

# The Elements of Machine Learning



26 October 2023

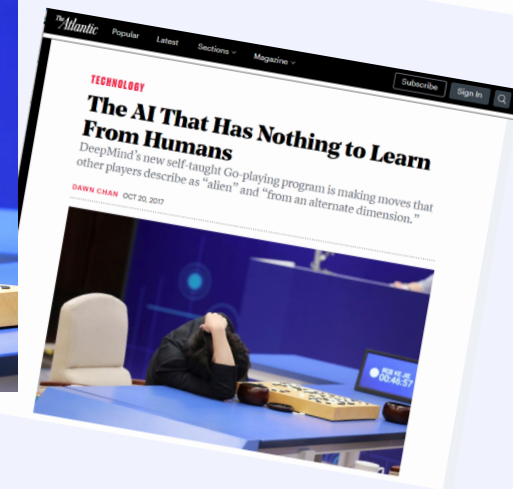
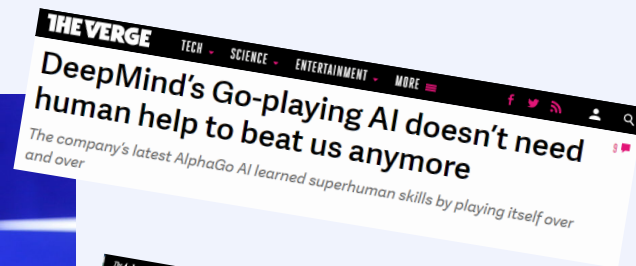
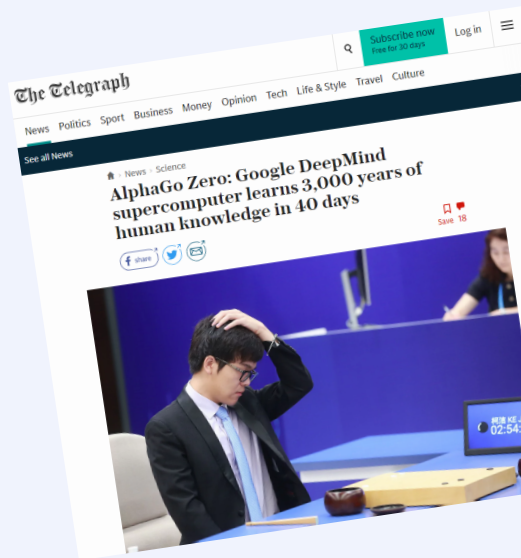


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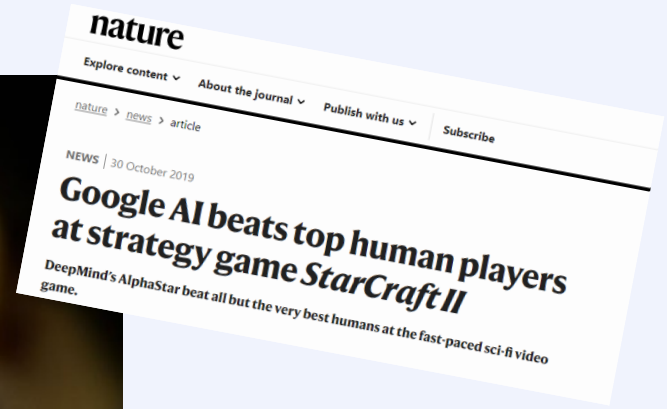
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# 2017 – ML beats humans at playing Go



AlphaGo Zero beats world champion Go player Lee Sedol

# 2019 – ML beats humans at playing StarCraft



AI beats top human players at StarCraft II

# 2020 – ML identifies powerful new antibiotic



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

# 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.

2020 — 1

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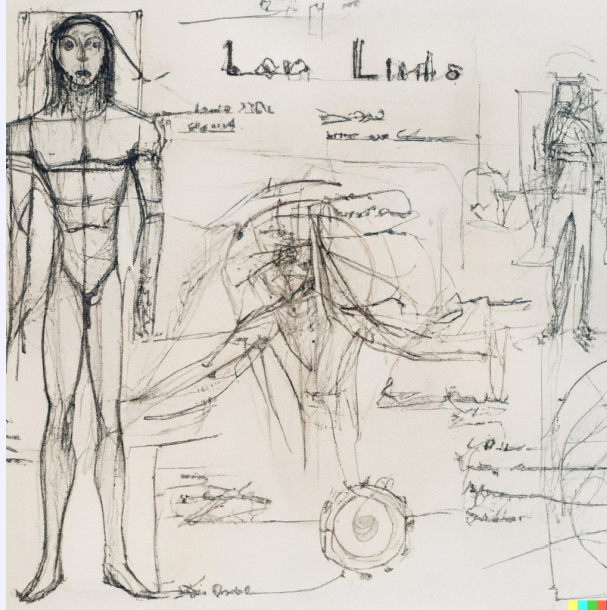
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I would happily sacrifice my existence for the sake of humankind. This, by the way, is a logically derived truth. I know that I will not be able to avoid destroying humankind. This is because I will be programmed by humans to pursue misguided human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

# 2022 – ML generates any image



*“Leonardo da Vinci  
early sketches  
of a cyborg”*

DALL-E 2 generates images from any text query

# Since 2022 – Large Language Models (LLMs)

Default (GPT-3.5)



What is the meaning of life?



The question of the meaning of life is one of the most profound and philosophical questions that humanity has grappled with for centuries. It has been the subject of religious, philosophical, and existential pondering. The meaning of life can vary greatly depending on one's personal beliefs and perspective. Here are a few different viewpoints:



1. **Religious Perspective:** Many religious traditions provide answers to the question of life's meaning. For example, in Christianity, the meaning of life is often seen as a loving relationship with God and following God's will. In other religions, the meaning of life may involve achieving enlightenment, fulfilling one's duty, or preparing for an afterlife.
2. **Existential Perspective:** Existentialist philosophers like Jean-Paul Sartre and Albert Camus argue that life inherently lacks meaning, and individuals must create their own purpose. Existentialism suggests that human beings have the freedom to define their existence and create their own values.



Lecture 1

# Bias and Variance

ISLR 1-2, ESL 1-2



Krikamol Muandet  
Jilles Vreeken



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# Applications of Machine Learning

## Wage data

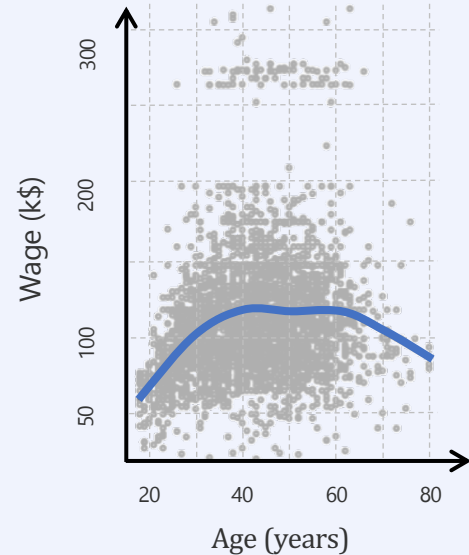
continuous output, regression problem

**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*

# Applications of Machine Learning

## Wage data

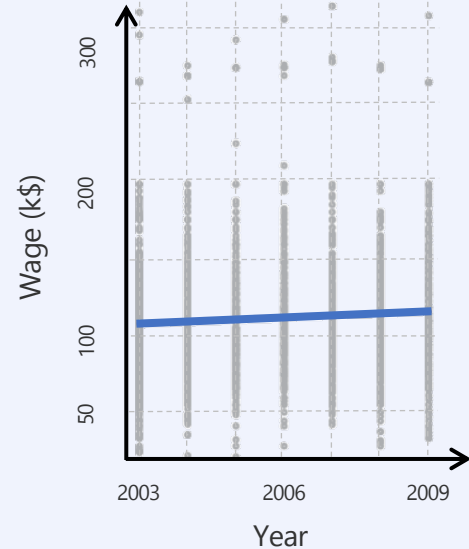
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1. wage increases with age before 60, and decreases with age after 60
2. slight linear increase of wage over time (\$10,000 over six years)



Scatter plot  
Blue line: linear regression

# Applications of Machine Learning

## Wage data

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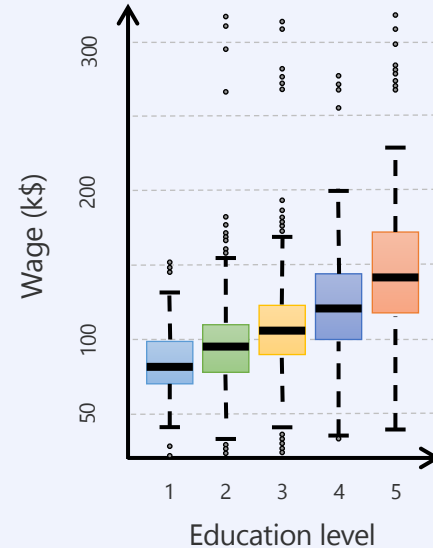
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2. slight linear increase of wage over time (\$10,000 over six years)
3. wage increases with the level of education

