# Optimization in R

Computational Economics Practice
Winter Term 2015/16
ISR

# Outline

# Today's Lecture

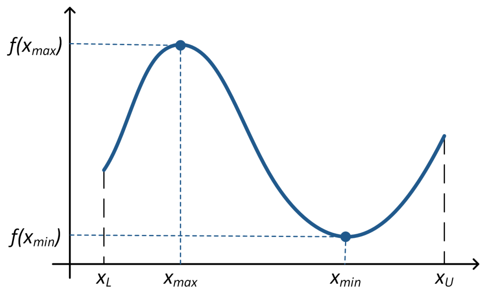
## Objectives

1. Being able to characterize different optimization problems
2. Learn how to solve optimization problems in R
3. Understand the idea behind common optimization algorithms

## Outline

# Mathematical Optimization

- Optimization uses a rigorous mathematical model to determine the most efficient solution to a described problem
- One must first identify an objective
  - Objective is a quantitative measure of the performance
  - Examples: profit, time, cost, potential energy
  - In general, any quantity (or combination thereof) represented as a single number



# Classification of Optimization Problems

**Common groups**

1. Linear Programming (LP)
   - Objective function and constraints are both linear
   - $\min_{\boldsymbol{x}} \boldsymbol{c}^T \boldsymbol{x} \quad \text{s. t.} \quad A\boldsymbol{x} \leq \boldsymbol{b}$ and $\boldsymbol{x} \geq 0$
2. Quadratic Programming (QP)
   - Objective function is quadratic and constraints are linear
   - $\min_{\boldsymbol{x}} \boldsymbol{x}^T Q \boldsymbol{x} + \boldsymbol{c}^T \boldsymbol{x} \quad \text{s. t.} \quad A\boldsymbol{x} \leq \boldsymbol{b}$ and $\boldsymbol{x} \geq 0$
3. Non-Linear Programming (NLP): objective function or at least one constraint is non-linear

**Solution strategy**

- Each problem class requires its own algorithms
  $\rightarrow$ R has different packages for each class
- Often, one distinguishes further, e. g. constrained vs. unconstrained
  - Constrained optimization refers to problems with equality or inequality constraints in place

# Optimization in R

- Common R packages for optimization

| **Problem type** | **Package** | **Routine** |
|---|---|---|
| General purpose (1-dim.) | Built-in | `optimize(...)` |
| General purpose ($n$-dim.) | Built-in | `optim(...)` |
| Linear Programming | `lpSolve` | `lp(...)` |
| Quadratic Programming | `quadprog` | `solve.QP(...)` |
| Non-Linear Programming | `optimize` | `optimize(...)` |
| | `optimx` | `optimx(...)` |
| General interface | `ROI` | `ROI_solve(...)` |

- All available packages are listed in the CRAN task view “Optimization and mathematical programming”

  URL: `https://cran.r-project.org/web/views/Optimization.html`

# Optimization in R

- Basic argument structure of a solver is always the same
- Format of such a generic call

```
optimizer(objective, constraints, bounds=NULL,
          types=NULL, maximum=FALSE)
```

- Routines usually provide an interface, which allows to switch between different algorithms

**Built-in optimization routines**

- `optimize(...)` is for 1-dimensional optimzation
- `optim(...)` is for *n*-dimensional optimization
  - Golden section search (with successive 2nd degree polynomial interpolation)
  - Aimed at continuous functions
  - Switching to dedicated routines usually achieves a better convergence

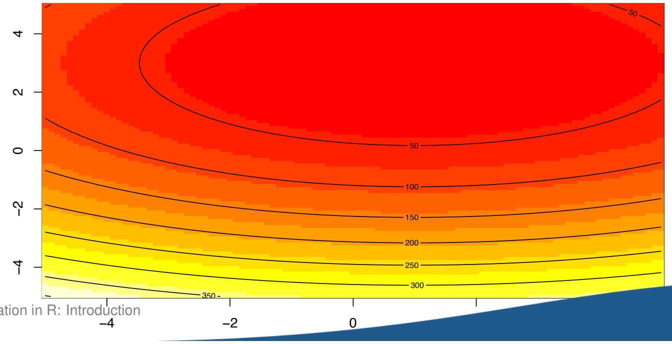
## Built-In Optimization in R

- `optim(x0, fun, ...)` is for *n*-dimensional general purpose optimization
  - Argument `x0` sets the initial values of the search
  - `fun` specifies a function to optimize over
  - Optional, named argument `method` chooses an algorithm

**Example**

- Define objective function

```
f <- function(x) 2*(x[1]-1)^2 + 5*(x[2]-3)^2 + 10
```



## Built-In Optimization in R

- Call optimization routine

```r
r <- optim(c(1, 1), f)
```

- Check if the optimization converged to a minimum

```r
r$convergence == 0  # TRUE if converged

## [1] TRUE
```

