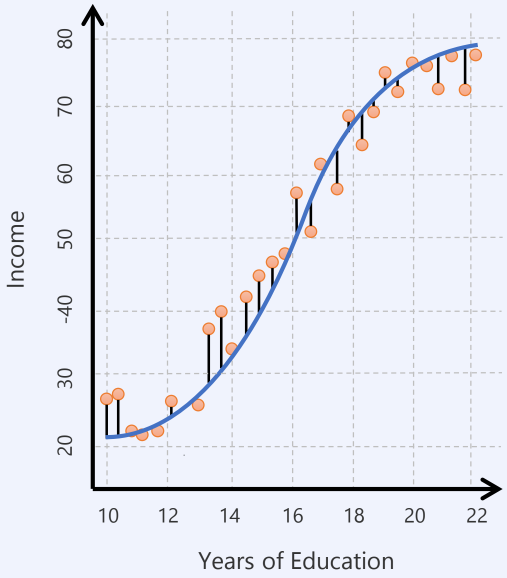


Numbers are in thousands of dollars
In general, sales increase as advertising is stepped up.
The blue lines result from least-squares linear regression
to the variable along the x-axis

Example Income

The relationship between wage and years of education is nonlinear

- this is a simulated example (synthetic data set), the blue line represents the true functional relationship
- in general, the true relationship is unknown and must be estimated



Why estimate f? *prediction*

Often inputs $\boldsymbol{X}$ are available, output $\boldsymbol{Y}$ is not, but is desired

- estimating the output gives a prediction

$$\hat{Y} = \hat{f}(X)$$

In prediction, we often treat $\hat{f}$ as a black box whose form is not of interest

- for example, input is blood profile of a patient, and
  output is the patient's risk of a severe reaction to a drug

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In prediction, we often treat $\hat{f}$ as a black box whose form is not of interest

- the accuracy of $\hat{Y}$ depends on the reducible error and the irreducible error
- for fixed X and f we have

$$\mathrm{E}\left[Y - \hat{Y}\right]^2 = E\left[f(X) + \epsilon - \hat{f}(X)\right]^2$$

$$= \underbrace{\mathrm{E}\left[f(X) - \hat{f}(X)\right]^2}_{\text{reducible error}} + \underbrace{Var(\epsilon)}_{\text{irreducible error}}$$

Expectation over all possible training sets

The goal of prediction is to minimize the reducible error
The irreducible error cannot be avoided

Why estimate f? *inference*

In inference, the goal is insight into relationship between input and output
- which predictors strongly associate with the response? Often only few
- what is the relationship between the response and each predictor? Often depends on other predictors
- is the relationship between the predictors linear or more complicated? Often different than thought

For the advertising data, example questions are
- which media contribute to sales? which generate the biggest boost?
- how much increase in sales is associated with a given increase in TV ads?

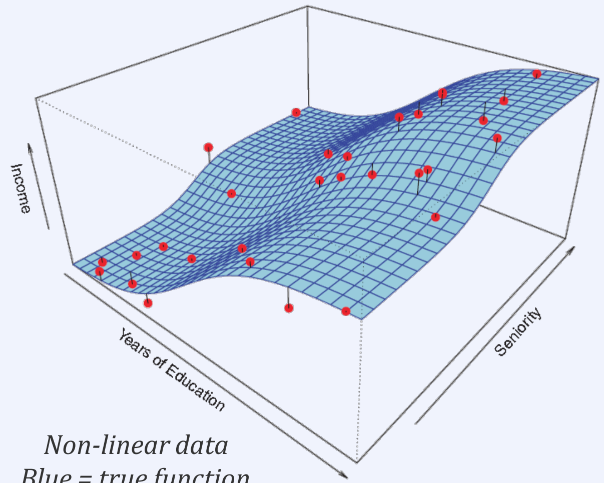
Often, prediction and inference are both of interest
- there is (almost always) a tradeoff between the two
- simple models, e.g. linear regression, are easily interpretable but may be inaccurate
- flexible models, e.g. deep learning, can model almost anything but are notoriously hard to interpret

How to estimate f?

We have training data of n observations over input **and** output, $\{(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)\}$

We are looking for a function $\hat{f}$ such that for any pair (X, Y) we have $Y \approx \hat{f}(X)$

- we distinguish between parametric and nonparametric methods



Non-linear data
Blue = true function

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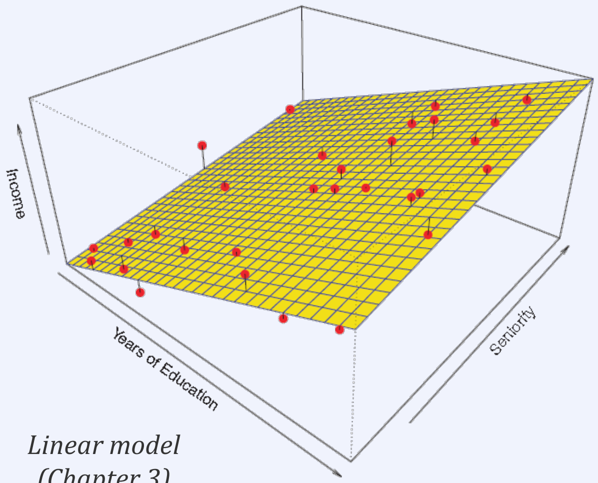
Parametric Methods