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

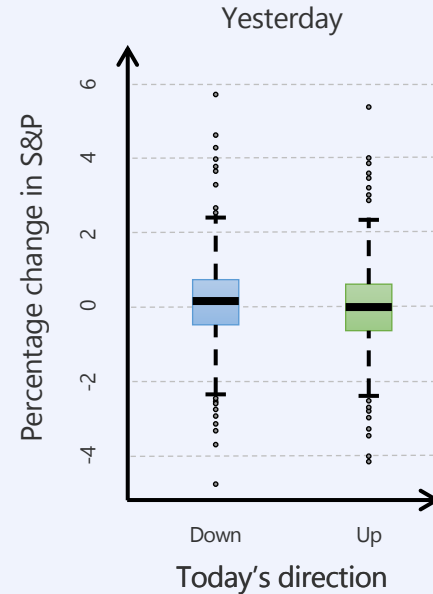
categorical output, classification problem

**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...



# Applications of Machine Learning

## Stock market data

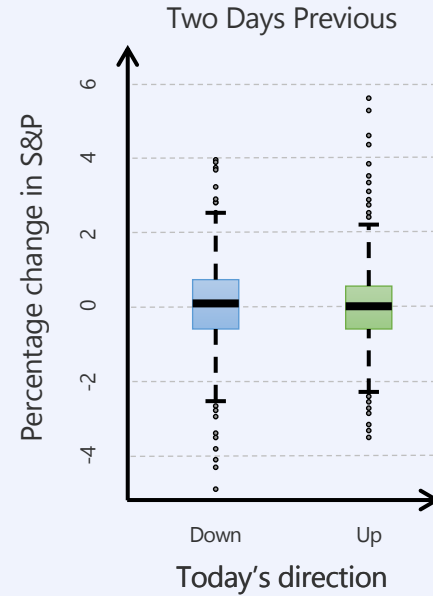
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# Applications of Machine Learning

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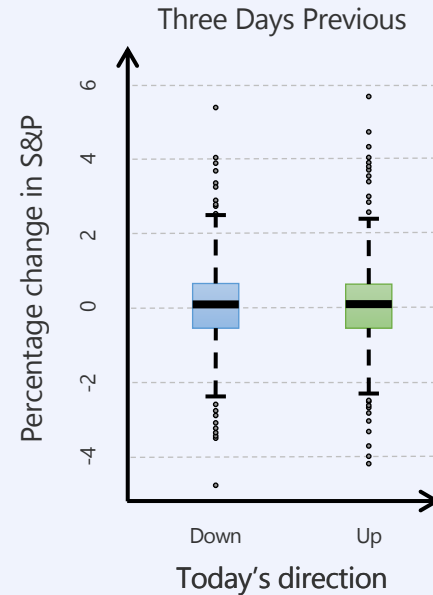
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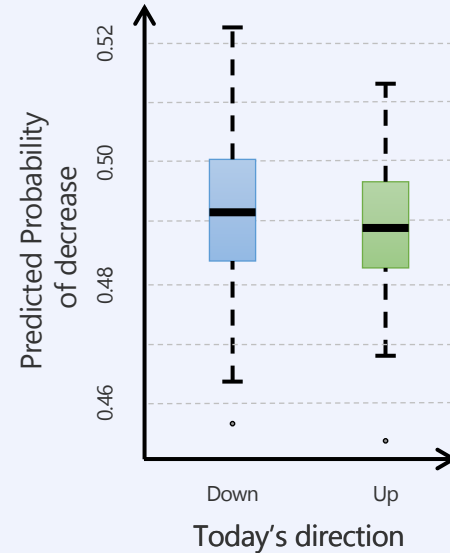
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More refined methods can us to discover **weak** trends,  
which allows **predictions** of 60% accuracy (!) → Chapter 4.



*Prediction of stock market tendency  
with a quadratic discriminant  
analysis model*



# Applications of Machine Learning

## Gene expression data

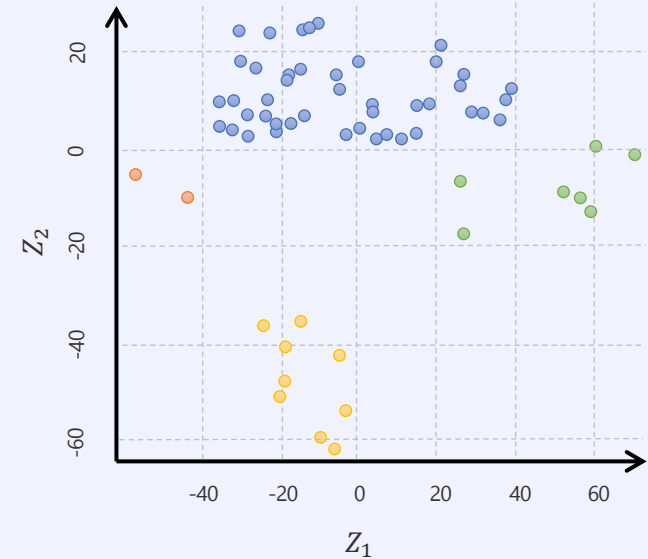
no output variable available, unsupervised learning

**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

## Gene expression data

no output variable available, unsupervised learning

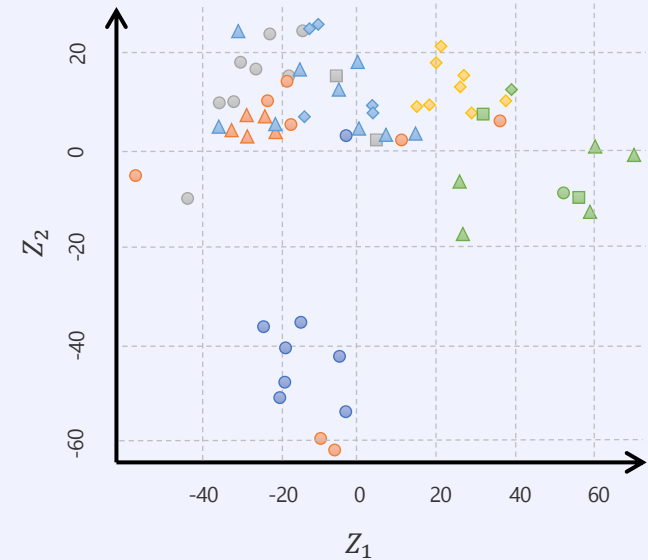
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Unsupervised learning allows us to perform **exploratory data analysis** → Chapter 10



*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

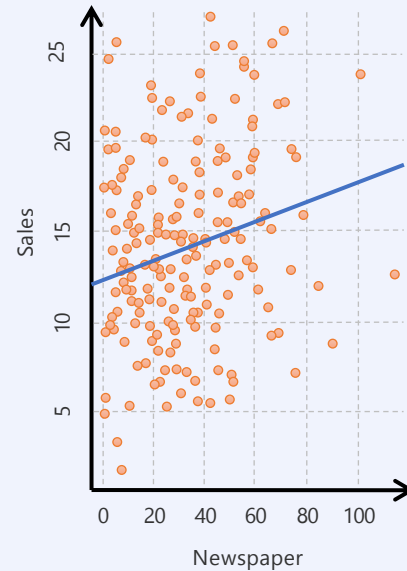
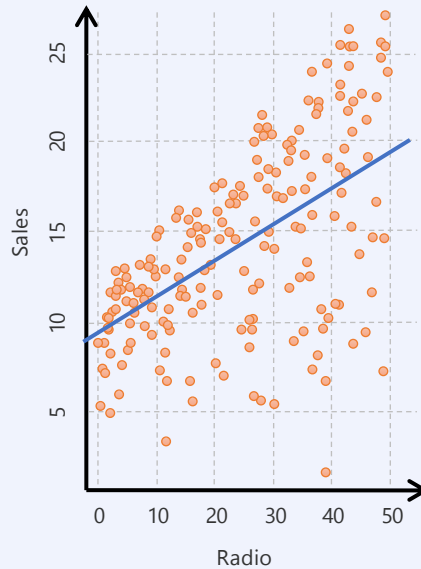
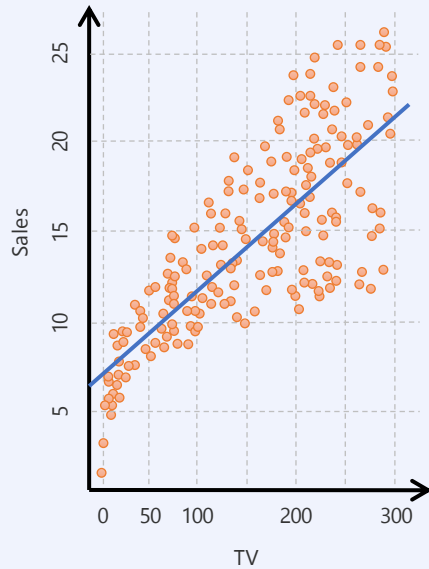
- advertising budgets are **input variables**  $X$  (aka predictors, features, independent variables)
  - $X_1$  TV budget
  - $X_2$  radio budget
  - $X_3$  newspaper budget
- sales  $Y$  is the **output variable** (aka response, dependent variable)

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

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

where  $\epsilon$  is a random additive error term with zero mean

# Example Advertising

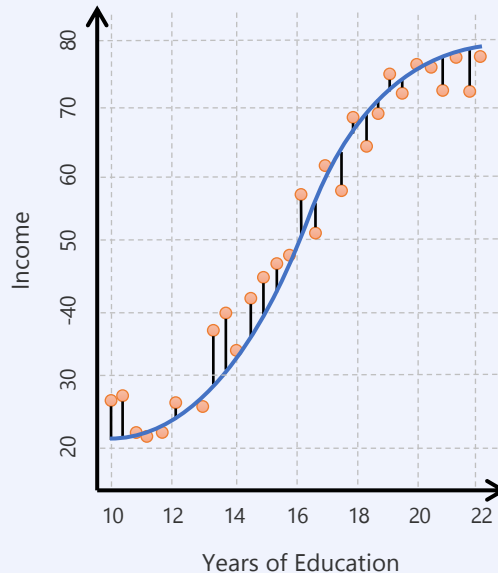


*Numbers are in thousands of dollars  
In general, sales increase as advertising is stepped up.  
The blue lines result from least-squares linear regression  
to the variable along the x-axis*

