What is Machine Learning?

Oxford Spring School in Advanced Research Methods, 2022

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Day 1/5

Introduction

This course

5×3 hour sessions, covering:

1. Introduction to ML and maximum likelihood estimation
2. ML extensions to regression
3. Tree-based methods
4. Neural networks
5. Ensemble methods

The logic:

- Understand the underlying mechanics of parameter estimation
- Start from a modeling strategy we are familiar with...
- ... and move on to algorithmically more complicated cases
- Build on the same foundational concepts across each day

Balancing a course on machine learning

- ML is a broad and contested domain
  - Within each sub-domain, there is a lot of potential (mathematical) detail
  - Easy to get stuck in the thickets of estimation
- Shouldn't lose sight of practical research problems
- Therefore we will not cover some topics:
  - Unsupervised methods
  - Clustering algorithms
  - (Text-specific ML models)

This course prioritises:

- Intuitive understanding of popular ML methods
- Transferability of fundamentals across ML strategies
- Relevance to our social science research streams

Session structure

Each session will be a mixture of:

- Lecture content and discussion
  - I will leave plenty of opportunities for questions
  - Building in some time for us to think through some applied problems
- Coding walkthroughs (approx. 1 hour)
  - Conducted in R using RStudio
  - Hands on experience using different algorithms
  - Many of which are very easy to implement

Slides and code are available at:
https://github.com/tsrobinson/ox_ml22

Today's session

Goals are threefold:

1. Introduce the topic of machine learning
   - What is ML?
   - How do we distinguish it from statistics?
   - What sort of problems might we apply it to?
2. Introduce key conceptual distinctions we will make throughout the course
3. Introduce maximum likelihood estimation
   - A key way in which ML parameters are estimated
   - Build our own logistic regression estimator

What is machine learning?

(Machine) learning and statistics

*"There are two cultures in the use of statistical modeling to reach **conclusions from data**. One assumes that the data are generated by a given stochastic data model. The other uses algorithmic models and treats the data mechanism as unknown" – Breiman 2001*

*"Statistical learning refers to a set of tools for modeling and understanding **complex** datasets. It is a recently developed area in statistics and blends with parallel developments in **computer science** and, in particular, machine learning" – James et al. 2013*

*"Machine learning is a subfield of **computer science** that is concerned with building algorithms which, to be useful, rely on a collection of examples of some phenomenon. . . " – Burkov 2019*

Machine learning

Expectation: I need a $1m super computer

Reality: It runs in minutes on a personal computer

Figure 1: Google: Tensor Processing Unit server rack

Why machine learning?

Machine learning can be:

- Powerful
  - With respect to computational efficiency
- Flexible
  - With respect to data generating processes
- Reduce the burden on the researcher
  - With respect to both generating data and estimating models

But ML is not a panacea!

- Cannot solve problems of poor research design
- *Can* be a black box

Machine learning and social science

ML can also introduce issues of its own:

Twitter apologises for 'racist' image-cropping algorithm

Users highlight examples of feature automatically focusing on white faces over black ones

Minority Report-style tech used to predict crime is 'prejudiced'

In his first interview since becoming surveillance commissioner, Fraser Sampson warns about accuracy of predictive policing technology

Prediction and inference

$$\hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_{1i} + e_i$$

ML typically focuses on prediction problems instead of inference problems:

- **Inference**: estimating the size/direction of the relationship between variables ($\hat{\boldsymbol{\beta}}$ problems)
- **Prediction**: estimating some outcome, using the relationships between variables ($\hat{\boldsymbol{y}}$ problems)

These two facets are connected:

- Knowing the size/direction of (all) relationships -> predict the outcome
- But we rarely know the true model
- Sometimes we can get good at $\hat{\boldsymbol{y}}$ problems without knowing $\hat{\boldsymbol{\beta}}$

Classification and prediction

Within $\hat{y}$ problems, we can distinguish two types:

- **Prediction** – estimating the value of a continuous variable (sometimes referred to as a "regression" problem) e.g.,
  - The ideology of a politician in 2D space
  - The number of votes received by a candidate
- **Classification** – estimating which *class* of a category an observation belongs to, e.g.,
  - Party identity (Republican/Democrat/Libertarian/Independent)
  - The topic of a tweet (foreign/domestic, pro/con)
  - Recidivism

