Optimization

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Today we are going to learn...

1. **Structure of Part II**
2. **Motivation: Why Optimize?**
3. **Newton's Method**
    - Finding a root
    - Finding a local minimum/maximum
    - Multidimensional Optimization
4. **Quasi-Newton Methods**
5. **Gradient Descent Methods**
6. **Derivative Free Methods**
    - Motivation
    - Nelder Mead Algorithm
    - Coding Nelder Mead
    - Using Nelder Mead

Structure

- We cover many different topics. This week: Optimization
- For each topic we consider the following
    - Motivation
    - Intuition
    - Mathematics
    - Code

Optimization in Business

- Many problems in business require something to be minimized or maximized
  - Maximizing Revenue
  - Minimizing Costs
  - Minimizing Delivery Time
  - Maximizing Financial Returns

Input and output

- For many of these problems there is some control over the input
  - Maximizing Revenue - Price
  - Minimizing Costs - Number of Workers
  - Minimizing Delivery Time - Driving Route
  - Maximizing Financial Returns - Portfolio weights

Optimization in Statistics

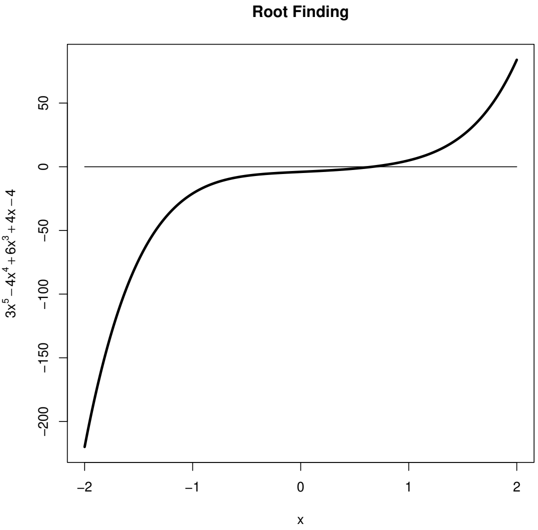
- In statistics, many estimators maximize or minimize a function
  - Maximum Likelihood
  - Least Squares
  - Method of Moments
  - Posterior Mode

- Suppose we want to find an minimum or maximum of a function $f(x)$
- Sometimes $f(x)$ will be very complicated
- Are there computer algorithms that can help?
- YES!
    - Newton's Method
    - Quasi-Newton
    - Nelder Mead

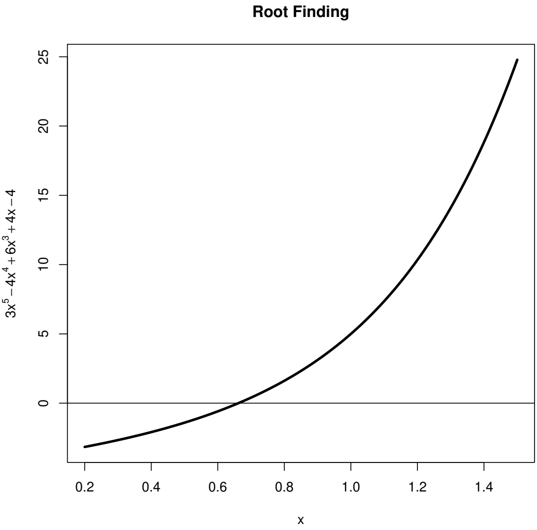
Root of a function

- Consider the problem of finding the **root** or **zero** a function.
- For the function $g(x)$ the **root** is the point x^* such that $g(x^*) = 0$
- An algorithm for solving this problem was proposed by Newton and Raphson nearly 500 years ago.
- We will use this algorithm to find the root of $g(x) = 3x^5 - 4x^4 + 6x^3 + 4x - 4$

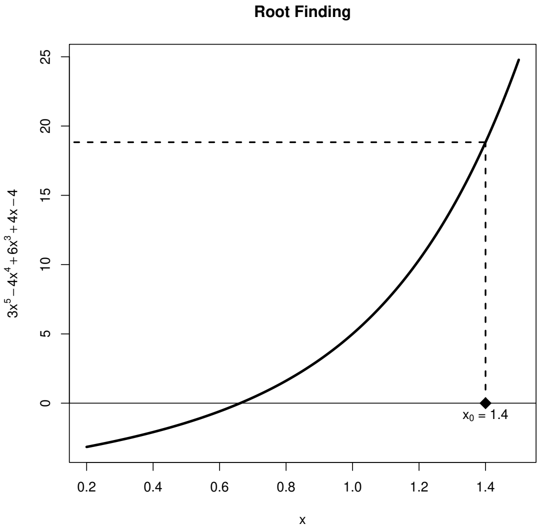
Root of a function



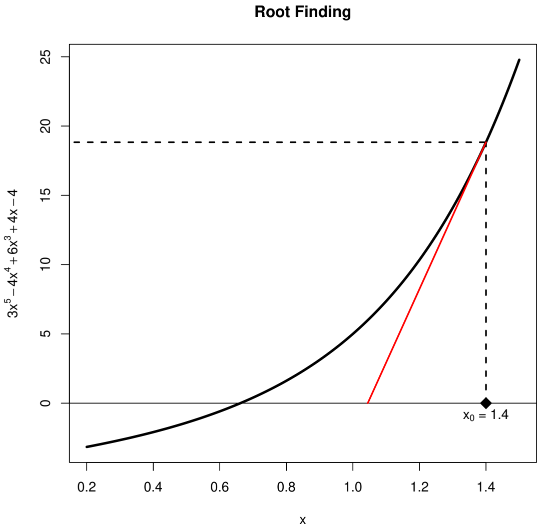
Root of a function



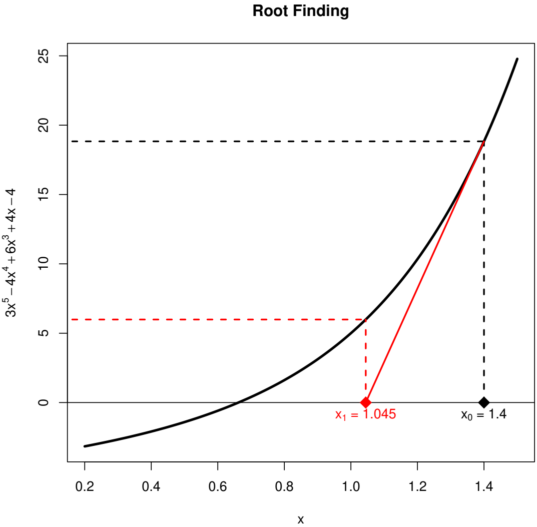
Initial Guess ($g(x_0) = 18.8$)



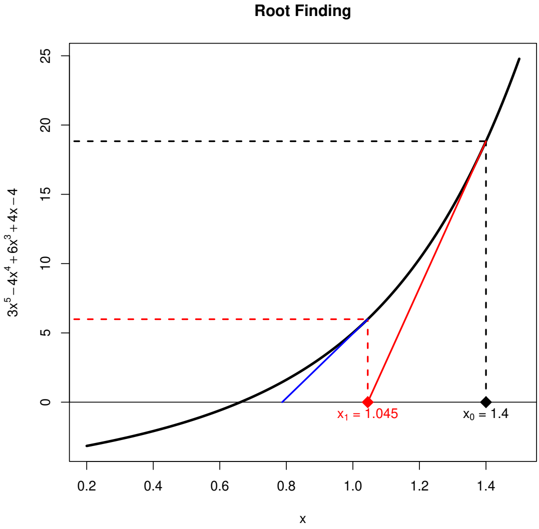
Tangent


Root Finding
$3x^5-4x^4+6x^3+4x-4$
x
0
5
10
15
20
25
0.2
0.4
0.6
0.8
1.0
1.2
1.4
x_0 = 1.4

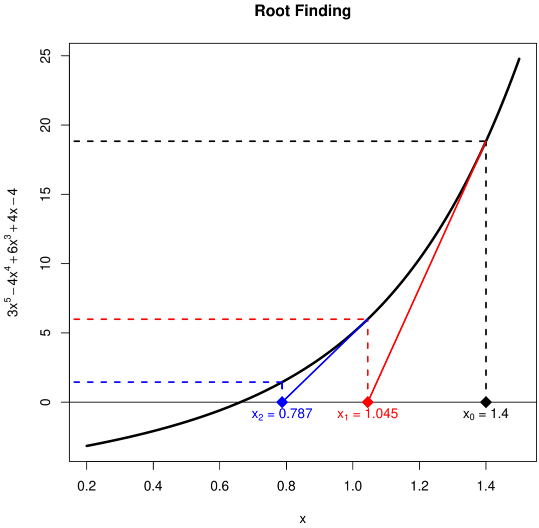
Now $g(x_1) = 6.0$


Root Finding
$3x^5 - 4x^4 + 6x^3 + 4x - 4$
0
5
10
15
20
25
0.2
0.4
0.6
0.8
1.0
1.2
1.4
x
x_1 = 1.045
x_0 = 1.4

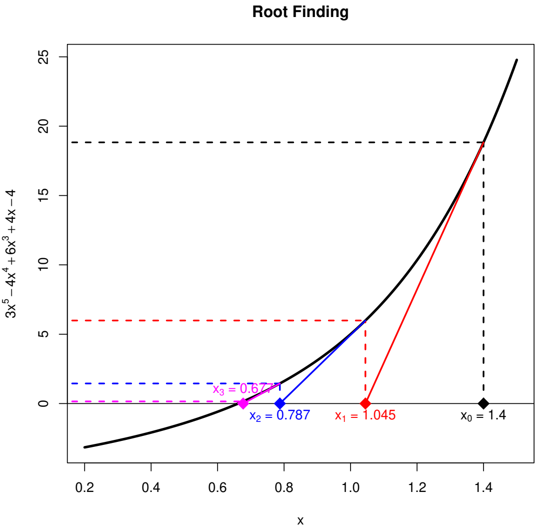
Do it again...