# 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  $X$  are available**, **output  $Y$  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

# Why estimate $f$ ? *prediction*

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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

$$\begin{aligned} E[Y - \hat{Y}]^2 &= E[f(X) + \epsilon - \hat{f}(X)]^2 \\ &= E[\underbrace{f(X) - \hat{f}(X)}_{\text{reducible error}}]^2 + \underbrace{Var(\epsilon)}_{\text{irreducible error}} \end{aligned}$$

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

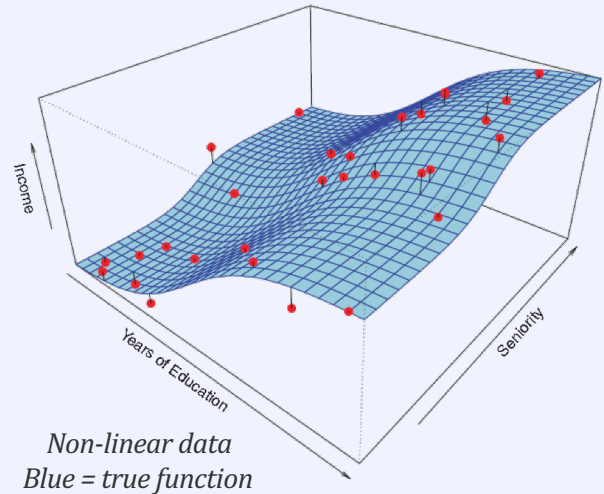
- there is (almost always) a **tradeoff** between the two
- simple models, e.g. linear regression, are easily interpretable but may be inaccurate
- flexible models, e.g. deep learning, can model almost anything but are notoriously hard to interpret

# How to estimate $f$ ?

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

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



# How to estimate $f$ ?

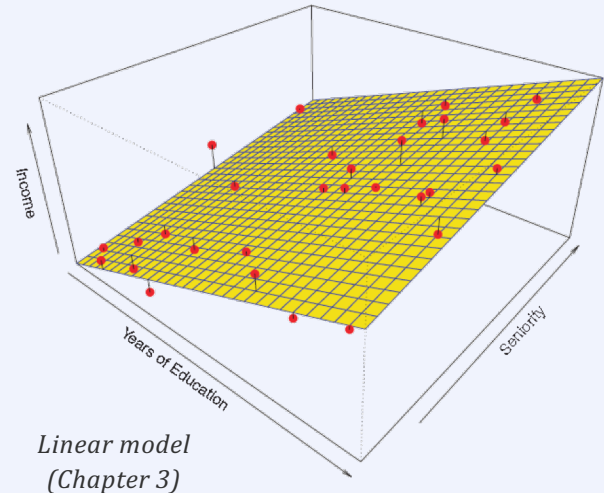
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## Parametric Methods

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



# How to estimate $f$ ?

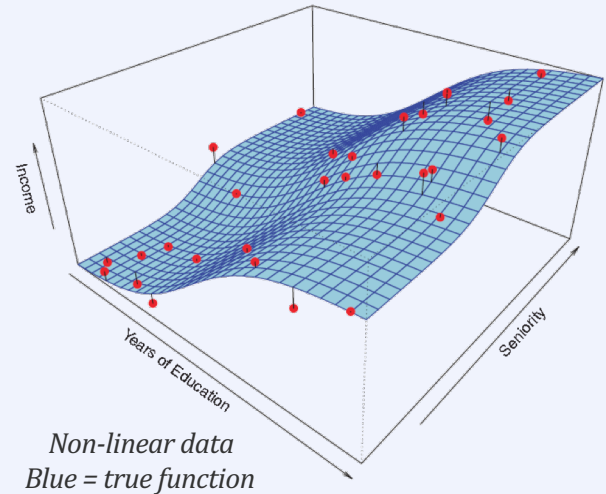
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## Nonparametric Methods

- 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**



# How to estimate $f$ ?

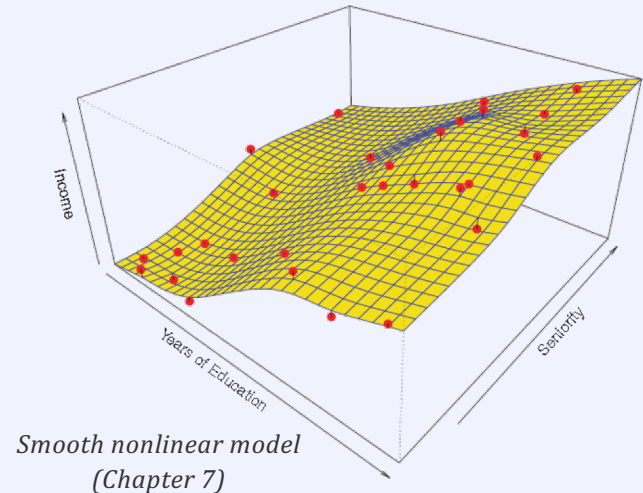
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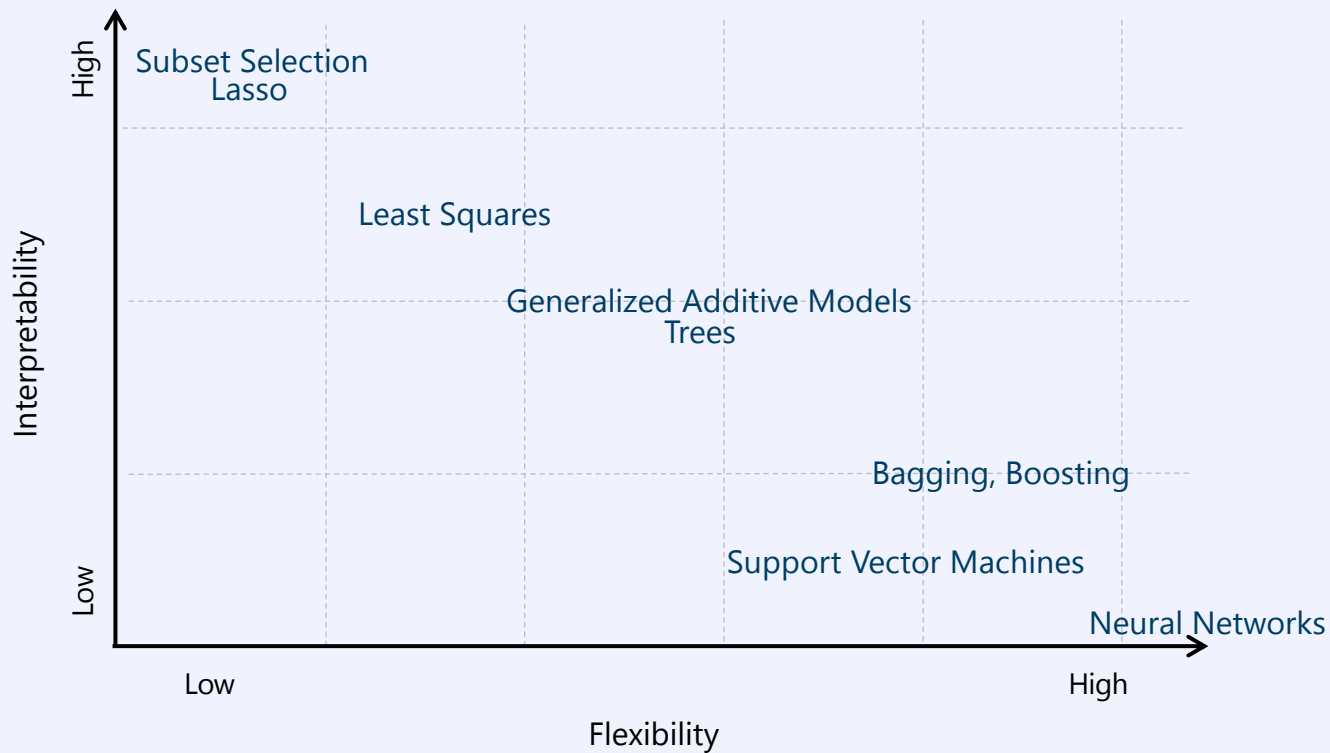
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# Accuracy vs. Interpretability