$\hat{Y}$ and $\hat{X}$ problems

We can also think about where the prediction problem lies:

- $\hat{\boldsymbol{y}}$ problems are about the dependent variable
  - To predict the probability of revolution...
  - ... or the weather tomorrow
  - These are not necessarily inferential problems
- But there are $\hat{\boldsymbol{X}}$ (independent variables) problems too:
  - Dimensions of interest that may be important to our theory, but which are:
    - Not directly observable (i.e. latent)
    - Difficult to measure "by hand"
  - We can make predictions over $\boldsymbol{X}$ so we can test our inferential theory

Supervised vs unsupervised methods

Supervised methods

- **Training data** are a set of labelled examples, where $\boldsymbol{y}$ is our target prediction
- We use these examples to "learn" the relationship between $\boldsymbol{y}$ and $\boldsymbol{X}$
- Then predict $\boldsymbol{y}$ for a *new* unlabelled dataset (i.e. where the target variable is not observed)

Learning the relationship:

$$\underbrace{\begin{bmatrix} 1 \\ 0 \\ 0 \\ \vdots \\ 1 \end{bmatrix}}_{\mathbf{y}^{\text{TRAIN}}} \quad \underbrace{\begin{bmatrix} 3.3 & 1.1 & 0 \\ 2.7 & 0.8 & 0 \\ 1.8 & 0.1 & 1 \\ \vdots & \vdots & \vdots \\ 5 & 1.2 & 0 \end{bmatrix}}_{\mathbf{X}^{\text{TRAIN}}}$$

Predicting on new data

$$\mathbf{X}^{\text{TEST}} = \begin{bmatrix} 3.5 & 1.9 & 1 \\ 5.4 & 0.3 & 0 \\ 1.7 & 0.5 & 1 \end{bmatrix}$$

Notation

Algebra

Throughout the course, we will follow the notation set out in Burkov (2019):

- θ and x are scalar - i.e. a single number
  - E.g., $\theta = 3.141$, $x = 1$ etc.
- $\boldsymbol{\theta}$ and $\boldsymbol{x}$ are vectors - i.e. an ordered list of scalar values
  - E.g., $\boldsymbol{\theta} = [0.5, 3, 2]$
- $\boldsymbol{\Theta}$ and $\mathbf{X}$ are matrices
  - E.g.,

$$\mathbf{X} = \begin{bmatrix} 1 & 5 \\ 24 & -3 \end{bmatrix}$$

  - $\mathbf{x}^{(k)}$ is the kth column of $\boldsymbol{X}$
  - $\mathbf{x_i}$ is the ith row in matrix $\mathbf{X}$
  - $x_i^{(k)}$ is the kth element of the row vector $\boldsymbol{x_i}$

Probability notation

Let p denote a probability distribution *function* that returns the probability of an event or observation:

- $p(A) = 0.5$ means the probability of event A is 0.5
- All probabilities are bounded between 0 and 1
  - $0 \leq p(A) \leq 1$

Conditional probabilities means the probability of an event **given** the value of another variable

- $p(A|c) = 0.25$

Probability rules

Probabilities have some nice features:

- $p(A \text{ and } B) = p(A)p(B|A)$
- If $p(A) \perp p(B)$, then $p(B|A) = p(B)$

As a result:

- If $p(A) \perp p(B)$, then $p(A \text{ and } B) = p(A)p(B)$
- These rules explain why the probability of two coin-flips is $= 0.25$:
  - $P(\text{Flip 1} = \text{Heads}) = 0.5$
  - $P(\text{Flip 2} = \text{Heads}|\text{Flip 1} = \text{Heads}) = P(\text{Flip 1} = \text{Heads})$
  - $P(\text{Flip 1} = \text{Heads *and* Flip 2} = \text{Heads}) = 0.5 \times 0.5 = 0.25$

Notation quiz

What are the following:

1. $\mathbf{a}$
2. y_i
3. $\boldsymbol{\beta}$
4. β
5. $\boldsymbol{\Theta}$

If $p(A) = 0.5$, $p(B) = 0.1$, and $p(B|A) = 0.3$:

6. Is $p(A) \perp p(B)$?
7. What is $p(A \text{ and } B)$?

Maximum Likelihood Estimation (a gentle introduction)

Bayes Theorem (from a frequentist perspective)

$$\underbrace{P(A|B)}_{\text{Posterior}} = \frac{\overbrace{P(B|A)}^{\text{Likelihood}} \times \overbrace{P(A)}^{\text{Prior}}}{\underbrace{P(B)}_{\text{Evidence}}}$$

We can use Bayes formula to estimate the posterior probability of some parameter $\boldsymbol{\theta}$:

$$p(\boldsymbol{\theta}|\mathbf{X}) \propto p(\mathbf{X}|\boldsymbol{\theta}) \times p(\boldsymbol{\theta}),$$

where $\mathbf{X}$ is the data.