Root Finding
25
20
15
10
5
0
$3x^5-4x^4+6x^3+4x-4$
0.2
0.4
0.6
0.8
1.0
1.2
1.4
x
x_1 = 1.045
x_0 = 1.4

Now $g(x_2) = 1.4$


Root Finding
$3x^5-4x^4+6x^3+4x-4$
0
5
10
15
20
25
0.2
0.4
0.6
0.8
1.0
1.2
1.4
x
x_2 = 0.787
x_1 = 1.045
x_0 = 1.4

...and again: $g(x_3) = 0.2$



Finding the Tangent

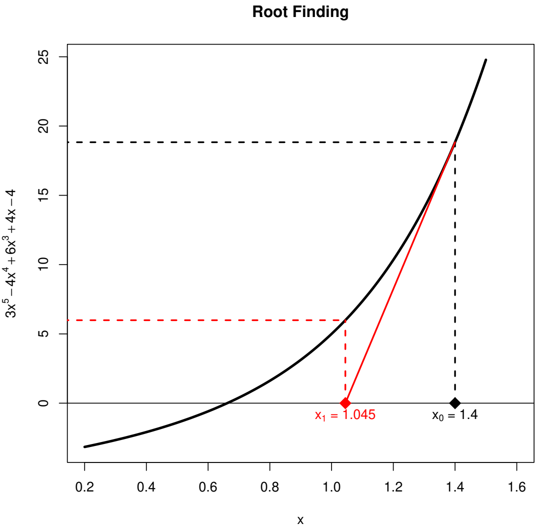
- To find the tangent evaluate the first derivative of $g(x)$.
- The function is

$$g(x) = 3x^5 - 4x^4 + 6x^3 + 4x - 4 \tag{1}$$

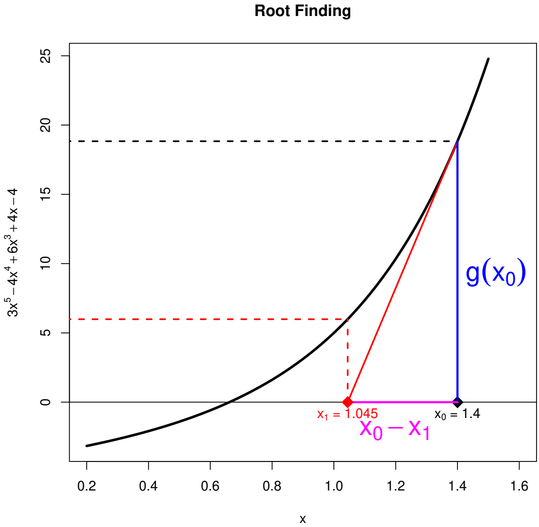
- The first derivative is

$$g'(x) = 15x^4 - 16x^3 + 18x^2 + 4 \tag{2}$$

Find the crossing point



Find the crossing point



Find the crossing point

From basic Geometry

$$g'(x_0) = \frac{g(x_0)}{x_0 - x_1} \tag{3}$$

Rearrange

$$x_0 - x_1 = \frac{g(x_0)}{g'(x_0)} \tag{4}$$

$$-x_1 = -x_0 + \frac{g(x_0)}{g'(x_0)} \tag{5}$$

$$x_1 = x_0 - \frac{g(x_0)}{g'(x_0)} \tag{6}$$

Stopping Rule

- With each step the algorithm should get closer to the root.
- However, it can run for a long time without reaching the **exact** root
- There must be a **stopping rule** otherwise the program could run forever.
- Let ϵ be an extremely small number e.g. 1×10^{-10} called the **tolerance level**
- If $|g(x^*)| < \epsilon$ then the solution is close enough and there is a root at x^*

Newton-Raphson Algorithm

1. Select initial value x_0 and set $n = 0$
2. Set $x_{n+1} = x_n - \frac{g(x_n)}{g'(x_n)}$
3. Evaluate $|g(x_{n+1})|$
    - If $|g(x_{n+1})| \leqslant \epsilon$ then stop.
    - Otherwise set $n = n + 1$ and go back to step 2.

Your task

Write R code to find the root of $g(x) = 3x^5 - 4x^4 + 6x^3 + 4x - 4$
Tips:

- Write functions for $g(x)$ and $g'(x)$ first.
- These can be inputs into a function that carries out the Newton Raphson method. Code should be flexible.
- Use loops!

Another Problem

- Now use your Newton-Raphson code to find the root of $g(x) = \sqrt{|x|}$
- The derivative has two parts

$$g'(x) = \begin{cases} 1/\sqrt{x} & \text{if } x > 0 \\ -1/\sqrt{-x} & \text{if } x < 0 \end{cases} \tag{7}$$

- Use 0.25 as the starting value

Learn from mistakes

- Newton-Raphson does not always converge
- Be careful using *while*. Avoid infinite loops.
- Don't always assume the answer given by code is correct. Check carefully!
- Print warning messages in code

Next Example

Next example:

$$g(x) = xe^{-x^2} - 0.4(e^x + 1)^{-1} + 0.2 \tag{8}$$

Try two different starting values

- Starting value $x_0 = 0.5$
- Starting value $x_0 = 0.6$

Next Example

Next example:

$$g(x) = x^3 - 2x^2 - 11x + 12 \tag{9}$$

Try two different starting values

- Starting value $x_0 = 2.35287527$
- Starting value $x_0 = 2.35284172$

Next Example

Next example:

$$g(x) = 2x^3 + 3x^2 + 5 \tag{10}$$

Try two different starting values

- Starting value $x_0 = 0.5$
- Starting value $x_0 = 0$

Learn from mistakes

- For some functions, using some certain starting values leads to a series that **converges**, while other starting values lead to a series that **diverges**
- For other functions different starting values converge to different roots.
- Be careful when choosing the initial value.
- Newton-Raphson doesn't work if the first derivative is zero.
- When can this happen?

Rough Proof of Quadratic Convergence

- Can we prove anything about the rate of convergence for the Newton Raphson Method?
- To do so requires the **Taylor Series**
- Let $f(x)$ have a root at α. The Taylor approximation states that

$$f(\alpha) \approx f(x_n) + f'(x_n)(\alpha - x_n) + \frac{1}{2}f''(x_n)(\alpha - x_n)^2 \tag{11}$$

- The quality of the approximation depends on the function and how close x_n is to α

Rough Proof of Convergence

- Since α is a root, $f(\alpha) = 0$ This implies

$$0 \approx f(x_n) + f'(x_n)(\alpha - x_n) + \frac{1}{2} f''(x_n)(\alpha - x_n)^2 \tag{12}$$

- Dividing by $f'(x_n)$ and rearranging gives:

$$\frac{f(x_n)}{f'(x_n)} + (\alpha - x_n) \approx \frac{-f''(x_n)}{2f'(x_n)}(\alpha - x_n)^2 \tag{13}$$

- More rearranging

$$\alpha - \left(x_n - \frac{f(x_n)}{f'(x_n)} \right) \approx \frac{-f''(x_n)}{2f'(x_n)} (\alpha - x_n)^2 \tag{14}$$

- The term in brackets on the left hand side is the formula used to update x in the Newton Raphson method

$$(\alpha - x_{n+1}) \approx \frac{-f''(x_n)}{2f'(x_n)} (\alpha - x_n)^2 \tag{15}$$

- This can be rewritten in terms of errors $e_{n+1} = \alpha - x_{n+1}$ and $e_n = \alpha - x_n$

$$e_{n+1} \approx \frac{-f''(x_n)}{2f'(x_n)} e_n^2 \tag{16}$$

Conclusion

- Why did we spend so much time on finding roots of an equation?
- Isn't this topic meant to be about optimization?
- Can we change this algorithm slightly so that it works for optimization?

Finding a maximum/minimum

$$\max f(x) \Longleftrightarrow f'(x) = 0$$

- Suppose we want to find an minimum or maximum of a function $f(x)$
- First order condition: Find the derivative $f'(x)$ and find x^* such that $f'(x^*) = 0$
- This is the same as finding a root of the first derivative. We can use the Newton Raphson algorithm on the first derivative.