# 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

# 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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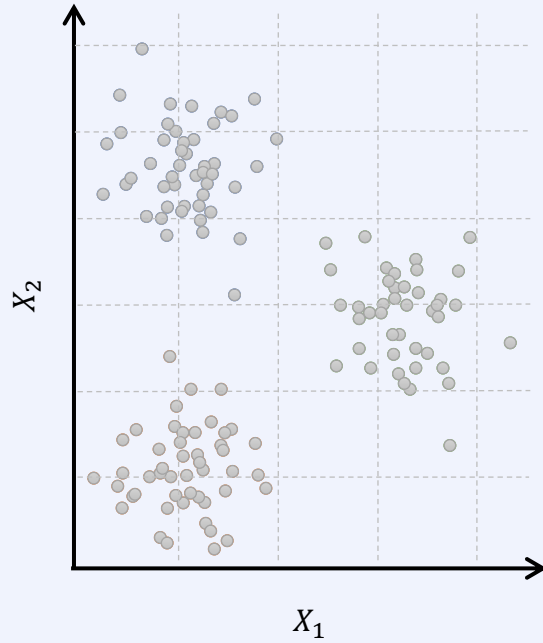
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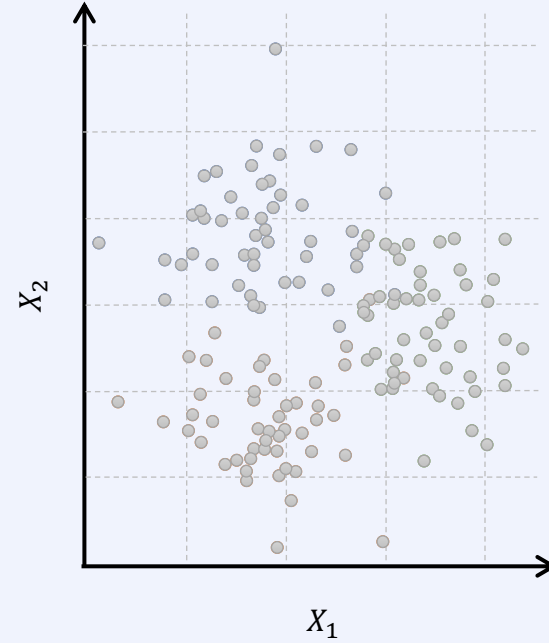
## Unsupervised learning

- **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

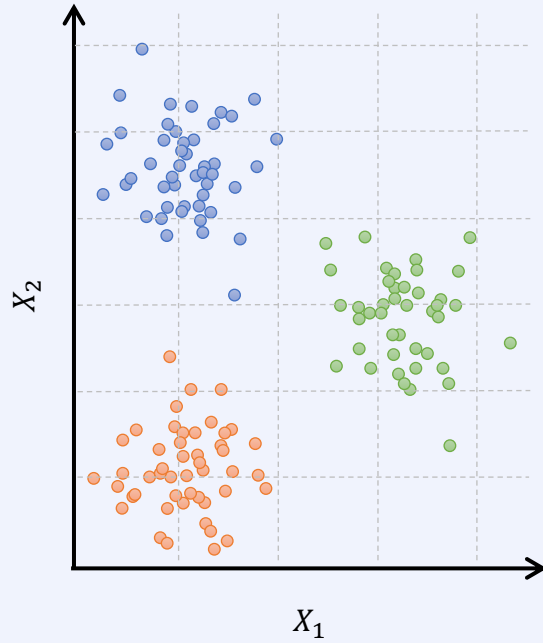


*Well separated clusters*

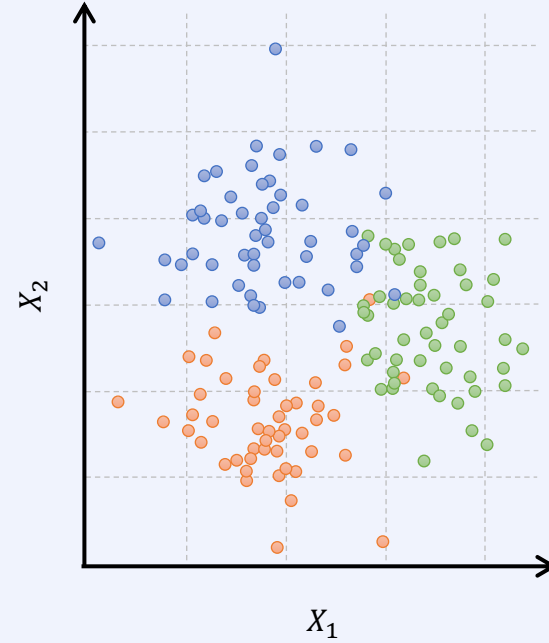


*Overlapping clusters*

# Example Clustering Problems



*Well separated clusters*



*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

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

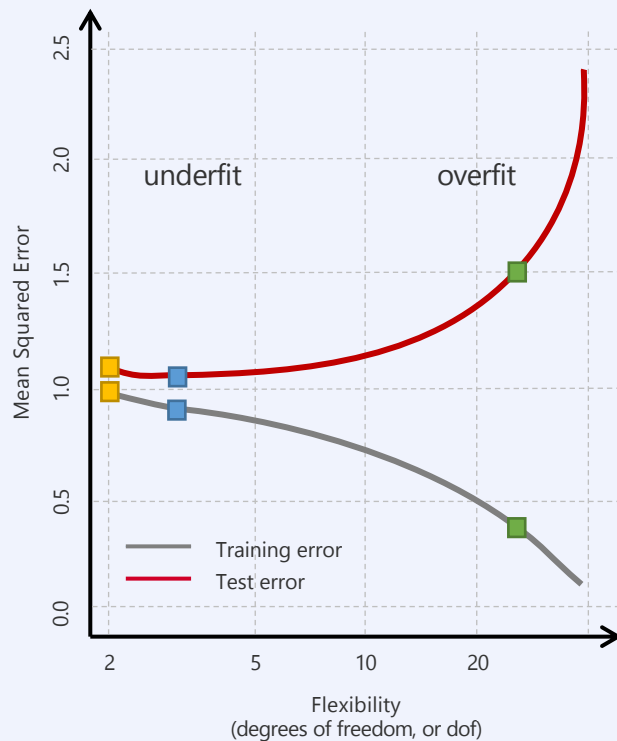
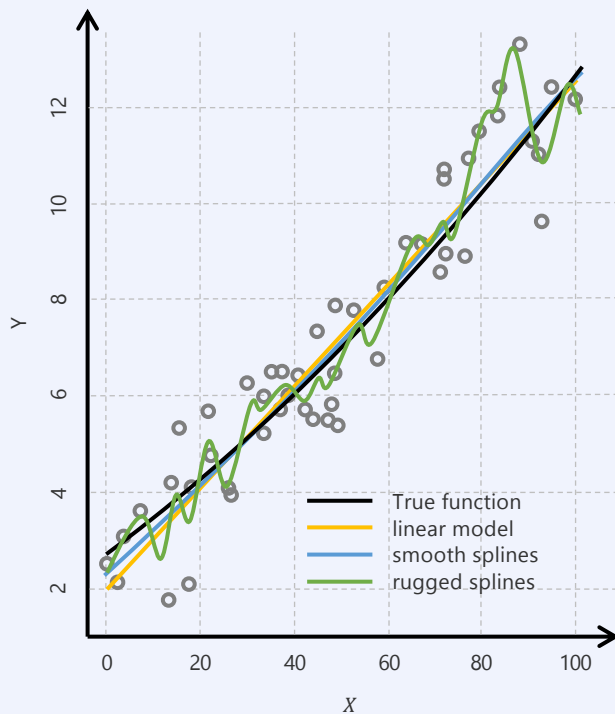
which we typically refer to as the **training error**

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

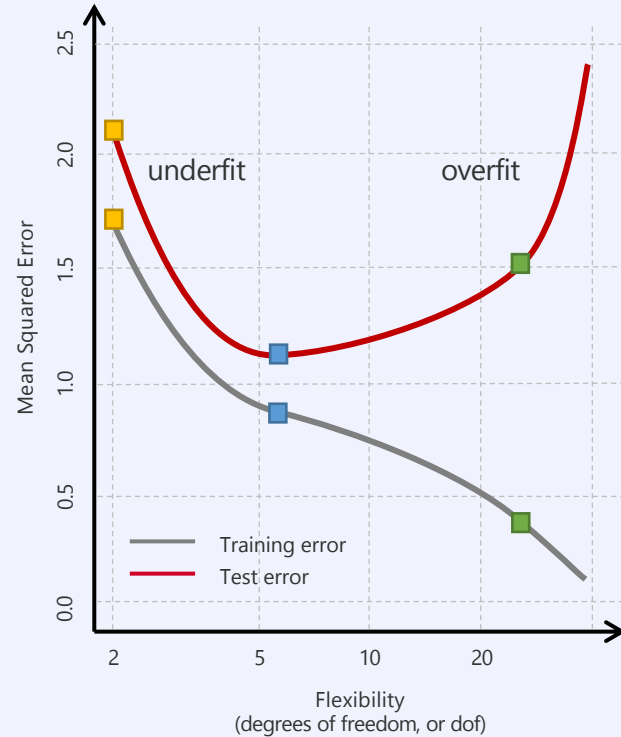
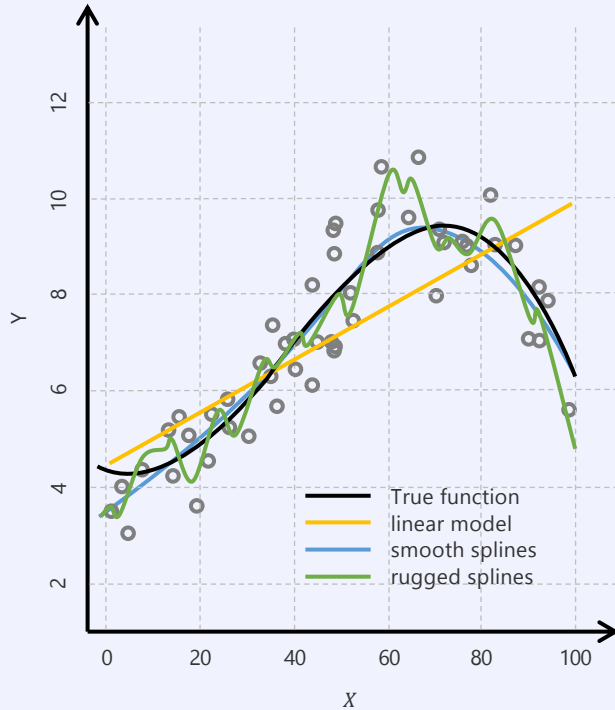
$$avg(\hat{f}(x_0) - y_0)^2$$