Likelihood function

Let's suppose that we have no prior knowledge over $\boldsymbol{\theta}$, so we'll drop the prior and focus specifically on the likelihood:

$$\mathcal{L}(\boldsymbol{\theta}) = p(\mathbf{X}|\theta)$$

How would we calculate this?

$$\begin{aligned}\mathcal{L}(\boldsymbol{\theta}) &= p(\mathbf{x_1}|\boldsymbol{\theta}) \times p(\mathbf{x_2}|\boldsymbol{\theta}) \times \ldots \times p(\mathbf{x_n}|\boldsymbol{\theta}) \\ &= \prod_{i=1\ldots N} p(\mathbf{x}_i|\boldsymbol{\theta})\end{aligned}$$

i.e. the product of the probability of each observations within $\mathbf{X}$, given $\boldsymbol{\theta}$.

What does this assume?

Comparing likelihoods

Suppose we have two alternative values of $\boldsymbol{\theta}$: $\boldsymbol{\theta^{(1)}}, \boldsymbol{\theta^{(2)}}$. We can calculate the likelihood *ratio* (LR) of these two possible parameter values:

$$LR = \frac{\mathcal{L}(\boldsymbol{\theta^{(1)}})}{\mathcal{L}(\boldsymbol{\theta^{(2)}})}$$

If $LR > 1$, which parameter value would we pick?

Maximum likelihood estimation

We can generalise this for all possible values of θ:

$$\arg\max_{\boldsymbol{\theta} \in \Theta} \mathcal{L}(\boldsymbol{\theta}) = \prod_{i=1 \ldots N} p(\mathbf{x}_i | \boldsymbol{\theta})$$

i.e., from the set of all possible parameter values Θ, find the parameter value that maximises the likelihood function.

Hence, **maximum** likelihood estimation.

- How we calculate $p(\mathbf{x}_i | \boldsymbol{\theta})$ will depend on the functional form of the underlying distribution
- We'll explore this specifically with respect to logistic regression later on today

Why is this maximum likelihood a useful concept?

Numeric overflow

Multiplying many small numbers means we soon lose the power to calculate them precisely

- R double-precision numbers range from 2×10^{-308} to 2×10^{308}
- If 400 observations have $p_{\boldsymbol{\theta}} = 0.01$, $\mathcal{L}(\boldsymbol{\theta})$ will be outside the computable range

What if we take the log?

- The log function is strictly increasing
- $Log(a \times b) = Log(a) + Log(b)$ so we can simply add the values

With the logged likelihood function we do not have the problem of numeric overflow!

Negative log-likelihood

We can also calculate the *negative* log-likelihood:

- I.e. put a minus sign in front!
- We then *minimise* the negative log-likelihood
- We typically want to minimise rather than maximise because many of our procedures for optimisation are based on the former
- But, broadly, this is just semantics:
  - Minimising the negative log-likelihood is the same as maximising the log-likelihood

Logistic regression

Logistic regression:

- Allows us to estimate β parameters when we have a binary outcome variable
- More broadly, it is a **binary classification** algorithm – what is the probability that $y_i = 1$ given a vector of features $\mathbf{x_i}$?

We can write the logistic regression function as,

$$f_{\boldsymbol{\theta},b}(\mathbf{X}) = \frac{1}{1 + e^{-(\boldsymbol{\theta}\mathbf{X}+b)}}.$$

The goal is to find the *best* values of $\boldsymbol{\theta}$ and b that "explains" the data

- Let's include b within $\boldsymbol{\theta}$ s.t. $\boldsymbol{\theta} = [b, \theta_1, \cdots, \theta_k]$

MLE of logistic regression

For a given vector of scalar values $\boldsymbol{\theta}$, we can ask what the likelihood of the data is given those values

How do we construct this?