Newton's algorithm for finding local minima/maxima

$f(x)$ max

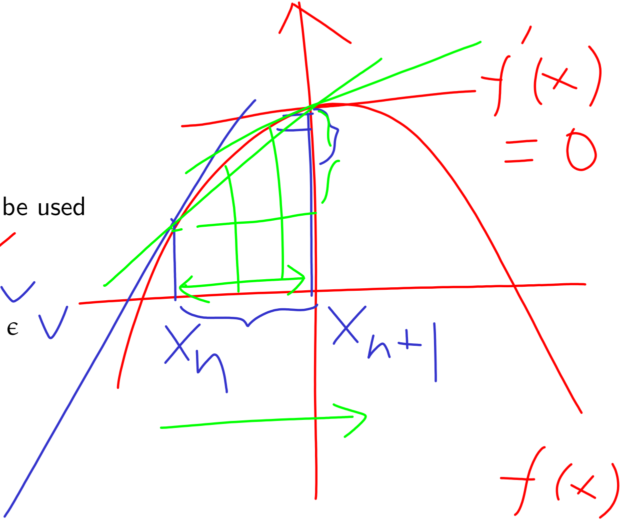
$g(x)$

1. Select initial value x_0 and set $n = 0$
2. Set $x_{n+1} = x_n - \frac{f'(x_n)}{f''(x_n)}$ $g'(x)$
3. Evaluate $|f'(x_{n+1})|$
   - If $|f'(x_{n+1})| < \epsilon$ then stop.
   - Otherwise set $n = n + 1$ and go back to step 2.

Different Stopping Rules

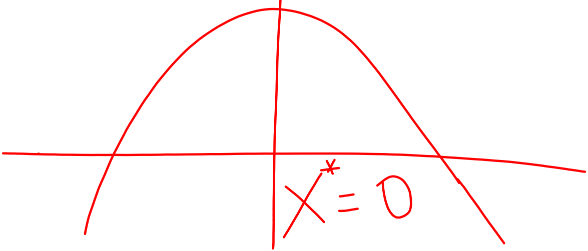
Three stopping rules can be used

- $|f'(x_n)| \leqslant \epsilon$ ✓
- $|x_n - x_{n-1}| \leqslant \epsilon$ ✓
- $|f(x_n) - f(x_{n-1})| \leqslant \epsilon$ ✓

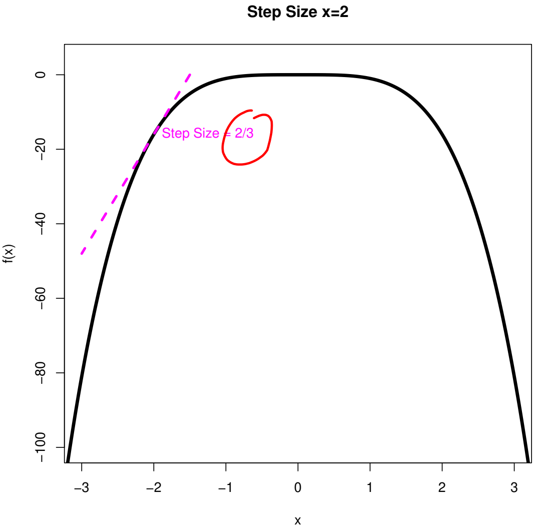


Intuition

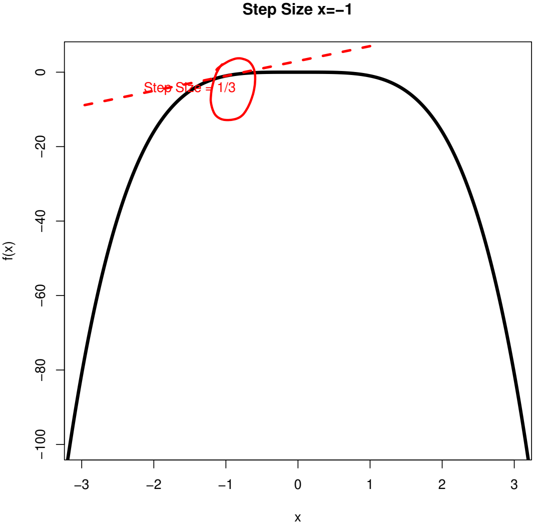
- Focus the **step size** $-\frac{f'(x)}{f''(x)}$.
- The **signs** of the derivatives control the **direction** of the next step.
- The **size** of the derivatives control the **size** of the next step.
- Consider the concave function $f(x) = -x^4$ which has $f'(x) = -4x^3$ and $f''(x) = -12x^2$. There is a maximum at $x^* = 0$



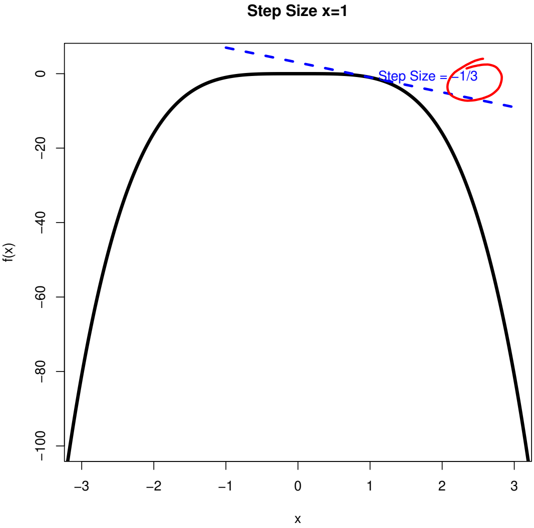
Role of first derivative



Role of first derivative



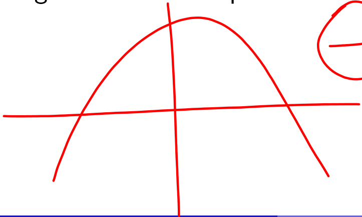
Role of first derivative



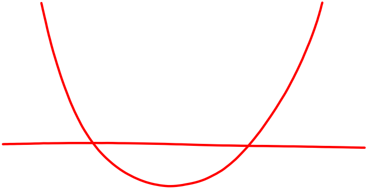
Role of first derivative

$-f(x)$

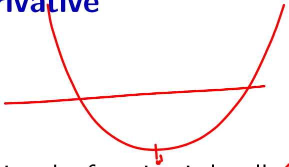
- If $f''(x)$ is negative the function is locally **concave**, and the search is for a local **maximum**
- To the left of this maximum $f'(x) > 0$
- Therefore $-\frac{f'(x)}{f''(x)} > 0$.
- The next step is to the right.
- The reverse holds if $f'(x) < 0$
- Large absolute values of $f'(x)$ imply a steep slope. A big step is needed to get close to the optimum. The reverse hold for small absolute value of $f'(x)$.



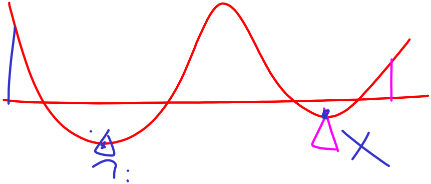
$-$



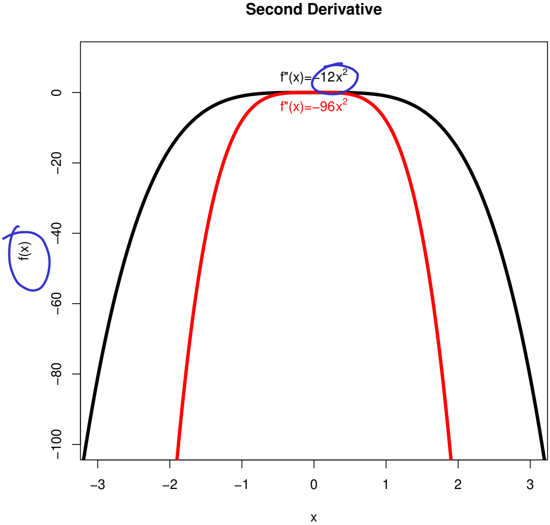
Role of first derivative



- If $f''(x)$ is positive the function is locally **convex**, and the search is for a local **minimum**
- To the left of this maximum $f'(x) < 0$
- Therefore $-\frac{f'(x)}{f''(x)} > 0$.
- The next step is to the right.
- The reverse holds if $f'(x) > 0$
- Large absolute values of $f'(x)$ imply a steep slope. A big step is needed to get close to the optimum. The reverse hold for small absolute value of $f'(x)$.



Role of second derivative



Role of second derivative

- Together with the sign of the first derivative, the sign of the second derivative controls the direction of the next step.
- A larger second derivative (in absolute value) implies a more curvature
- In this case smaller steps are need to stop the algorithm from overshooting.
- The opposite holds for a small second derivative.

Functions with more than one input

$$f(\underbrace{x_1 \quad x_2 \quad \cdots \quad x_p}_{\boldsymbol{X}}) = f(\boldsymbol{X})$$

- Most interesting optimization problems involve **multiple** inputs.
  - In determining the most risk efficient portfolio the return is a function of many weights (one for each asset).
  - In least squares estimation for a linear regression model, the sum of squares is a function of many coefficients (one for each regressor).
- How do we optimize for functions $f(\boldsymbol{x})$ where $\boldsymbol{x}$ is a vector?

Derviatives

- Newton's algorithm has a simple update rule based on first and second derivatives.
- What do these derivatives look like when the function is $y = f(\boldsymbol{x})$ where y is a scalar and $\boldsymbol{x}$ is a $d \times 1$ vector?

First derivative

$$x = \begin{bmatrix} x_1 \\ \vdots \\ x_d \end{bmatrix} \qquad y = f(x)$$

Simply take the **partial derivatives** and put them in a vector

$$\frac{\partial y}{\partial \mathbf{x}} = \begin{pmatrix} \frac{\partial y}{\partial x_1} \\ \frac{\partial y}{\partial x_2} \\ \vdots \\ \frac{\partial y}{\partial x_d} \end{pmatrix} \begin{matrix} x_1 \\ \\ \\ x_d \end{matrix} \tag{17}$$

This is called the **gradient** vector.