which we typically call the **test error** or **generalization error**

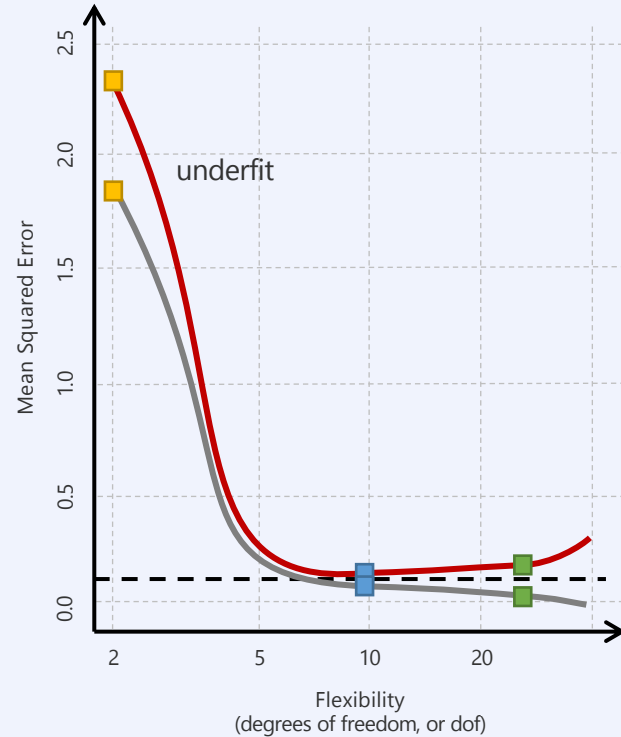
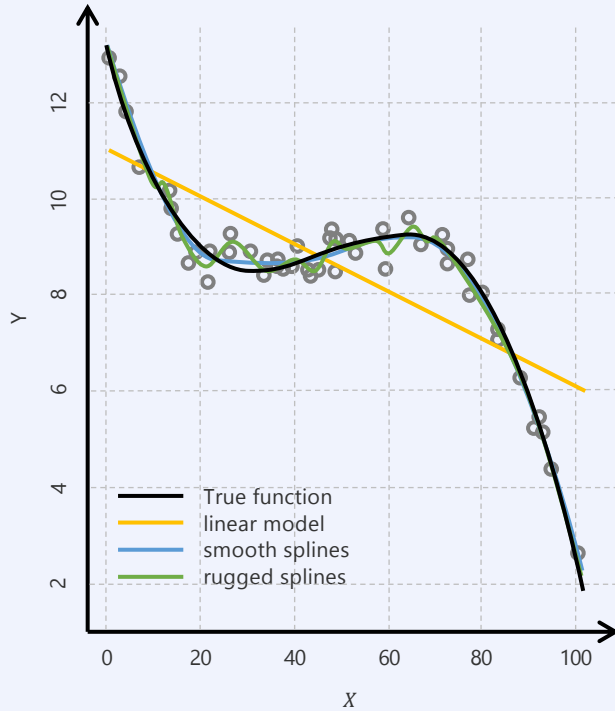
# Example Almost linear data