- If $y_i = 1$, we want the $f_{\boldsymbol{\theta}}(\mathbf{x_i})$
- But if $y_i = 0$ we want the inverse, i.e. $(1 - f_{\boldsymbol{\theta}}(\mathbf{x_i}))$
- We can combine these two using a mathematical "logic gate":

$$\mathcal{L}_{\boldsymbol{\theta}} = f_{\boldsymbol{\theta}}(\mathbf{X})^{\boldsymbol{y}} \times (1 - f_{\boldsymbol{\theta}}(\mathbf{X}))^{(1-\boldsymbol{y})},$$

  as when $y_i = 0, x^{y_i} = 1$ and $x^{(1-y_i)} = x$, and vice versa.

Simplifying, since $f_{\boldsymbol{\theta}}(\boldsymbol{x_i}) = \hat{y}_i$:

$$\mathcal{L}_{\boldsymbol{\theta}} = \hat{\boldsymbol{y}}^{y}(1 - \hat{\boldsymbol{y}})^{1-y}$$

MLE optimization

We can then apply our "tricks" to make the computation easier:

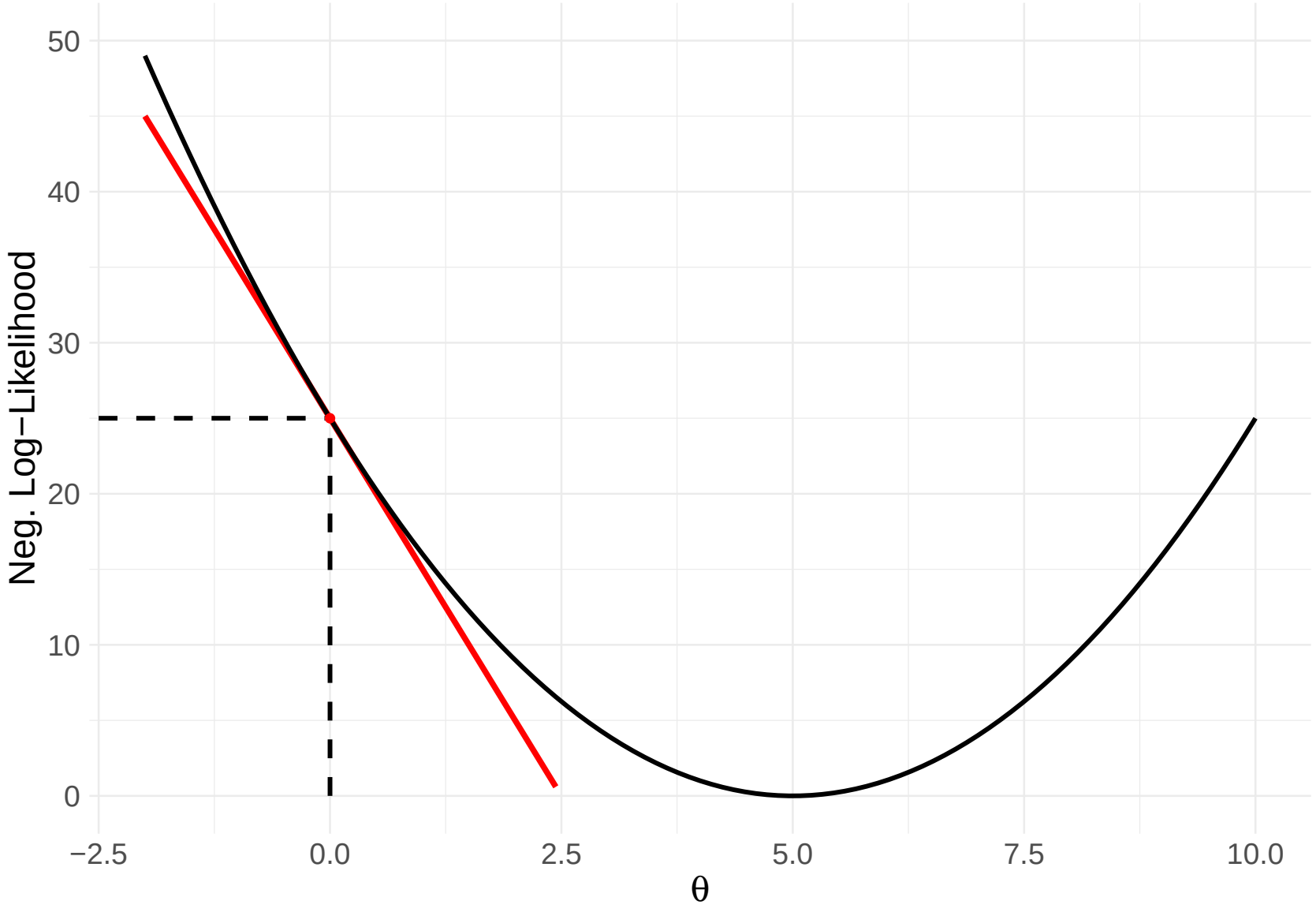
$$-Log(\mathcal{L}_{\boldsymbol{\theta}}) = -\sum_{i=1}^{N} Log(\mathcal{L}_{\boldsymbol{\theta}}(\mathbf{x_i})),$$