$d \times 1$

An example

$$x = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

The function

$$y = x_1^2 - x_1 x_2 + x_2^2 + e^{x_2} \tag{18}$$

Has gradient vector

$$\frac{\partial y}{\partial \mathbf{x}} = \begin{pmatrix} 2x_1 - x_2 \\ -x_1 + 2x_2 + e^{x_2} \end{pmatrix}_{2 \times 1} \tag{19}$$

Second derivative

Simply take the second order **partial derivatives**. This will give a matrix

$$\frac{\partial\left(\frac{\partial y}{\partial x}\right)_{d\times 1}}{x'}$$

$d\times d$

$$\frac{\partial y}{\partial \mathbf{x}\partial \mathbf{x}'} = \begin{pmatrix} \frac{\partial^2 y}{\partial x_1^2} & \frac{\partial^2 y}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 y}{\partial x_1 \partial x_d} \\ \frac{\partial^2 y}{\partial x_2 \partial x_1} & \frac{\partial^2 y}{\partial x_2^2} & \cdots & \frac{\partial^2 y}{\partial x_2 \partial x_d} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 y}{\partial x_d \partial x_1} & \frac{\partial^2 y}{\partial x_d \partial x_2} & \cdots & \frac{\partial^2 y}{\partial x_d^2} \end{pmatrix} \tag{20}$$

$d\times d$

∂

This is called the **Hessian** matrix.

An example

The function

$$y = x_1^2 - x_1 x_2 + x_2^2 + e^{x_2} \tag{21}$$

Has Hessian matrix

$$\frac{\partial y}{\partial \mathbf{x} \partial \mathbf{x}'} = \begin{pmatrix} 2 & -1 \\ -1 & 2 + e^{x_2} \end{pmatrix} \tag{22}$$

Preliminaries for matrix derivatives I

1. The derivative of a vector $\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{bmatrix}$, by a scalar x is written (in numerator layout notation) as

$$\frac{\partial \mathbf{y}}{\partial x} = \begin{bmatrix} \frac{\partial y_1}{\partial x} \\ \frac{\partial y_2}{\partial x} \\ \vdots \\ \frac{\partial y_m}{\partial x} \end{bmatrix}.$$

In vector calculus the derivative of a vector y with respect to a scalar x is known as the tangent vector of the vector y, $\frac{\partial \mathbf{y}}{\partial x}$

Preliminaries for matrix derivatives II

2. **The derivative of a scalar y by a vector $\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$**, is written (in numerator layout notation) as

$$\frac{\partial y}{\partial \mathbf{x}} = \begin{bmatrix} \frac{\partial y}{\partial x_1} & \frac{\partial y}{\partial x_2} & \cdots & \frac{\partial y}{\partial x_n} \end{bmatrix}.$$

3. **The second order derivatives of a scalar y by a vector $\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$** is written (in numerator layout notation) as

Preliminaries for matrix derivatives III

$$
\begin{aligned}
\frac{\partial^2 y}{\partial \mathbf{x} \partial \mathbf{x}'} = \frac{\partial}{\partial \mathbf{x}'}\left[\frac{\partial y}{\partial \mathbf{x}}\right] &= \frac{\partial}{\partial \mathbf{x}'}\begin{bmatrix} \frac{\partial y}{\partial x_1} & \frac{\partial y}{\partial x_2} & \cdots & \frac{\partial y}{\partial x_n} \end{bmatrix} \\
&= \begin{bmatrix}
\frac{\partial^2 y}{\partial x_1^2} & \frac{\partial^2 y}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 y}{\partial x_1 \partial x_n} \\
\frac{\partial^2 y}{\partial x_2 \partial x_1} & \frac{\partial^2 y}{\partial x_2^2} & \cdots & \frac{\partial^2 y}{\partial x_2 \partial x_n} \\
\vdots & \vdots & \ddots & \vdots \\
\frac{\partial^2 y}{\partial x_m \partial x_1} & \frac{\partial^2 y}{\partial x_m \partial x_2} & \cdots & \frac{\partial^2 y}{\partial x_m \partial x_m}
\end{bmatrix}.
\end{aligned}
$$

4. The derivative of a vector function (a vector whose components are functions) $\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{bmatrix}$, with respect to an input vector, $\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$, is written (in numerator layout notation) as

Preliminaries for matrix derivatives IV

$$\frac{\partial \mathbf{y}}{\partial \mathbf{x}} = \begin{bmatrix} \frac{\partial y_1}{\partial x_1} & \frac{\partial y_1}{\partial x_2} & \cdots & \frac{\partial y_1}{\partial x_n} \\ \frac{\partial y_2}{\partial x_1} & \frac{\partial y_2}{\partial x_2} & \cdots & \frac{\partial y_2}{\partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial y_m}{\partial x_1} & \frac{\partial y_m}{\partial x_2} & \cdots & \frac{\partial y_m}{\partial x_n} \end{bmatrix}.$$

5. The derivative of a matrix function Y by a scalar x is known as the tangent matrix and is given (in numerator layout notation) by

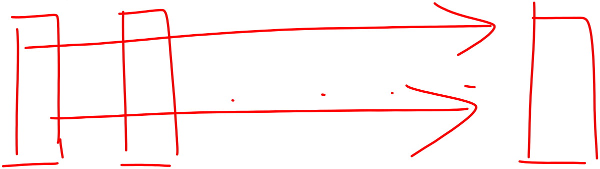
$$\frac{\partial \mathbf{Y}}{\partial x} = \begin{bmatrix} \frac{\partial y_{11}}{\partial x} & \frac{\partial y_{12}}{\partial x} & \cdots & \frac{\partial y_{1n}}{\partial x} \\ \frac{\partial y_{21}}{\partial x} & \frac{\partial y_{22}}{\partial x} & \cdots & \frac{\partial y_{2n}}{\partial x} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial y_{m1}}{\partial x} & \frac{\partial y_{m2}}{\partial x} & \cdots & \frac{\partial y_{mn}}{\partial x} \end{bmatrix}.$$

Preliminaries for matrix derivatives V

6. The derivative of a scalar y function of a matrix X of independent variables, with respect to the matrix X, is given (in numerator layout notation) by

$$\frac{\partial y}{\partial \mathbf{X}} = \begin{bmatrix} \frac{\partial y}{\partial x_{11}} & \frac{\partial y}{\partial x_{21}} & \cdots & \frac{\partial y}{\partial x_{p1}} \\ \frac{\partial y}{\partial x_{12}} & \frac{\partial y}{\partial x_{22}} & \cdots & \frac{\partial y}{\partial x_{p2}} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial y}{\partial x_{1q}} & \frac{\partial y}{\partial x_{2q}} & \cdots & \frac{\partial y}{\partial x_{pq}} \end{bmatrix}.$$

Newton's algorithm for multidimensional optimization



We can now generalise the update step in Newton's method:

$$\underset{d\times 1}{x_{n+1}} = x_n - \left(\underset{d\times d}{\frac{\partial^2 f(\mathbf{x})}{\partial \mathbf{x} \partial \mathbf{x}'}}\right)^{-1} \underset{d\times 1}{\frac{\partial f(\mathbf{x})}{\partial \mathbf{x}}} \qquad (23)$$

$c' \times 1$

Now write code to minimise $y = x_1^2 - x_1 x_2 + x_2^2 + e^{x_2}$

The linear regression model, a revisit

lm(y~x)

$$\beta = \begin{bmatrix} \beta_0 \\ \vdots \\ \beta_p \end{bmatrix}$$

- Consider the linear regression model with multiple covariates,

$$y_i = \beta_0 + \beta_1 x_1 + \ldots + \beta_p x_p + \epsilon_i$$

where $\epsilon_i \sim N(0, \sigma^2)$

- What is the gradient and Hessian matrix for the log likelihood ($\mathcal{L}$) with respect to the parameter vector $\boldsymbol{\beta} = (\beta_0, \ldots, \beta_p)$?

$$\nabla \log \mathcal{L}(\beta) \quad c$$

$$\frac{\partial \log \mathcal{L}}{\partial \boldsymbol{\beta}} = ? \quad \begin{bmatrix} \\ \\ \end{bmatrix}_{(p+1)\times 1}$$

$$\frac{\partial^2 \log \mathcal{L}}{\partial \boldsymbol{\beta} \partial \boldsymbol{\beta}'} = ? \quad \begin{bmatrix} & & \\ & & \\ & & \end{bmatrix}_{(p+1)^2}$$

Maximum likelihood Estimate for linear models

①

$$V = \begin{bmatrix}\beta_0\\ \vdots\\ \beta_p\\ \hline \sigma^2\end{bmatrix} \leftarrow 1/0$$

- Assume you want to make a regression model

$$y_i = \beta_0 + \beta_1 x_i + \epsilon_i$$

  where $\epsilon_i \sim N(0, \sigma^2)$

$$\frac{\partial \log L}{\partial V}$$

- What is the (log) likelihood function?
- What are the unknown parameters?
- How do we estimate the parameters? Let's consider three situations
  - When $\beta_0 = 1$ and $\sigma^2 = 1$ known.
  - When $\sigma^2 = 1$ known.
  - Neither β nor σ is known.