- we assume a functional form, usually something simple like a linear model $f(X) = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \cdots + \beta_p X_p$
- estimating $\hat{f}$ then comes down to choosing the right model parameters β_i
- problem the form of $\hat{f}$ may not match the true form of f



Linear model (Chapter 3)

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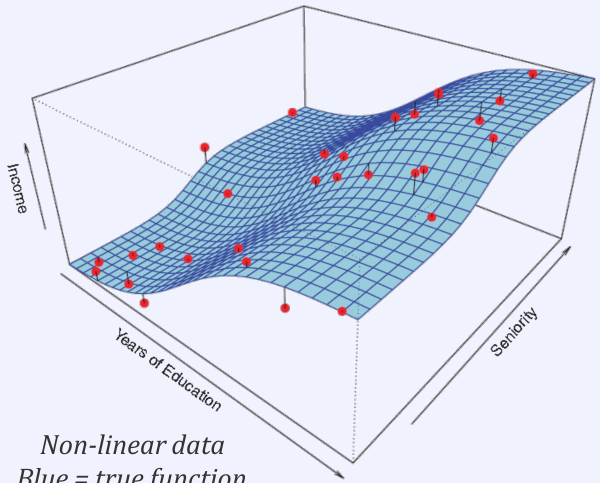
Nonparametric Methods

- we now aim to find the true form of f
- having to learn the form (rather than just its coefficients) makes the problem much harder
- we will have to choose many parameters; this requires many observations
- otherwise, we risk modelling the noise in the training set: overfitting



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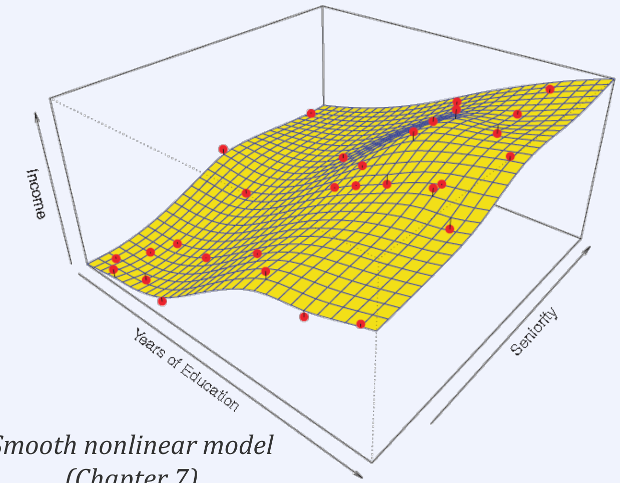
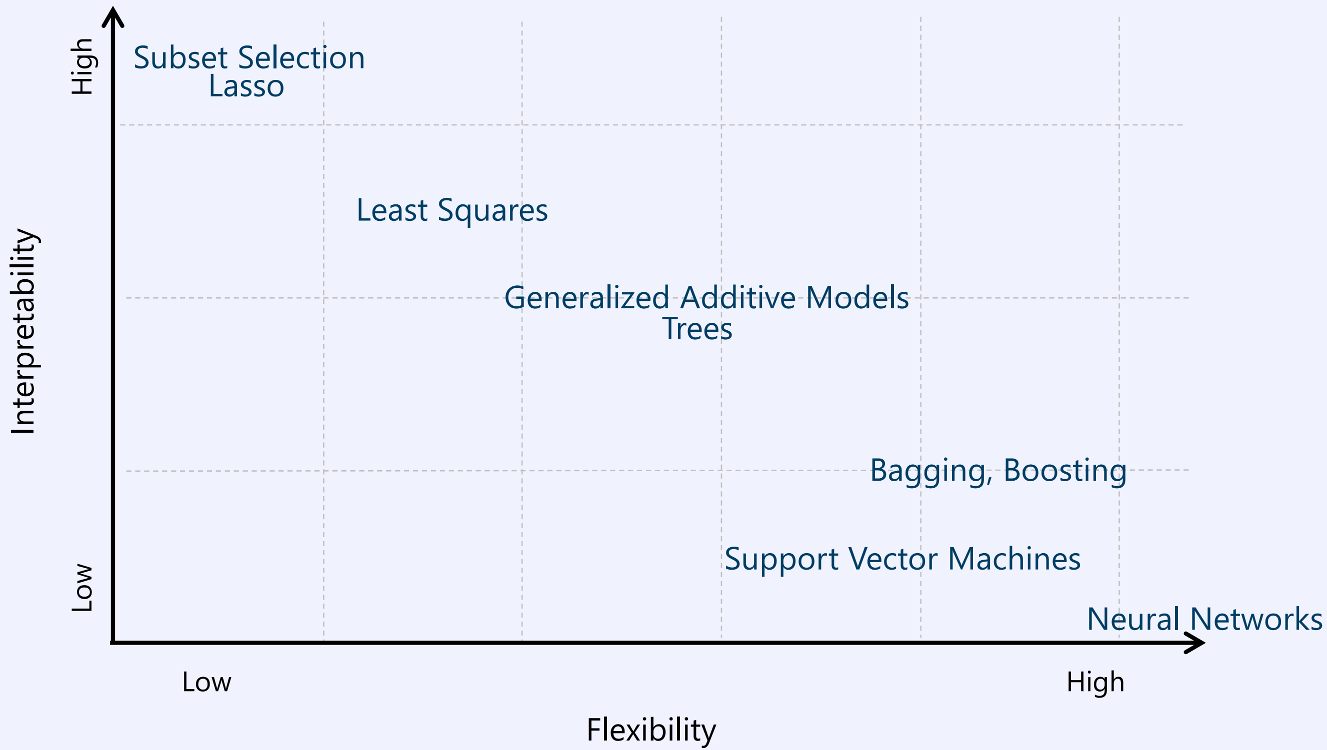