with the goal of minimising this quantity through choosing $\boldsymbol{\theta}$.

How exactly do we minimize this function?

- Unlike OLS, where there is a closed form solution, it is not possible to analytically minimize the negative log-likelihood of the logistic regression
- We therefore have to use computation to iterate through values of $\boldsymbol{\theta}$ to approximate the minima

Minimising the negative log-likelihood in one dimension



Gradient descent algorithm

To find the minimum of the negative log-likelihood we:

1. Choose a value for the starting parameter θ
2. Calculate the slope of the function at that point
3. Adjust our value of θ in the *opposite* direction to the slope coefficient's sign
4. Recalculate the slope, and repeat 2-4

We can generalise this to $\boldsymbol{\theta}$:

- Let $Q(\boldsymbol{\theta})$ be the negative log likelihood function
- Calculate the **gradient** vector of the function in k-dimensions
- Adjust each parameter $\theta_k \in \boldsymbol{\theta}$ by the negative of the corresponding gradient element

$$\theta_k = \theta_k - \frac{\partial Q(\boldsymbol{\theta})}{\partial \theta_k}$$

Logistic regression gradient

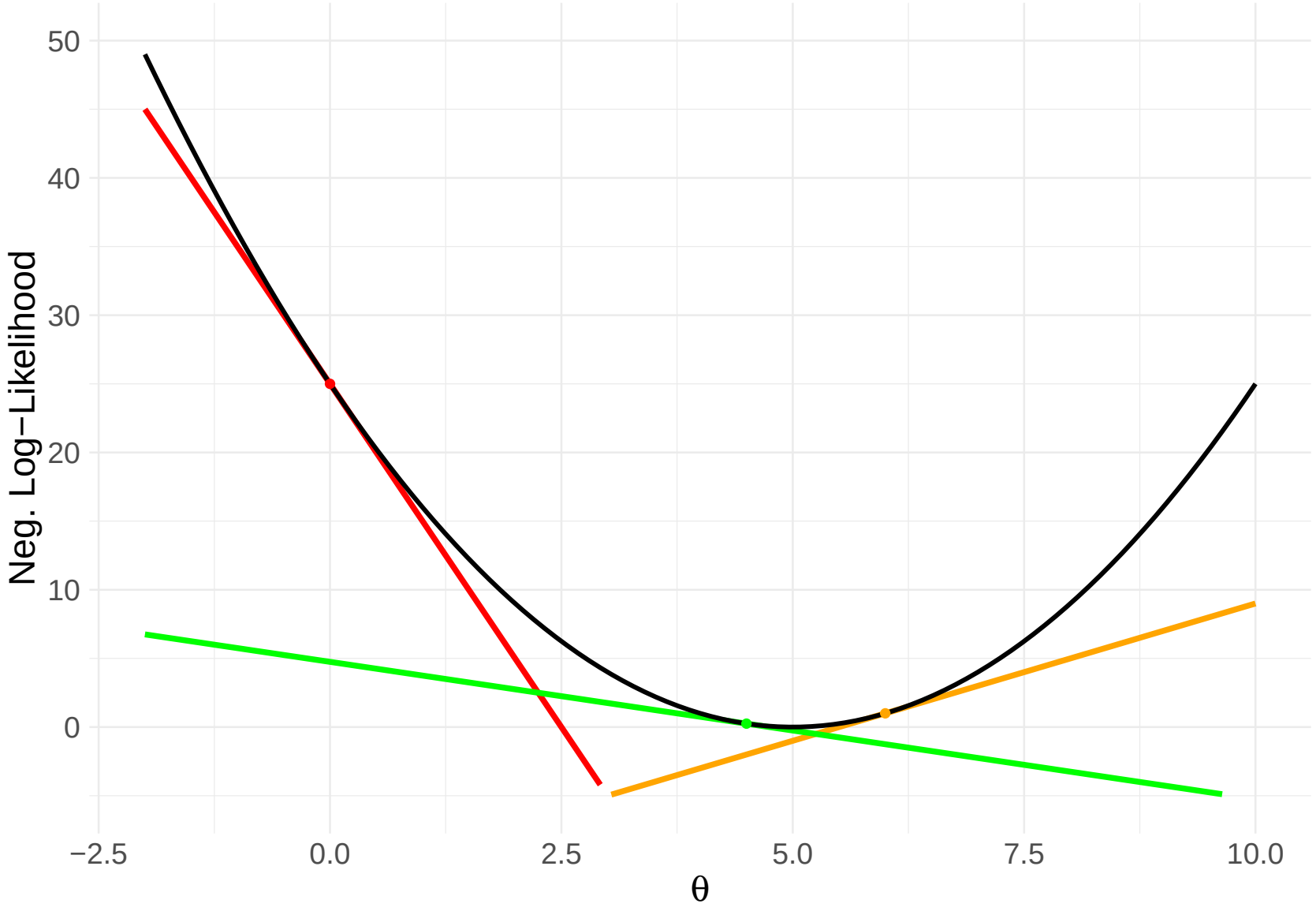
The partial derivative for any predictor $\boldsymbol{x}^{(j)}$ for the *logistic* cost function is:

$$\frac{\partial Q^{\text{Logit}}}{\partial \theta_k} = \left(f_{\theta_k}(\boldsymbol{X}) - \boldsymbol{y}\right)\boldsymbol{x}^{(k)}$$

Hence the gradient of the function's curve for any vector of logistic parameters $\boldsymbol{\theta}$ can be described as:

$$\boldsymbol{\nabla} = \begin{bmatrix} \frac{\partial Q^{\text{Logit}}(\boldsymbol{\theta})}{\partial \theta_1} \\ \frac{\partial Q^{\text{Logit}}(\boldsymbol{\theta})}{\partial \theta_2} \\ \vdots \\ \frac{\partial Q^{\text{Logit}}(\boldsymbol{\theta})}{\partial \theta_k} \end{bmatrix}$$

Progression of the descent algorithm



Learning rate

As we iteratively adjust the value of our parameter:

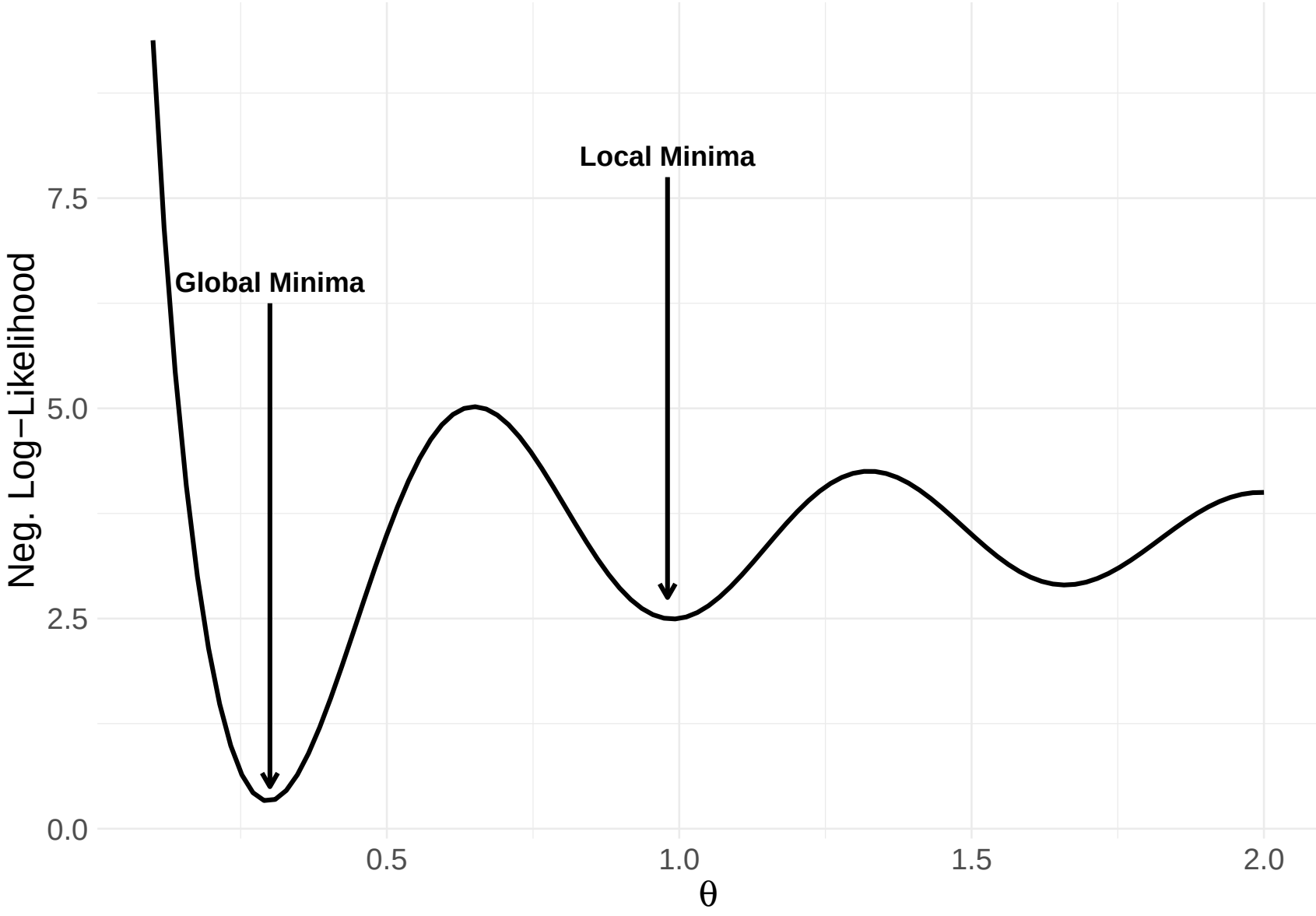
- It's possible we keep jumping over the minima
- Or we get stuck in a rut and the estimator fails to find an even better parameter choice

So we can scale the impact of the current gradient on the new parameter choice:

- Let's call this hyperparameter the **learning rate** (λ)
- $\boldsymbol{\theta}_{\text{New}} = \boldsymbol{\theta} - \lambda \boldsymbol{\nabla}$

The choice of λ is down to the researcher:

- Overly-large values will prevent minimisation
- Overly small values may take too long, or risk converging on *local* minima