②

① σ

② σ^2, if <0

$\sigma^2 = f$

- Write down the likelihood function with respect to the unknown parameters.
- Write down the gradient for the likelihood function.
- Write down the Hessian for the likelihood function.
- Use Newton's method to obtain the best parameter estimate.

$$\boxed{\sigma^2 > 0}$$

(*)

③ $\log(\sigma^2)$

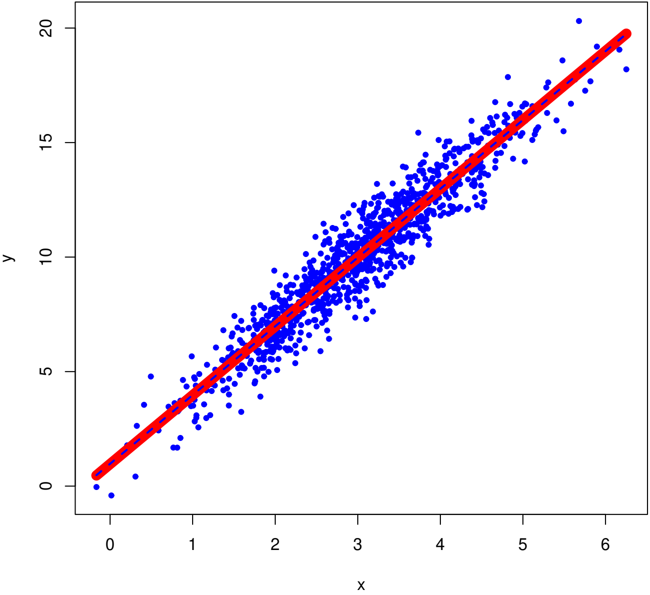
$= 0$

Optimizing the likelihood function by using `optim()`

```
## Generate some data
beta0 <- 1
beta1 <- 3
sigma <- 1
n <- 1000
x <- rnorm(n, 3, 1)
y <- beta0 +x*beta1 + rnorm(n, mean = 0, sd = sigma)
plot(x, y, col = "blue", pch = 20)

## The optimization
optimOut <- optim(c(0, -1, 0.1), logNormLikelihood,
                  control = list(fnscale = -1),
                  x = x, y = y)
beta0Hat <- optimOut$par[1]
beta1Hat <- optimOut$par[2]
sigmaHat <- optimOut$par[3]
yHat <- beta0Hat + beta1Hat*x

plot(x, y, pch = 20, col = "blue")
points(sort(x), yHat[order(x)], type = "l", col = "red", lwd = 2)
```

Comparison with OLS

```
myLM <- lm(y~x)
myLMCoef <- myLM$coefficients
yHatOLS <- myLMCoef[1] + myLMCoef[2]*x

plot(x, y, pch = 20, col = "blue")
points(sort(x), yHat[order(x)], type = "l", col = "red", lwd = 10)
points(sort(x), yHatOLS[order(x)], type = "l",
       col = "blue", lty="dashed", lwd = 2, pch = 20)
```



0
5
10
15
20
y
0
1
2
3
4
5
6
x

Vector Newton-Raphson Algorithm: The logit model

↬ Estimate logit model with ungrouped (individual) data

- **The idea**: using maximum likelihood method with binomial distribution.
- One owns a house ($Y = 1$) or do not own a house ($Y = 0$) can be represented with **Bernoulli distribution**

$$Pr(y; p) = p^y (1-p)^{1-y} \quad \text{for } y \in \{0, 1\}.$$

- The log likelihood function is as follows

$$l(\beta) = \sum_{n=1}^{N} \{y_i \log P_i + (1-y_i)\log(1-P_i)\}$$

where

$$P_i = \frac{1}{1+\exp(-(\beta_1+\beta_2 X_{2i}+...+\beta_p X_{pi}))}$$

- Note that the sum of n Bernoulli samples will be **binomial** distributed.
- To obtain $\hat{\beta}$, use Newton-Raphson algorithm

$$\beta^{new} = \beta^{old} - \left(\frac{\partial^2 l(\beta)}{\partial\beta\partial\beta'}\right)^{-1} \frac{\partial l(\beta)}{\partial\beta}|_{\beta=\beta^{old}}$$

A harder example

- Use Newton's method to find the maximum likelihood estimate for the coefficients in a logistic regression. The steps are:
  - Write down likelihood function
  - Find the gradient and Hessian matrix
  - Code these up in R
  - Simulate some data from a logistic regression model.
  - Test your code.

Quasi-Newton Methods

- One of the most difficult parts of the Newton method is working out the derivatives especially the Hessian.
- However methods can be used to approximate the Hessian and also the gradient.
- These are known as Quasi-Newton Methods
- In general they will converge slower than pure Newton methods.

The BFGS algorithm

- The BFGS algorithm was introduced over several papers by Broyden, Fletcher, Goldfarb and Shanno.
- It is the most popular Quasi-Newton algorithm.
- The R function 'optim' also has a variation called L-BFGS-B.
- The L-BFGS-B uses less computer memory than BFGS and allows for box constraints

Box Constraints

- Box constraints have the form

$$l_i \leqslant x_i \leqslant u_i \quad \forall i \tag{24}$$

- In statistics this can be very useful. Often parameters are constrained
  - Variance must be greater than 0
  - For a stationary AR(1), coefficient must be between -1 and 1
  - Weights in a portfolio must be between 0 and 1 if short selling is prohibited.

Optim function in R

- The optim function in R requires at least two inputs
  - Initial values
  - The function that needs to be optimized
- By default it **minimises** a function.
- A function that computes the gradient vector can also be provided.
- The optimization method can be set (choices include BFGS, L-BFGS-B and Nelder-Mead)
- Lower and upper bounds can be set through the arguments *lower* and *upper* if the L-BFGS-B method is used.

Optim function in R

- Further arguments can be passed in an argument called *control*.
- Some things that can be included in this list are
  - Maximum number of iterations (*maxit*)
  - Information about the algorithm (*trace*)
  - How often to display information about the algorithm (*REPORT*)

Optim function in R

- The result of *optim* can be saved in an object that is a list containing
  - The value of the function at the turning point (*value*)
  - The optimal parameters (*par*)
  - Useful information about whether the algorithm has converged (*convergence*)
- For all algorithms *convergence*=0 if the algorithm has converged (slightly confusing)

Homework

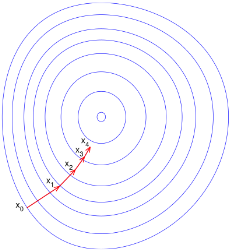
Use *optim* to carry out maximum likelihood for the

- Logistic regression model

Gradient Descent I

- Gradient descent is a **first-order** iterative optimization algorithm for finding the minimum of a function.
- To find a **local minimum** of a function using gradient descent, one takes steps proportional to the negative of the gradient (or approximate gradient) of the function at the current point.
- If, instead, one takes steps proportional to the positive of the gradient, one approaches a local maximum of that function; the procedure is then known as gradient ascent.
- Gradient descent is based on the observation that if the multi-variable function $F(\mathbf{x})$ is defined and differentiable in a neighborhood of a point **a** , then $F(\mathbf{x})$decreases **fastest** if one goes from **a** in the direction of the negative gradient of F at **a** ,$-\nabla F(\mathbf{a})$.
- It follows that, if $\mathbf{a}_{n+1} = \mathbf{a}_n - \gamma \nabla F(\mathbf{a}_n)$ for $\gamma \in \mathbb{R}_+$ small enough, then $F(\mathbf{a_n}) \geqslant F(\mathbf{a_{n+1}})$.

Gradient Descent II



- Gradient descent is relatively slow close to the minimum.
- Conversely, using a fixed small γ can yield poor convergence.

Stochastic Gradient Descent I

- Stochastic gradient descent (often abbreviated SGD) is an iterative method for optimizing an objective function with suitable smoothness properties (e.g. differentiable or subdifferentiable).
- It is called stochastic because the method uses randomly selected (or shuffled) samples to evaluate the gradients, hence SGD can be regarded as a stochastic approximation of gradient descent optimization.
- When used to minimize the function $F(x)$, a standard (or "**batch**") gradient descent method would perform the following iterations :

$$w := w - \eta \nabla Q(w) = w - \eta \sum_{i=1}^{n} \nabla Q_i(w)/n$$

  where η is a step size (sometimes called the **learning rate** in machine learning).

- In many cases, the summand functions have a simple form that enables inexpensive evaluations of the sum-function and the sum gradient.

Stochastic Gradient Descent II

- Stochastic gradient descent is a popular algorithm for training a wide range of models in machine learning.
- **Averaged stochastic gradient descent**, is ordinary stochastic gradient descent that records an average of its parameter vector over time. That is, the update is the same as for ordinary stochastic gradient descent, but the algorithm also keeps track of

  $$\bar{w} = \frac{1}{t}\sum_{i=0}^{t-1} w_i.$$

  When optimization is done, this averaged parameter vector takes the place of w.