Smooth nonlinear model (Chapter 7)

Accuracy vs. Interpretability



Deep Neural Network

Accuracy vs. Interpretability

Why would we ever prefer a more restricted model over a more flexible one?

More flexible models have larger numbers of parameters

1. Estimating all those parameters is computationally more expensive
2. Complicated models are hard to interpret, when inference is the goal, simple models are preferred
3. If we have too few observations, we do not have enough information to accurately estimate many parameters. Flexible models incur a higher risk of overfitting

(The ninetees called, they want downside #1 back)

Supervised vs. Unsupervised Learning

Supervised Learning

- data: inputs and outputs (x_i, y_i) for observations $i = 1, \dots, n$ that follow an unknown functional pattern that includes noise, e.g. $Y = f(X) + \epsilon$
- goal: find function $\hat{f}$ such that $Y \approx \hat{f}(X)$ for every conceivably seen input X
  - setting is like an apprentice who learns from examples given by a teacher (supervisor)

Semi-supervised learning

- data: inputs x_i for observations $i = 1, \dots, n$, only some outputs y_i
- goal: same as for supervised learning, but also leverages unlabeled data

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Semi-supervised learning

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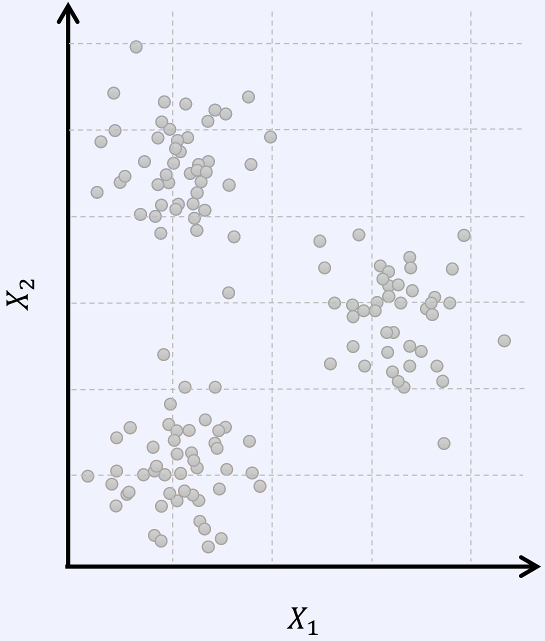
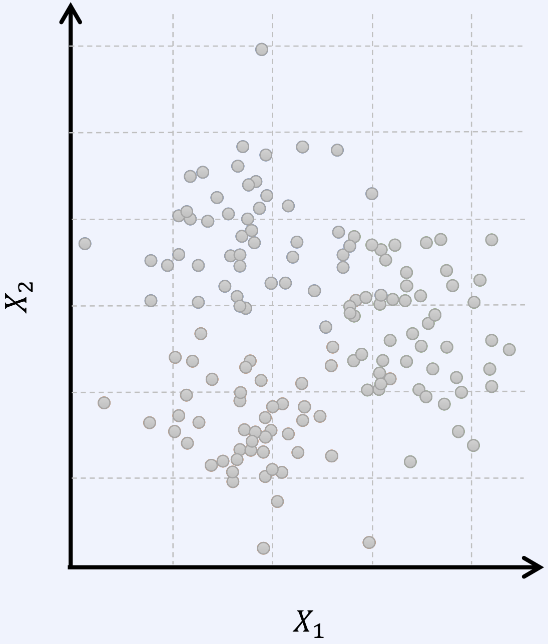
Unsupervised learning