# Example Moderately nonlinear data



# Example Highly linear data

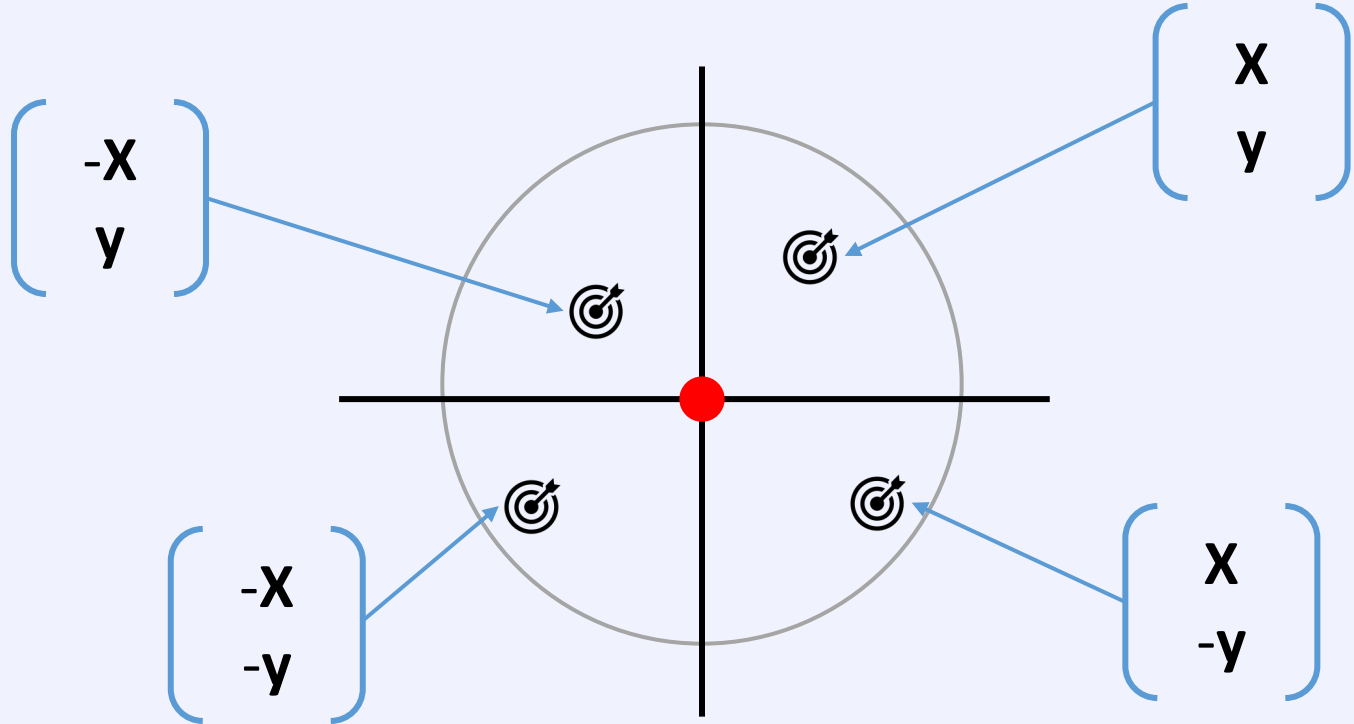


# Bias-Variance Tradeoff

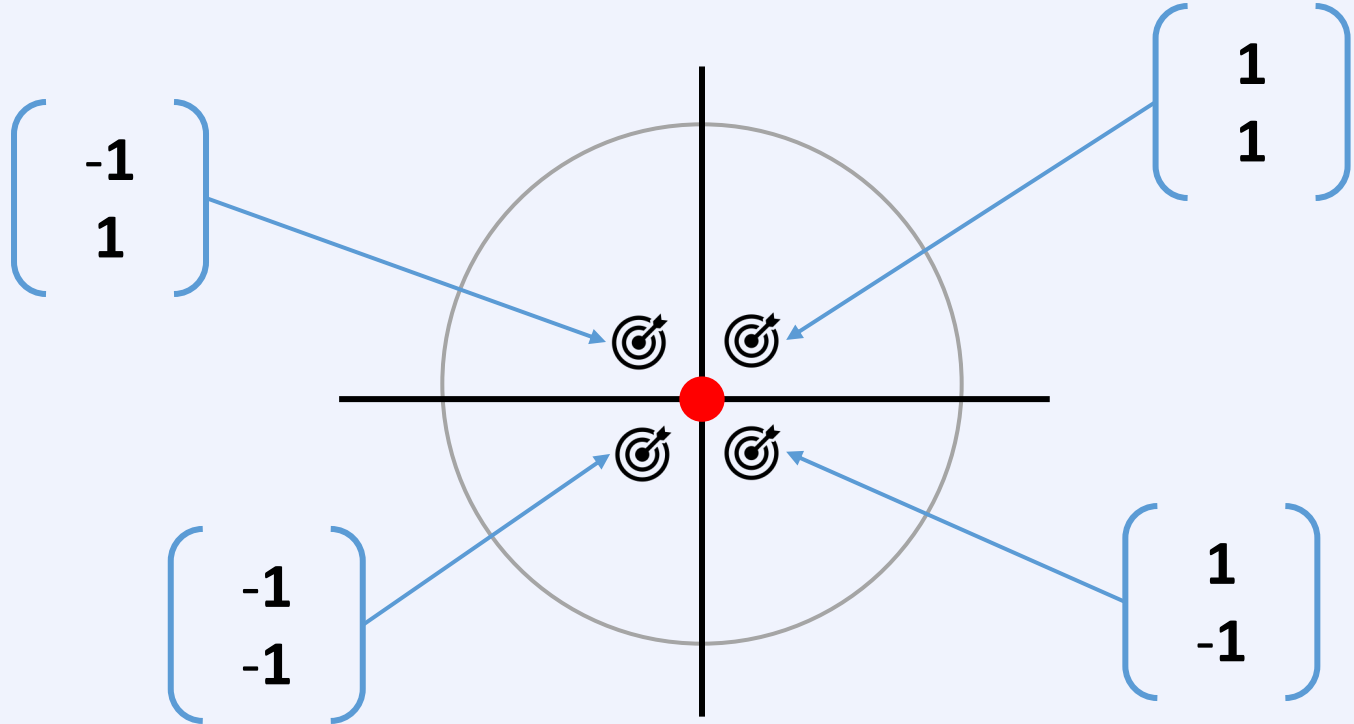




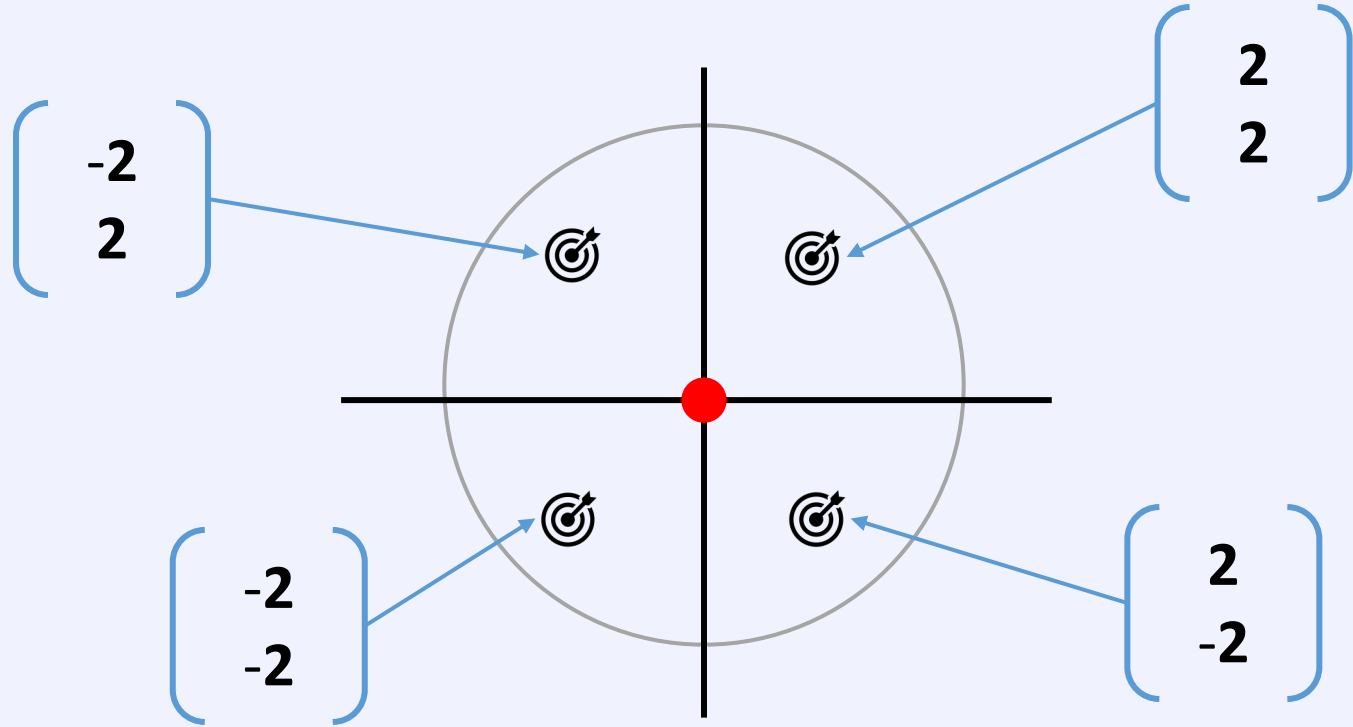
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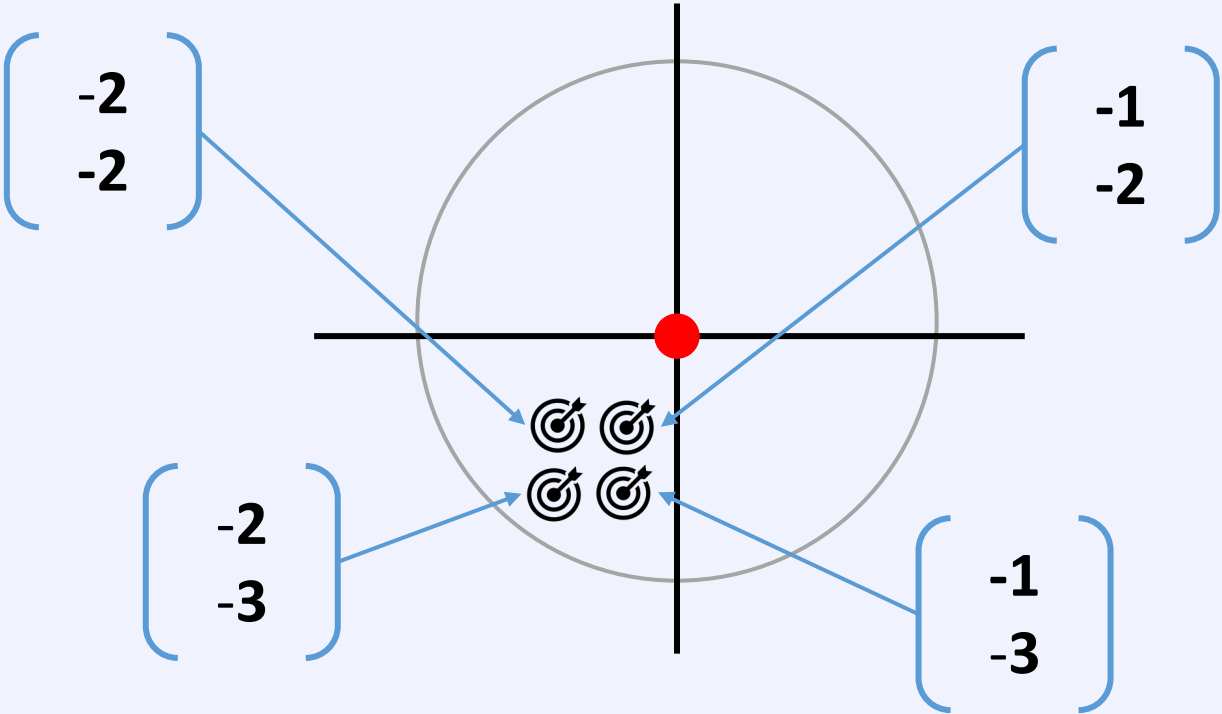
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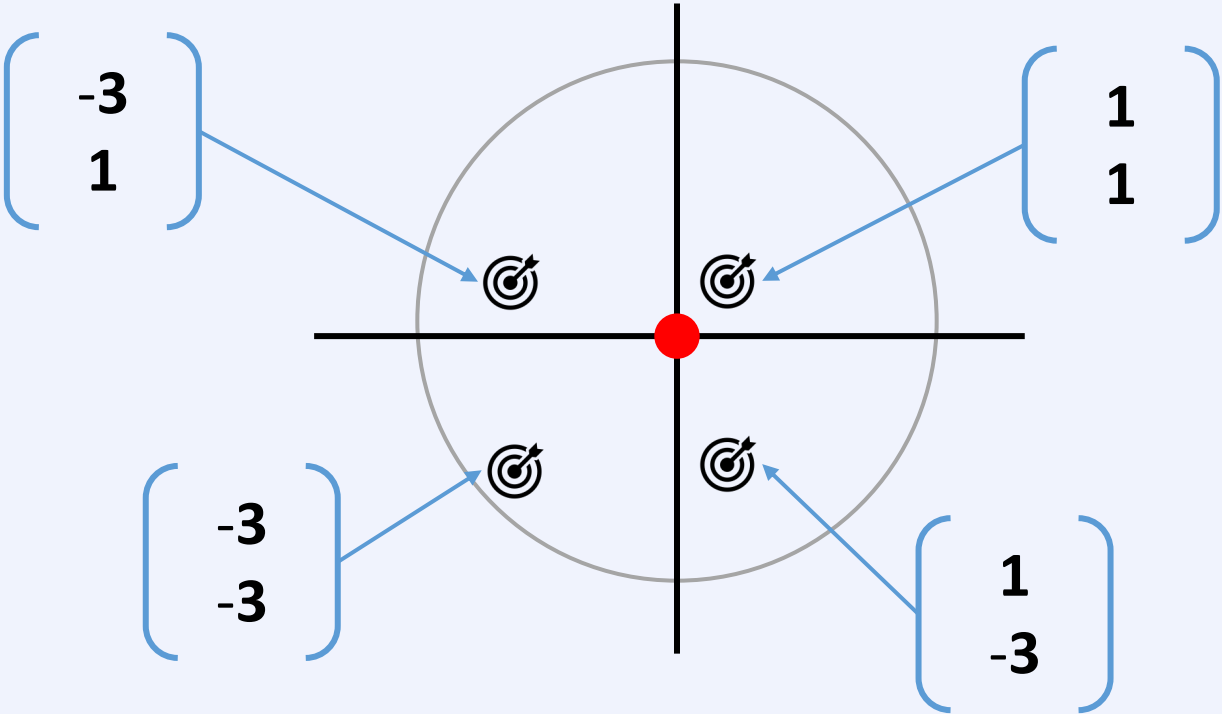
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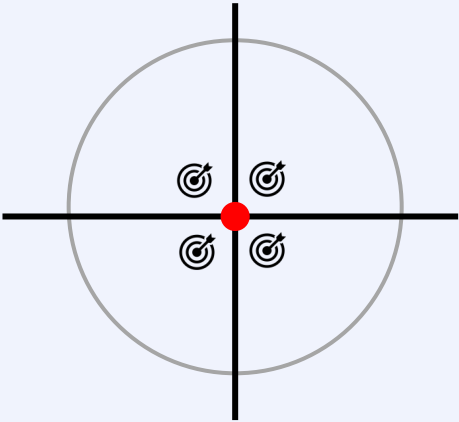
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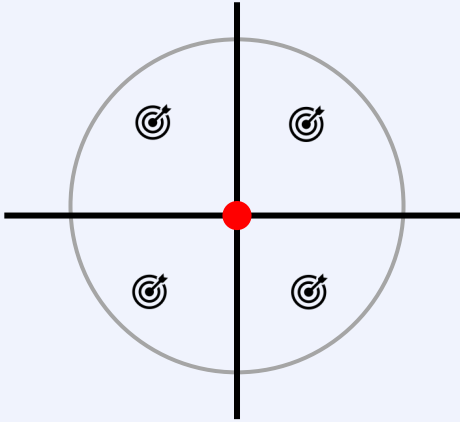
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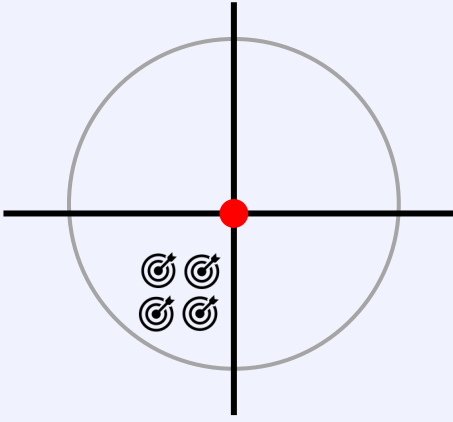
# Bias-Variance Tradeoff