Stochastic Gradient Descent III

- **Further Readings:**
  - **AdaGrad**: Duchi, John; Hazan, Elad; Singer, Yoram (2011). "Adaptive subgradient methods for online learning and stochastic optimization" (PDF). JMLR. 12: 2121–2159.
  - **Adam AdaMax**: Diederik P. Kingma, Jimmy Ba. "Adam: A Method for Stochastic Optimization", ICLR 2015. arXiv:1412.6980

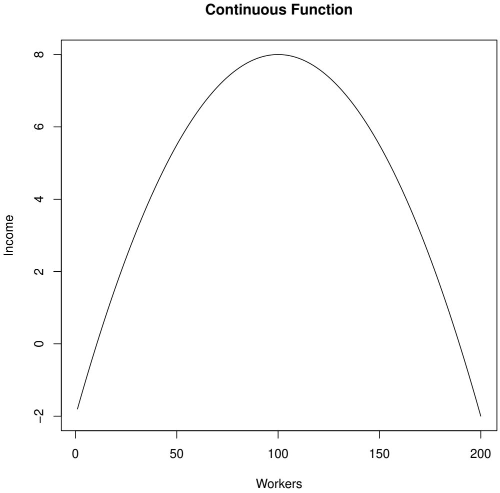
Discontinuous Functions

- The *Newton Method* requires first and second derivatives.
- If derivatives are not available the they can be approximated by *Quasi-Newton methods*
- What if the derivatives do not exist?
- This may occur if there are **discontinuities** in the function.

Business Example

- Suppose the aim is to optimize income of the business by selecting the number of workers.
- In the beginning adding more workers leads to more income for the business.
- If too many workers are employed, they may be less efficient and the income of the company goes down

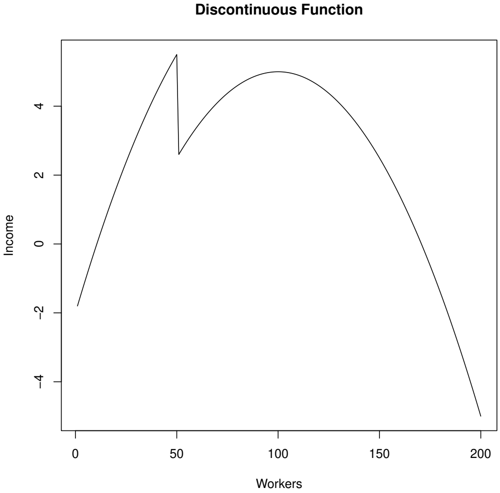
Business Example



Business Example

- Now suppose that there is a tax that the company must pay.
- Companies with less than 50 workers do not pay the tax
- Companies with more than 50 workers do pay the tax
- How does this change the problem?

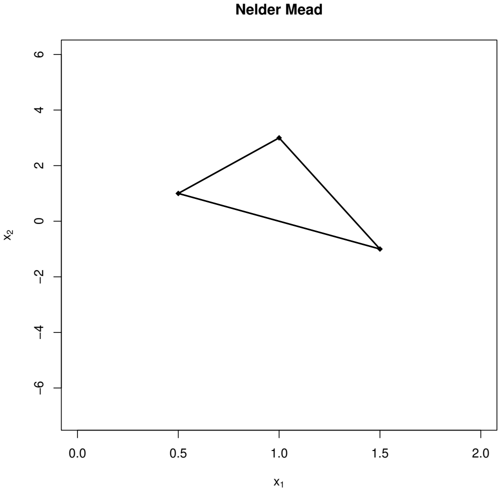
Business Example



The Nelder Mead Algorithm

- The Nelder Mead algorithm is robust even when the functions are discontinuous.
- The idea is based on evaluating the function at the vertices of an n-*dimensional simplex* where n is the number of input variables into the function.
- For two dimensional problems the n-*dimensional simplex* is simply a triangle, and each corner is one vertex
- In general there are $n + 1$ vertices.

A 2-dimensional simplex



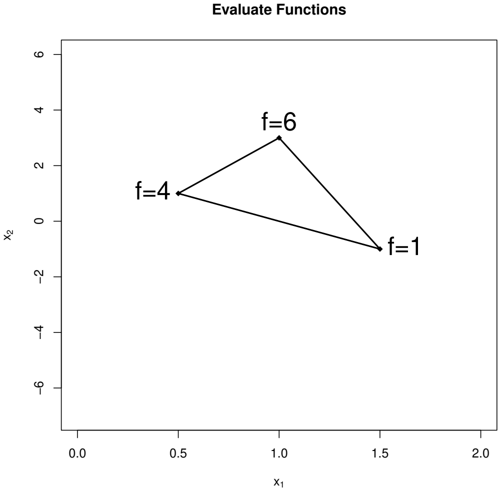
Step 1: Evaluate Function

- For each vertex $\mathbf{x}_j$ evaluate the function $f(\mathbf{x}_j)$
- Order the vertices so that

$$f(\mathbf{x}_1) \leqslant f(\mathbf{x}_2) \leqslant \ldots \leqslant f(\mathbf{x}_{n+1}) \tag{25}$$

- Suppose that the aim is to **minimize** the function, then $f(\mathbf{x}_{n+1})$ is the worst point.
- The aim is to replace $f(\mathbf{x}_{n+1})$ with a better point

A 2-dimensional simplex



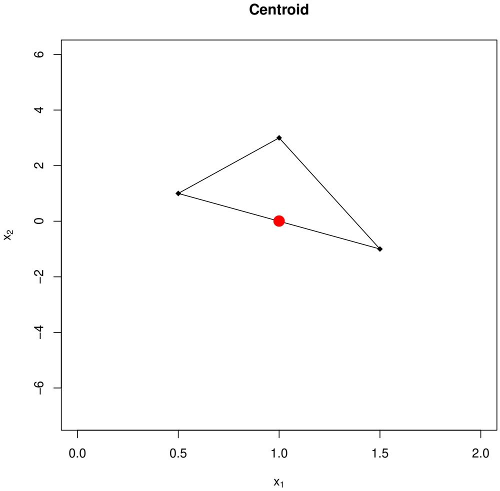
Step 2: Find Centroid

- After eliminating the worst point x_{n+1}, compute the **centroid** of the remaining n points

$$x_0 = \frac{1}{n}\sum_{j=1}^{n} x_j \tag{26}$$

- For the 2-dimensional example the centroid will be in the middle of a line.

Find Centroid



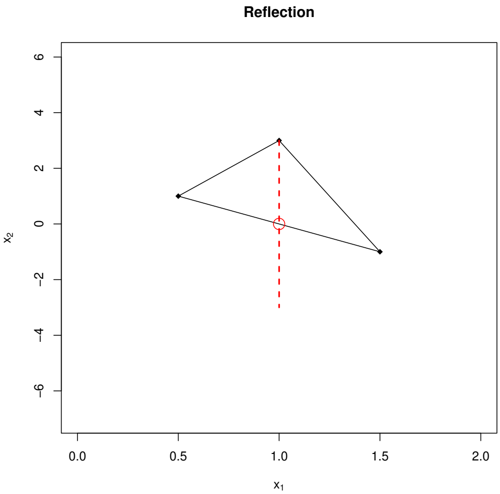
Step 3: Find reflected point

- Reflect the worst point around the centroid to get the **reflected point**.
- The formula is:

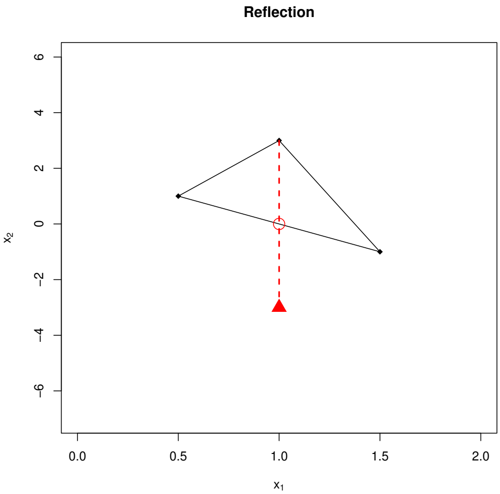
$$x_r = x_0 + \alpha(x_0 - x_{n+1}) \tag{27}$$

- A common choice is $\alpha = 1$.
- In this case the reflected point is the same distance from the centroid as the worst point.

Find Reflected point



Find Reflected point



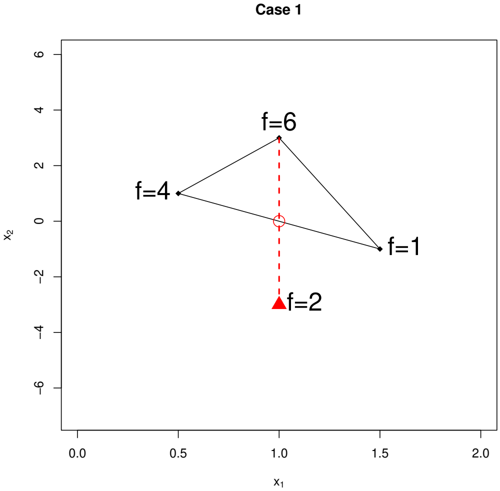
Three cases

1. $f(x_1) \leqslant f(x_r) < f(x_n)$
    - x_r is neither best nor worst point
2. $f(x_r) < f(x_1)$
    - x_r is the best point
3. $f(x_r) \geqslant f(x_n)$
    - x_r is the worst point

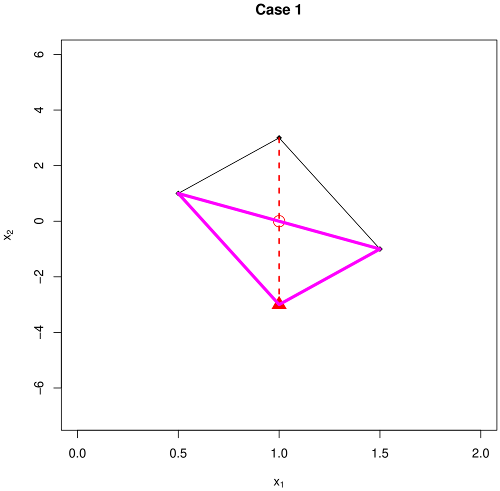
Case 1

In Case 1 a new simplex is formed with x_{n+1} replaced by the reflected point x_r. Then go back to step 1.