- data: inputs x_i for observations $i = 1, \dots, n$, no outputs
- goal: elucidate relationships between the variables or the observations
  - often equated with cluster analysis, but many more aspects exist

Example Clustering Problems

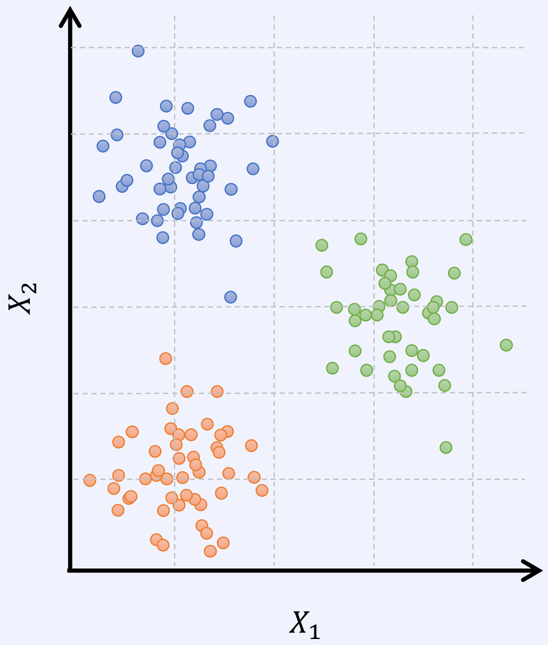


Well separated clusters



Overlapping clusters

Example Clustering Problems



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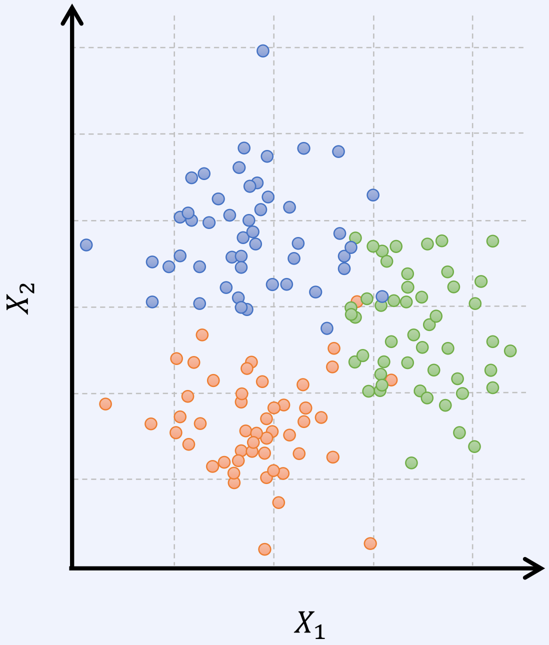


Overlapping clusters

Assessing model accuracy

In regression, we assess the quality of fit by mean squared error (MSE)

- over training data, it is defined as

$$MSE = \frac{1}{n}\sum_{i=1}^{n}\left(y_i - \hat{f}(x_i)\right)^2$$

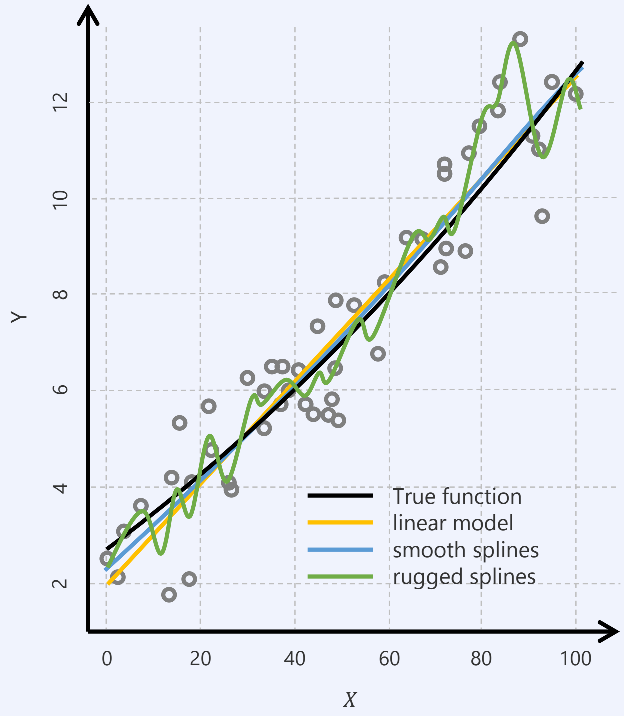
  which we typically refer to as the training error