Local Minima
Global Minima
Neg. Log−Likelihood
7.5
5.0
2.5
0.0
0.5
1.0
1.5
2.0
θ

Stochastic gradient descent

Gradient descent can be **expensive**:

- We have to evaluate all rows in our training data before making any updates to the parameters
- If we have lots of observations
    1. Each calculation takes a long time
    2. Take many iterations to optimise
- Instead we can use **stochastic gradient descent** (SGD)
    - Inspect the loss of each observation (or a random subset) individually
    - Update the coefficients based on each observation

Stochastic gradient descent

Under GD, for each iteration:

$$\theta_k \leftarrow \theta_k + \lambda \sum_{i=1}^{N} (y_i - f_{\theta_k}(\boldsymbol{x_i}))\boldsymbol{x_i}^{(k)}$$

Under SGD, for each iteration:

$$\theta_k \leftarrow \sum_{i=1}^{N} \theta_k + \lambda (y_i - f_{\theta_k}(\boldsymbol{x_i}))\boldsymbol{x_i}^{(k)}$$

- SGD typically converges a lot faster than GD
  - Every iteration we make N small changes to the parameter estimate
  - Computationally more efficient (we'll cover this more later in the week)
  - At the cost of some additional noise in the optimisation process

Coding workshop: writing our own logistic regression classifier