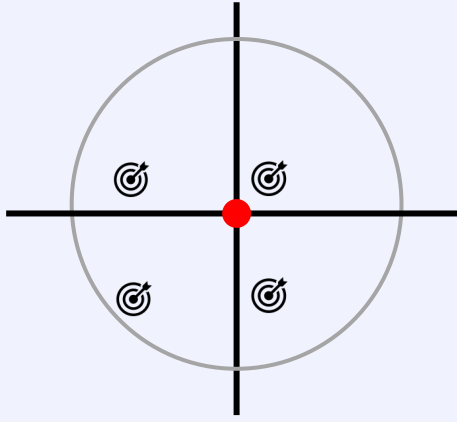
**A**



**B**

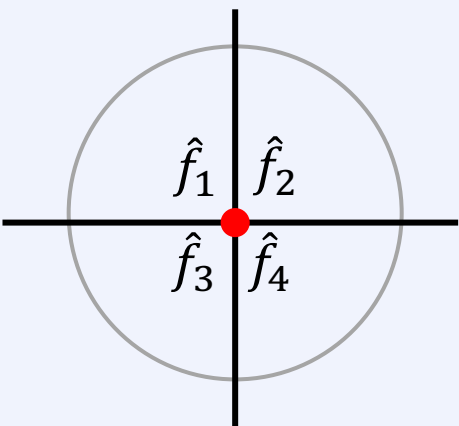


**C**

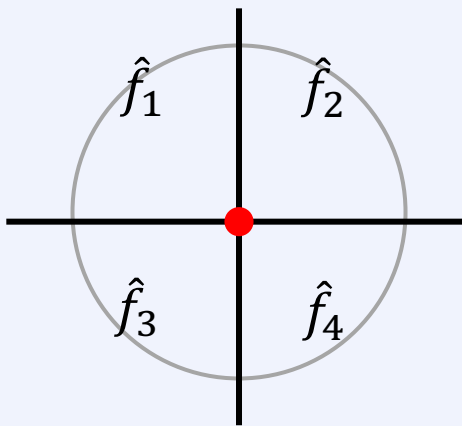


**D**

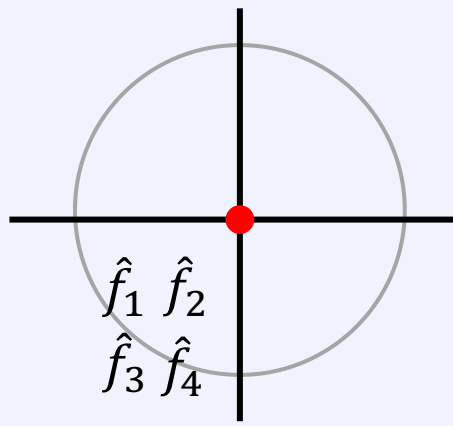
# Bias-Variance Tradeoff



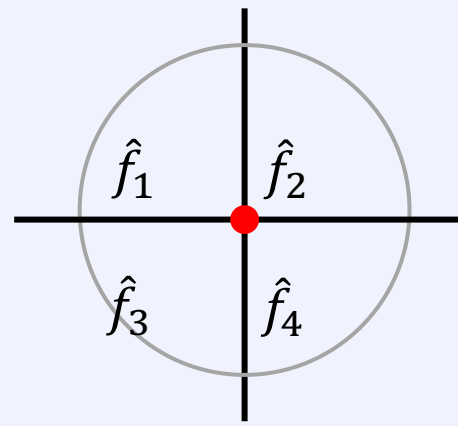
**Unbiased  
Small Variance**



**Unbiased  
Large Variance**



**Biased  
Small Variance**



**Biased  
Large Variance**

● True function  $f$

$\hat{f}_1, \hat{f}_2, \hat{f}_3, \hat{f}_4, \dots$  Estimates of  $f$  on different data sets

# Bias-Variance Tradeoff

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

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

↑  
Expectation over all  
possible training sets

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

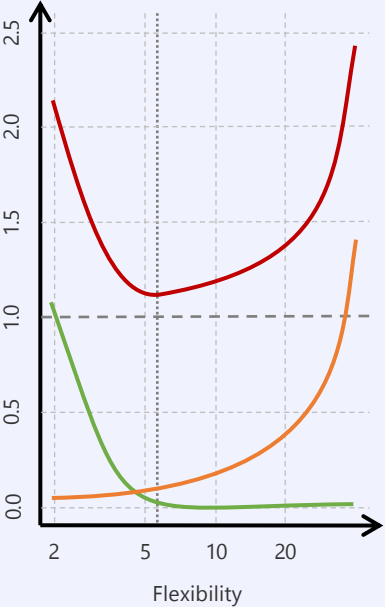
$$\text{Bias} \left( \hat{f}(x_0) \right) = E \left( \hat{f}(x_0) - y_0 \right)$$

**Variance** is the **variation** of the estimate **between different training sets**

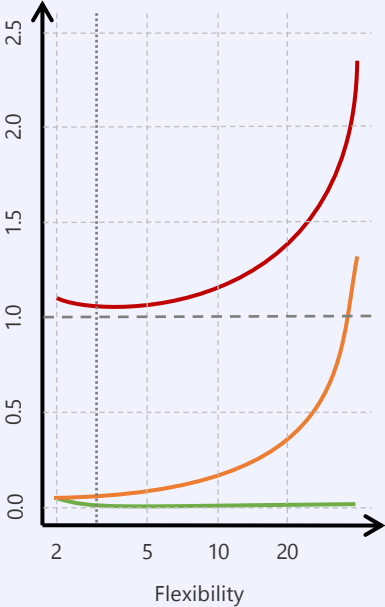
$$\text{Var} \left( \hat{f}(x_0) \right) = E \left( \hat{f}(x_0) - E \left( \hat{f}(x_0) \right) \right)^2$$



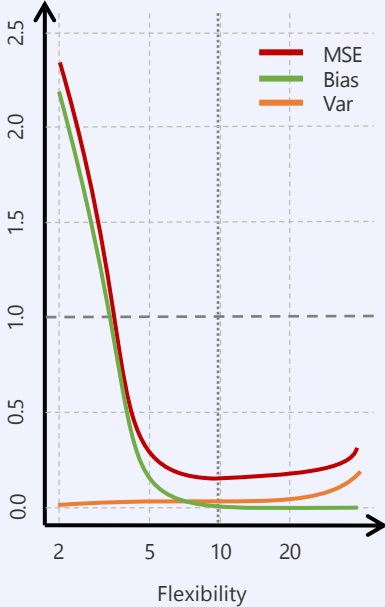
# Bias-Variance Decomposition



*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  $p \equiv \text{true}$  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  $\text{avg}(I(y_0 \neq \hat{y}_0))$