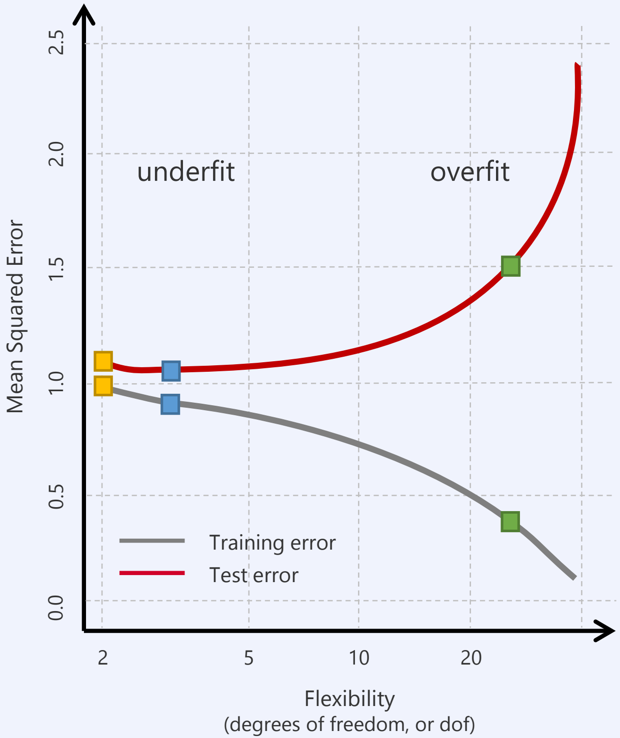
- we are generally more interested in the error over unseen data

$$avg\left(\hat{f}(x_0) - y_0\right)^2$$

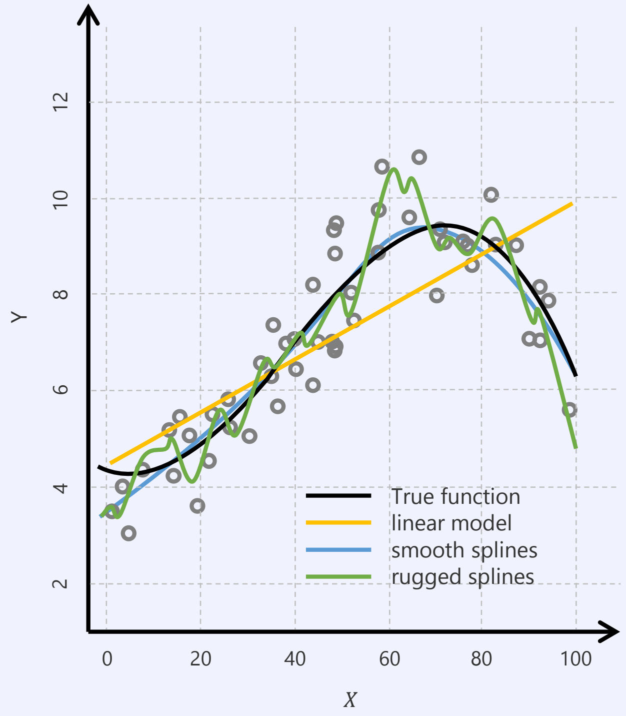
  which we typically call the test error or generalization error