Case 1



Case 1



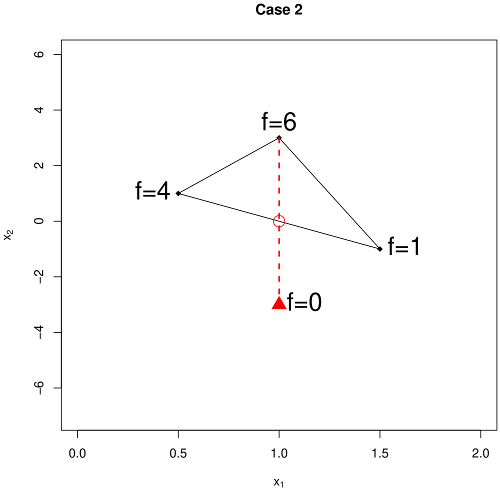
Case 2

In Case 2, $x_r < x_1$. A good direction has been found so we **expand** along that direction

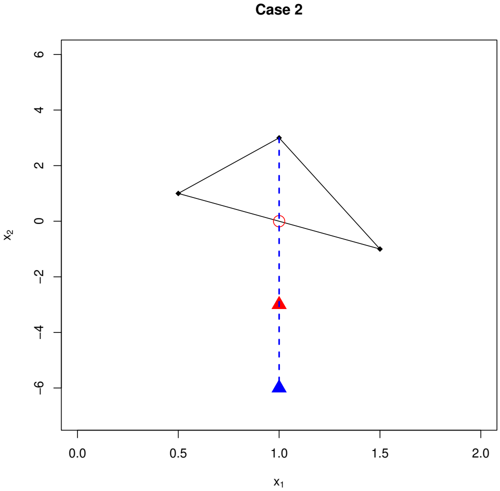
$$x_e = x_0 + \gamma(x_r - x_0) \tag{28}$$

A common choice is $\gamma = 2$

Case 2



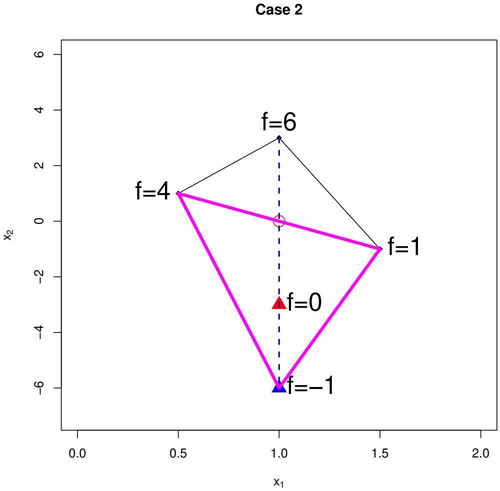
Case 2



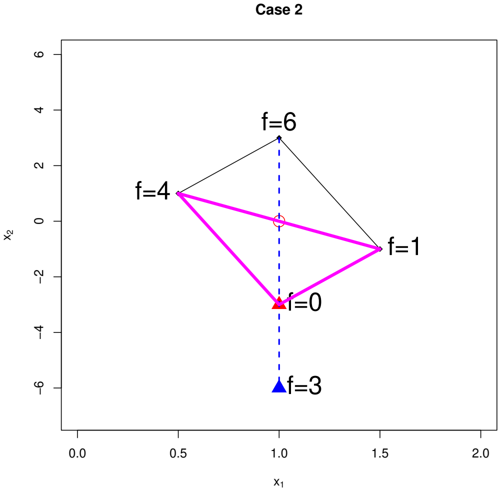
Choosing the expansion point

- Evaluate $f(\boldsymbol{x}_e)$.
- If $f(\boldsymbol{x}_e) < f(\boldsymbol{x}_r)$:
    - The expansion point is better than the reflection point. Form a new simplex with the expansion point
- If $f(\boldsymbol{x}_r) \leqslant f(\boldsymbol{x}_e)$:
    - The expansion point is not better than the reflection point. Form a new simplex with the reflection point.

Keep expansion point



Keep reflection point



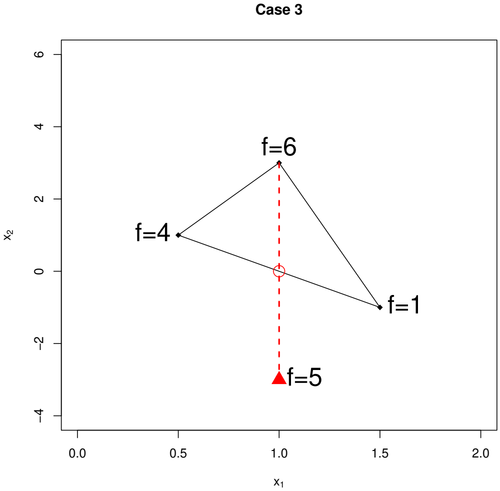
Case 3

Case 3 implies that there may be a valley between x_{n+1} and x_r so find the **contracted** point. A new simplex is formed with the contraction point if it is better than x_{n+1}

$$x_c = x_0 + \rho(x_{n+1} - x_0) \tag{29}$$

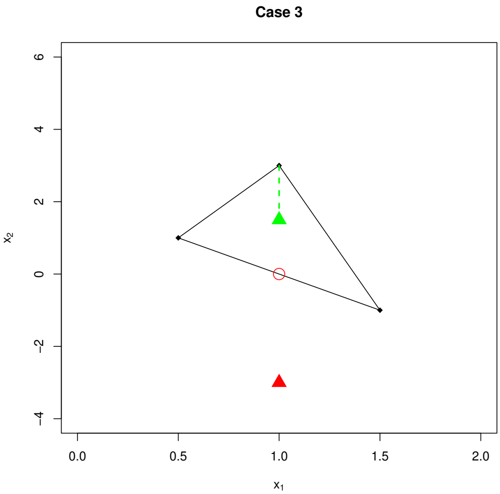
A common choice is $\rho = 0.5$

Case 3

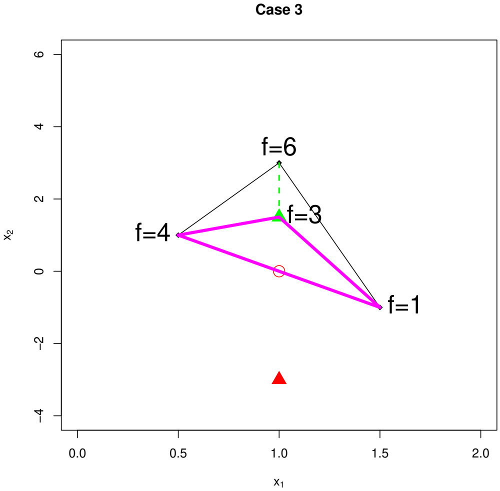


‘Valley’

Find Contraction point



New Simplex



Shrink

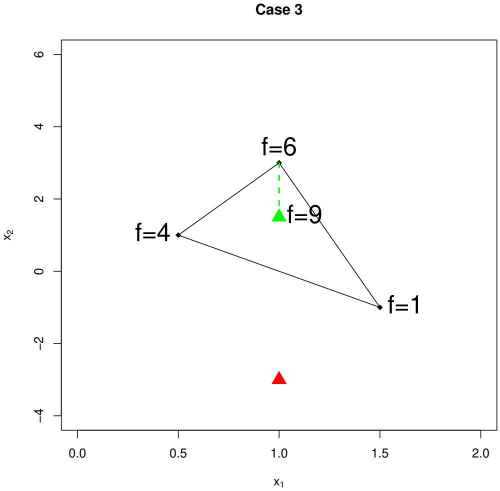
If $f(x_{n+1}) \leqslant f(x_c)$ then contracting away from the worst point does not lead to a better point. In this case the function is too irregular a smaller simplex should be used. Shrink the simplex

$$x_i = x_1 + \sigma(x_i - x_1) \tag{30}$$

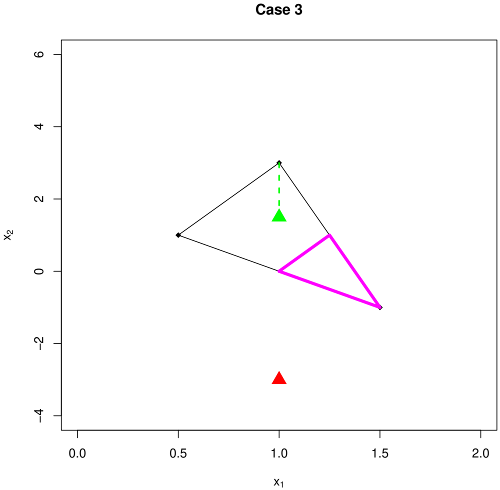
A popular choice is $\sigma = 0.5$

‘Egg Carton’