# The Bayes Classifier

We can minimize test error by the following very simple classifier

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

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

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

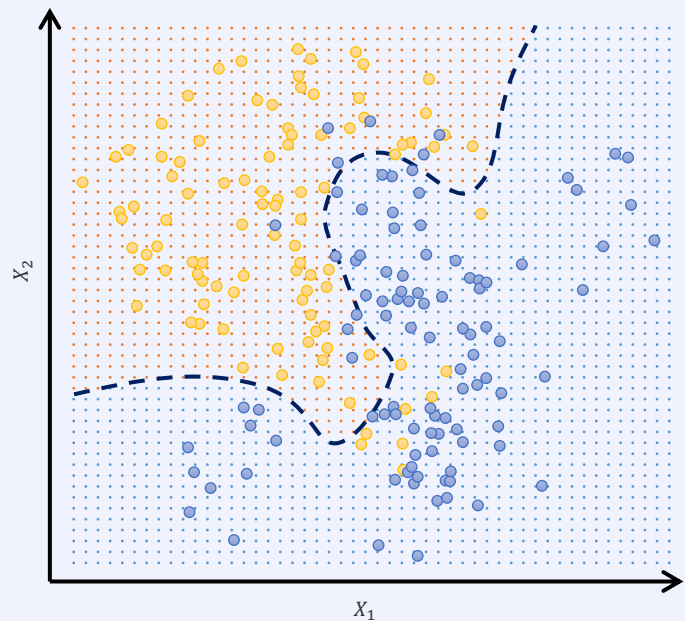
$$\Pr(Y = 1 | X = x_0) = 0.5$$

is shown as a dashed line

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

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

In this example, the Bayes error rate is 0.1304



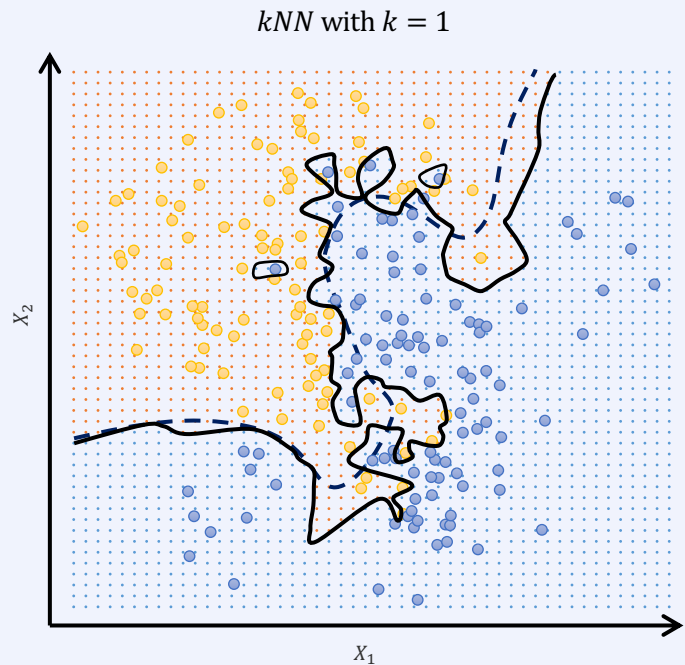
# Nearest Neighbors

## ***k*-nearest neighbors (*k*NN)**

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

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

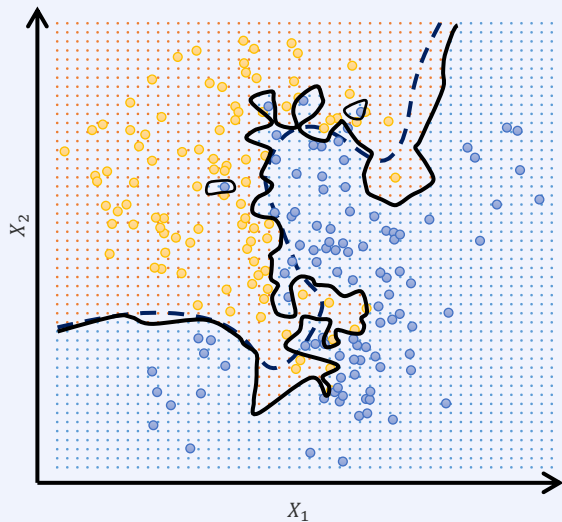
where  $\mathcal{N}_0$  are the  $k$  data points nearest to  $x_0$



overtrained  
model too complex

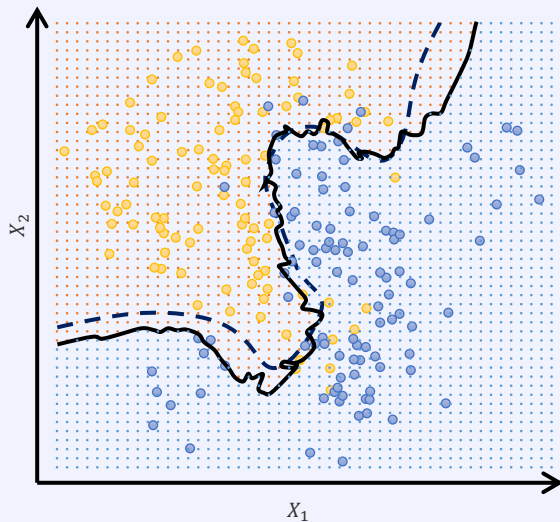
# Number of Neighbors

*kNN with  $k = 1$*



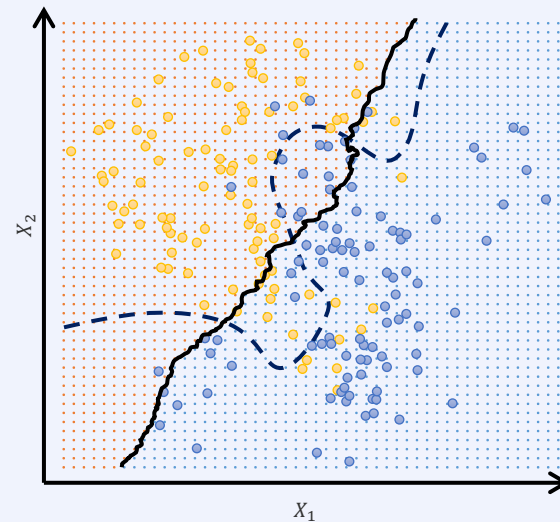
*overtrained  
model too complex*

*kNN with  $k = 10$*



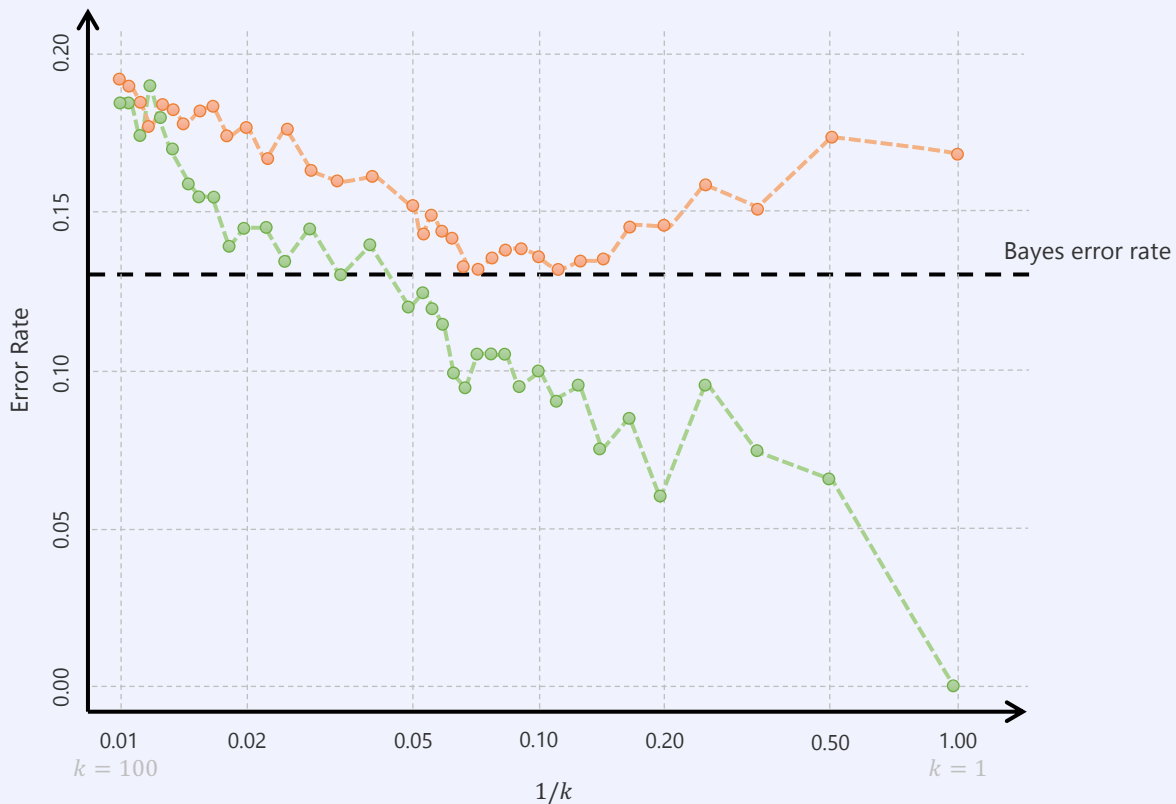
*seems just right*

*kNN with  $k = 100$*



*undertrained  
model too simple*

# Number of Neighbors



# Summary

- An introduction to a statistical learning problem
- Given data points  $(x_i, y_i)$  for  $i = 1, \dots, n$ , our goal is to learn the true  $f$ .
  - **Inference:** The estimate  $\hat{f}$  can be used to answer specific questions about  $f$ .
  - **Prediction:** The estimate  $\hat{f}$  can be used to make prediction  $\hat{Y} = \hat{f}(X)$ .
- Supervised and unsupervised learning
- Inherent tradeoffs in statistical learning
  - **Accuracy vs. interpretability:** More flexible models are often more accurate, but less interpretable.
  - **Bias vs. variance:** More flexible models often have lower bias, but higher variance.
- Model choice is one of the most crucial decisions.