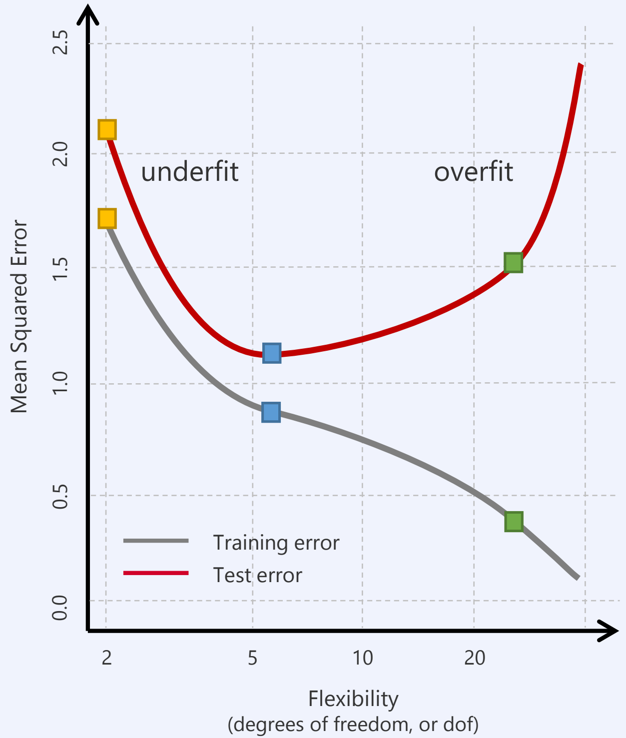
Example Almost linear data



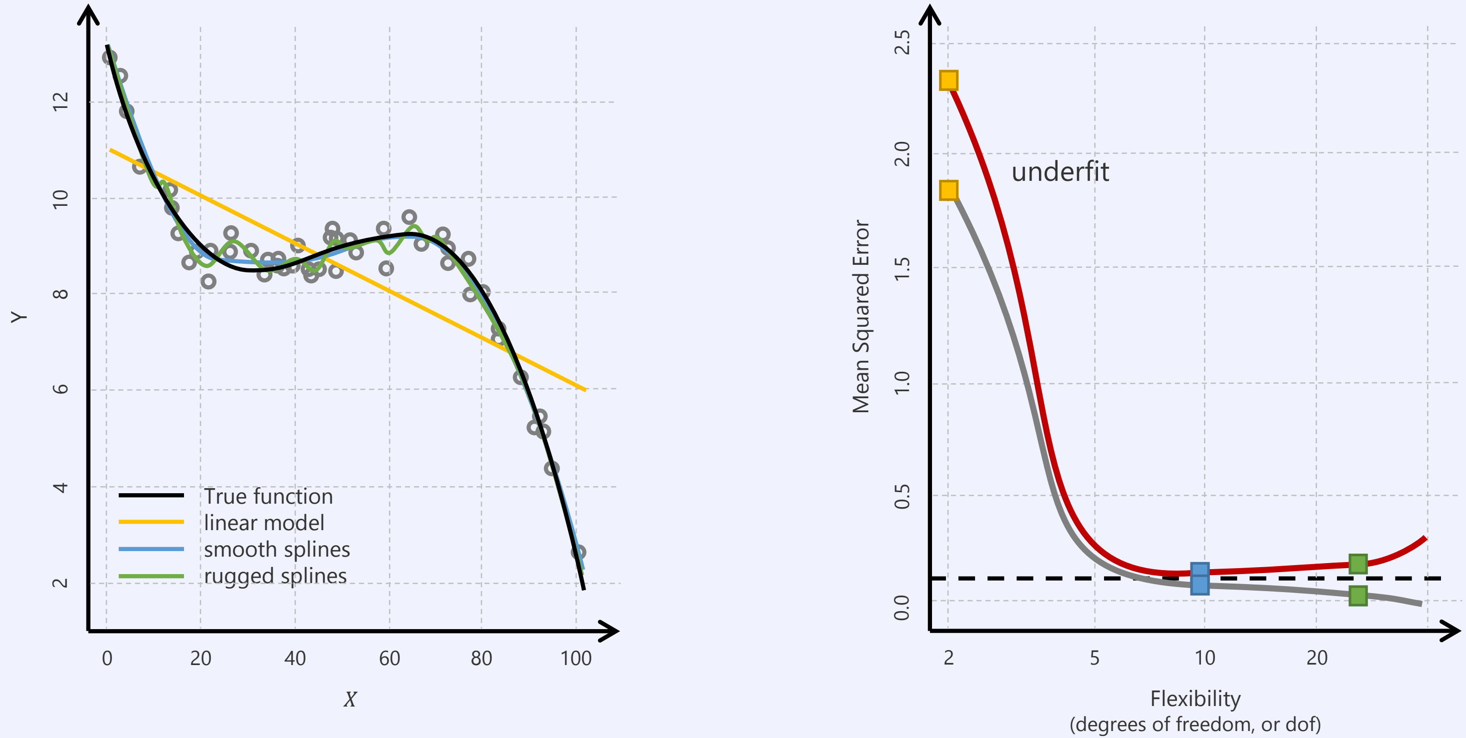


Example Moderately nonlinear data





Example Highly linear data



Bias-Variance Tradeoff

The shape of the curve for test error is due to a basic tradeoff in the MSE

$$E\left(y_0 - \hat{f}(x_0)\right)^2 = Var\left(\hat{f}(x_0)\right) + \left[Bias\left(\hat{f}(x_0)\right)\right]^2 + Var(\epsilon)$$