Contraction Point is worst



New Simplex



Summary

- Order points
- Find centroid
- Find reflected point
- Three cases:
  1. Case 1 $(f(\mathbf{x}_1) \leqslant f(\mathbf{x}_r) < f(\mathbf{x}_n))$: Keep $\mathbf{x}_r$
  2. Case 2 $(f(\mathbf{x}_r) < f(\mathbf{x}_1))$: Find $\mathbf{x}_e$.
     - If $f(\mathbf{x}_e) < f(\mathbf{x}_r)$ then keep $f(\mathbf{x}_e)$
     - Otherwise keep $f(\mathbf{x}_r)$
  3. Case 3 $(f(\mathbf{x}_r) \geqslant f(\mathbf{x}_n))$: Find $f(\mathbf{x}_c)$
     - If $f(\mathbf{x}_c) < f(\mathbf{x}_{n+1})$ then keep $f(\mathbf{x}_c)$
     - Otherwise Shrink

Your task

- Find the minimum of the function $f(\boldsymbol{x}) = x_1^2 + x_2^2$
- Use a triangle with vertices $(1, 1)$, $(1, 2)$, $(2, 2)$ as the starting simplex
- Don't worry about using a loop just yet. Try to get code that just does the first iteration.
- Don't worry about the stopping rule yet either

Use pseudo-code

Algorithm 1 Nelder Mead

```
Set initial simplex and evaluate function
Sort $f(x_1) \leqslant \ldots \leqslant f(x_n)$
Compute reflected point
if $f(x_1) \leqslant f(x_r) < f(x_n)$ then
    return $x_{n+1} \leftarrow x_r$
else if $f(x_r) < f(x_1)$ then
    Compute expanded point
    if $f(x_e) < f(x_r)$ then
        return $x_{n+1} \leftarrow x_e$
    else if $f(x_r) \leqslant f(x_e)$ then
        return $x_{n+1} \leftarrow x_r$
    end if
else if $f(x_n) \leqslant f(x_r)$ then
    Compute contracted point
end if
```

Lessons

- Break down a difficult problem into smaller problems.
- Use pseudo code in planning
- Use comments
- Use indents

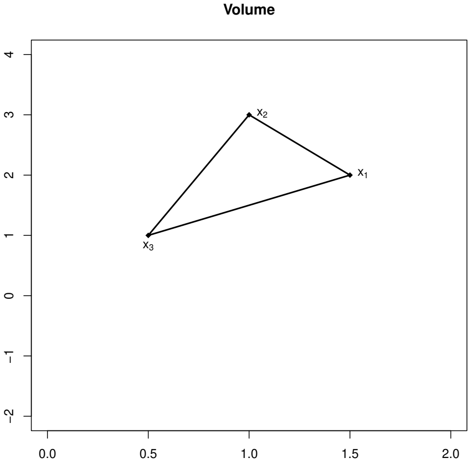
Stopping Rule for Nelder Mead

- As Nelder Mead gets close to (or reaches) the minimum, the simplex gets smaller and smaller.
- One way to know that Nelder Mead has converged is by looking at the volume of the simplex.
- To work out the volume requires some understanding between the relationship between matrix algebra and geometry.

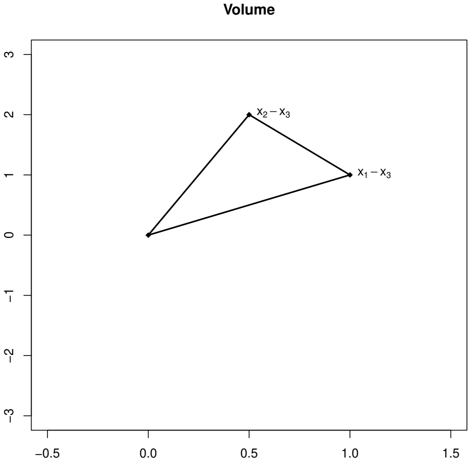
Stopping Rule for Nelder Mead

- Choose the vertex $\mathbf{x}_{n+1}$ (although choosing any other vertex will also work)
- Build the matrix $\tilde{X} = (\mathbf{x}_1 - \mathbf{x}_{n+1}, \mathbf{x}_2 - \mathbf{x}_{n+1}, \ldots, \mathbf{x}_n - \mathbf{x}_{n+1})$
- The volume of the simplex is $\frac{1}{2}|det(\tilde{X})|$

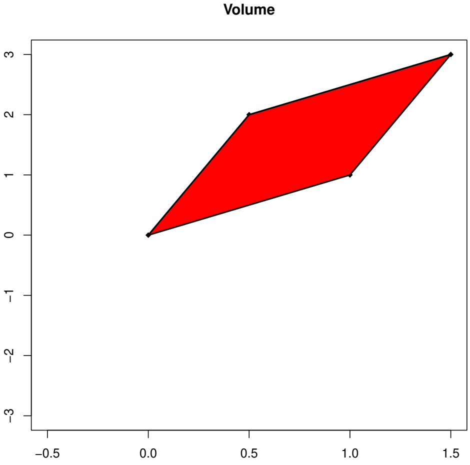
Why?



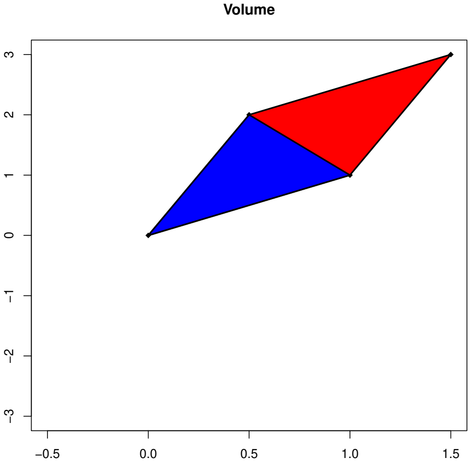
Translate



Determinant=Area of Trapezoid



Triangle=Half Trapezoid



Alternative formula

Some of you may have learnt the formula for the area of a triangle as:

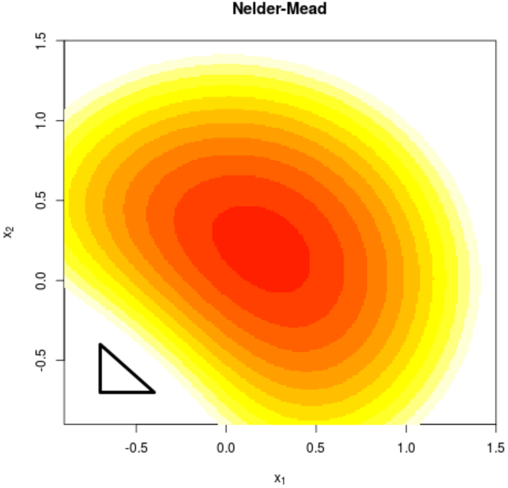
$$\frac{1}{2}\left|\det\begin{pmatrix} \boldsymbol{x}_1 & \boldsymbol{x}_2 & \boldsymbol{x}_3 \\ 1 & 1 & 1 \end{pmatrix}\right| \tag{31}$$

The two approaches are equivalent.

Questions

- In my code, where should I start the loop?
- Should it be a *for* loop or a *while* loop?
- What should the loop look like?

Visualizing Nelder Mead



Nelder Mead in ‘optim’

- Nelder Mead is the **default** algorithm in the R function *optim*
- It is generally slower than Newton and Quasi-Newton methods but is more stable for functions that are not smooth.
- Including the argument control=list(trace, REPORT=1) will print out details about each step of the algorithm.
- Slight different terminology is used for example ‘expansion’ is called ‘extension’

Box constraints in Nelder Mead

- It is not possible to impose box constraints in Nelder Mead.
- However it is possible to trick R. How?
- Suppose the problem is a minimization. We can use an *if* statement to force the function to be extremely large outside the box.
- This is not an option in BFGS since this induces a discontinuity in the function.

Some test functions

Use both Nelder Mead and L-BFGS-B to minimize the following

- Booth's Function:

$$f(\boldsymbol{x}) = (x_1 + 2x_2 - 7)^2 + (2x_1 + x_2 - 5)^2 \quad -10 \leqslant x_1, x_2 \leqslant 10$$

- Bukin Function N.6

$$f(\boldsymbol{x}) = 100\sqrt{\left|x_2 - \frac{x_1^2}{100}\right|} + \frac{|x_1 + 10|}{100} \qquad \begin{array}{c} -15 \leqslant x_1 \leqslant 5 \\ -3 \leqslant x_2 \leqslant 3 \end{array}$$

Summary

- This is the end of the optimization topic.
- You should now be familiar with
    - Newton's Method
    - Quasi Newton Method
    - Nelder Mead
- Hopefully you also improved your coding skills!

Summary

- Some important lessons:
  - If you can evaluate derivatives and Hessians then do so when implementing Newton and Quasi-Newton methods.
  - If there are discontinuities in the function then Nelder Mead may work better.
  - In any case the best strategy is to optimize using **more than one method** to check that results are robust.
  - Also pay special attention to **starting values**. A good strategy is to check that results are robust to a few different choices of starting values.