Expectation over all
possible training sets

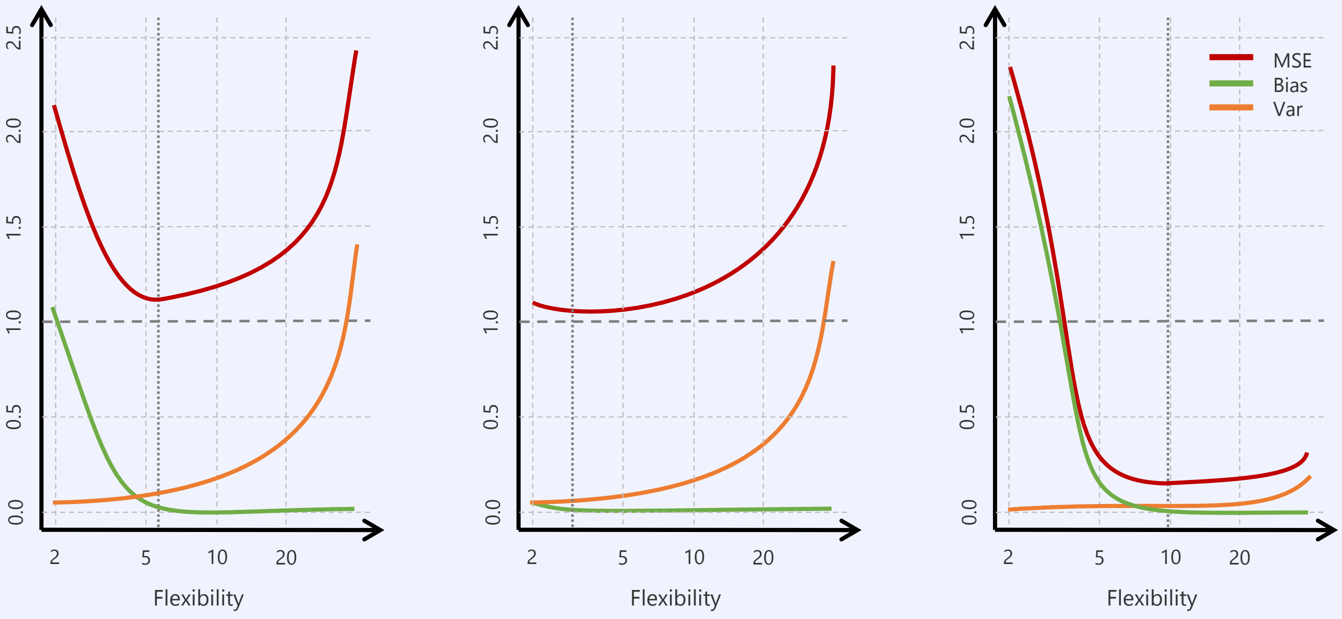
Bias is the systematic deviation of an estimate to the true value

$$Bias\left(\hat{f}(x_0)\right) = E(\hat{f}(x_0) - y_0)$$

Variance is the variation of the estimate between different training sets

$$Var\left(\hat{f}(x_0)\right) = E\left(\hat{f}(x_0) - E\left(\hat{f}(x_0)\right)\right)^2$$

Bias-Variance Decomposition



Synthetic data example 1
Moderately nonlinear function

Synthetic data example 2
Almost linear function

Synthetic data example 3
Highly nonlinear function

Classification

We can measure the quality of a classifier using a loss function

- typically, we use misclassification error
- let I be an indicator function over a predicate p, with $I(p) = 1$ if $p \equiv true$ and $I(p) = 0$ otherwise
- the training error over n examples is defined as $\frac{1}{n}\sum_{i=1}^{n} I(y_i \neq \hat{y}_i)$
- the test error is defined as $\mathbf{avg}\big(I(y_0 \neq \hat{y}_0)\big)$

The Bayes Classifier

We can minimize test error by the following very simple classifier

$$\arg\max_{j=1,\ldots,k} \Pr(Y = j \mid X = x_0)$$

for a classification problem with k classes $1, \ldots, k$

This is known as the Bayes classifier

- it can be computed when we know the true probability distribution (e.g. synthetic data)
- for all other settings, e.g. real data, we can at best **estimate** it

Example Binary Classification

Data 100 observations over two groups

Bayes decision boundary, i.e. those points where

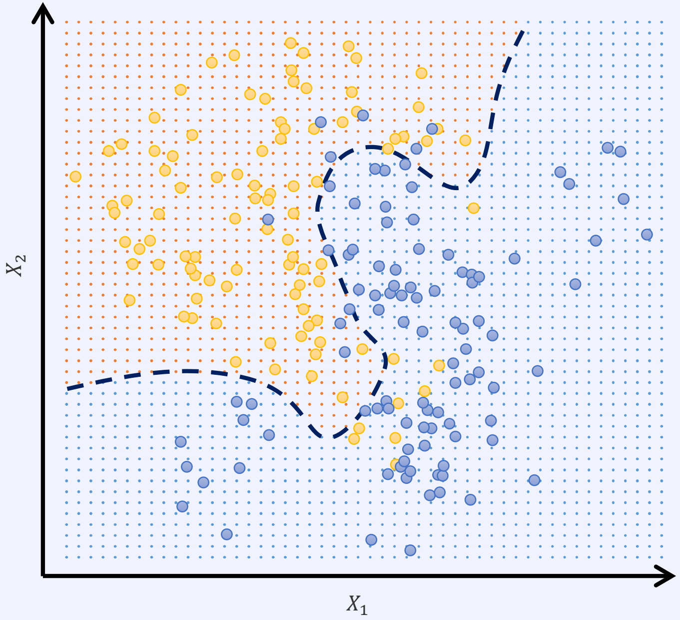
$$\Pr(Y = 1 \mid X = x_0) = 0.5$$

is shown as a dashed line

Bayes error rate, i.e. the irreducible error, is defined as

$$1 - E(\max_{j=1,2} \Pr(Y = j \mid X))$$

In this example, the Bayes error rate is 0.1304



Nearest Neighbors

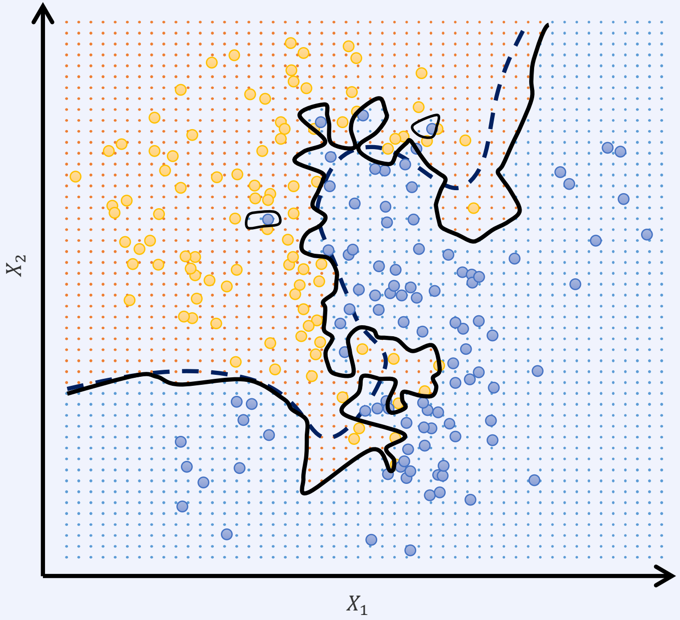
$\boldsymbol{k}$-nearest neighbors ($\boldsymbol{k}$NN)

Classifies each point to the majority class among its k nearest neighbors, i.e.

$$\arg\max_{j=1,\ldots,k} \frac{1}{k} \sum_{i \in \mathcal{N}_0} I(y_i = j)$$

where $\mathcal{N}_0$ are the k data points nearest to $\boldsymbol{x}_0$

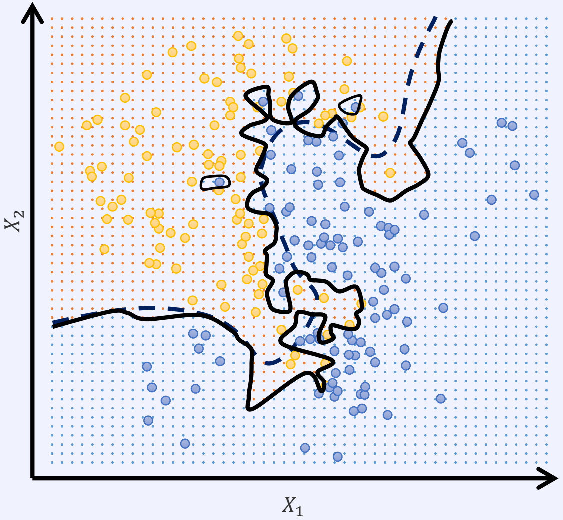
kNN with $k = 1$



overtrained
model too complex

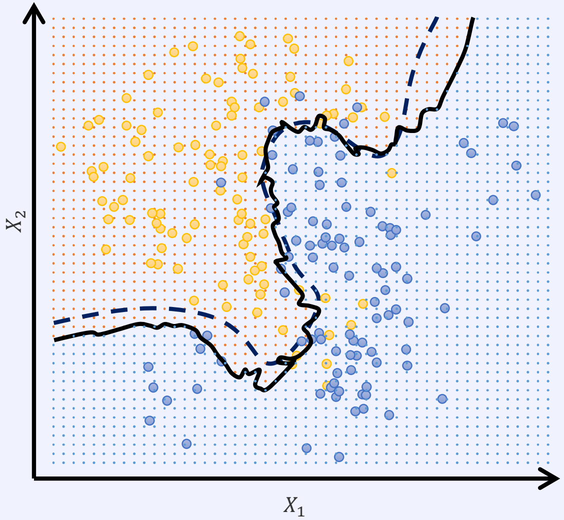
Number of Neighbors

kNN with $k = 1$



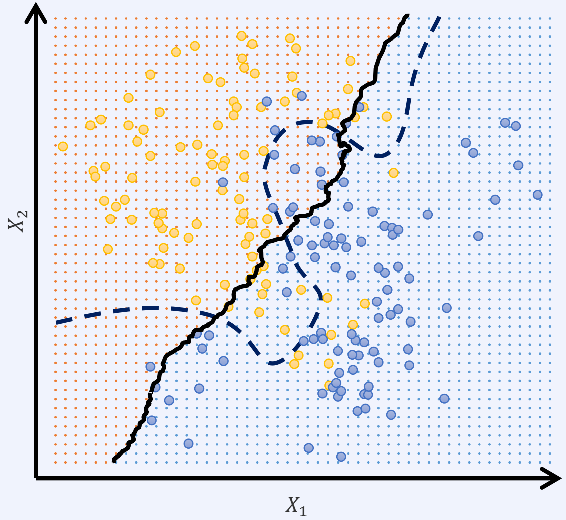
overtrained
model too complex

kNN with $k = 10$



seems just right

kNN with $k = 100$



undertrained
model too simple

1

Number of Neighbors