- Optimal input arguments

```r
r$par

## [1] 1.000168 3.000232
```

- Objective at the minimum

```r
r$value

## [1] 10
```

# Outline

# Linear Programming

**Mathematical specification**

1. Matrix notation

$$\underbrace{\min_{\boldsymbol{x}} \begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_n \end{bmatrix}^T \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}}_{\text{Objective}} \text{ s.t. } \underbrace{\begin{bmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & \dots & a_{mn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} \geq \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{bmatrix}}_{\text{First constraint}}, \underbrace{\begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} \geq 0}_{\text{Second constraint}}$$

2. Alternative formulation in a more compact form

$$\min_{\boldsymbol{x}} c^T \boldsymbol{x} = \min_{\boldsymbol{x}} c_1 x_1 + \cdots + c_n x_n$$

$$\text{subject to} \quad A\boldsymbol{x} \geq \boldsymbol{b}, \quad \boldsymbol{x} \geq 0$$

# Linear Programming

**Example**

1. Objective function
   - Goal is to maximize the total profit
   - Products A and B are sold at €25 and €20 respectively
2. Resource constraints
   - Product A requires 20 resource units, product B needs 12
   - Only 1800 resource units are available per day
3. Time constraints
   - Both products require a production time of 1/15 hour
   - A working day has a total of 8 hour

# Linear Programming

**Problem formulation**

- Variables: let $x_1$ denote the number of produced items of $A$ and $x_2$ of B
- Objective function maximizes the total sales

$$Sales_{\max} = \max_{x_1, x_2} 25\, x_1 + 20\, x_2 = \max_{x_1, x_2} \begin{bmatrix} 25 \\ 20 \end{bmatrix}^T \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

**Constraints**

- Constraints for resources and production time are given by

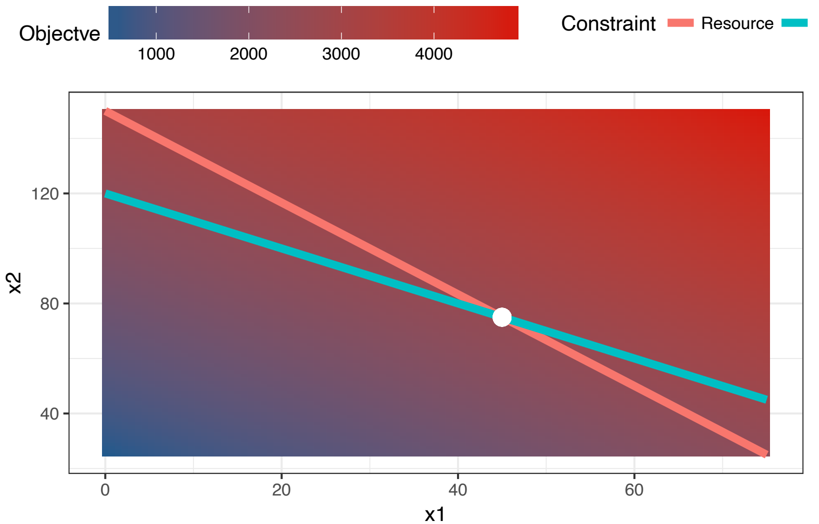
$$20\, x_1 + 12\, x_2 \leq 1800$$
$$\frac{1}{15} x_1 + \frac{1}{15} x_2 \leq 8$$

- Both constraints can also be rewritten in matrix form

$$\underbrace{\begin{bmatrix} 20 & 12 \\ \frac{1}{15} & \frac{1}{15} \end{bmatrix}}_{A} \underbrace{\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}}_{\boldsymbol{x}} \leq \underbrace{\begin{bmatrix} 1800 \\ 8 \end{bmatrix}}_{\boldsymbol{b}}$$

# Linear Programming

- Visualization of objective function and both constraints



## Linear Programming in R

- Package `lpSolve` contains routine `lp(...)` to solve linear optimization problems
- General syntax

```
lp(direction="min", objective.in, const.mat, const.dir,
   const.rhs)
```

  - `direction` controls whether to minimize or maximize
  - Coefficients $\boldsymbol{c}$ are encoded a vector `objective.in`
  - Constraints $A$ are given as a matrix `const.mat` with directions `const.dir`
  - Constraints $\boldsymbol{b}$ are inserted as a vector `const.rhs`

## Linear Programming in R

- Loading the package

```r
library(lpSolve)
```

- Encoding and executing the previous example

```r
objective.in <- c(25, 20)
const.mat <- matrix(c(20, 12, 1/15, 1/15), nrow=2,
                    byrow=TRUE)
const.rhs <- c(1800, 8)
const.dir <- c("<=", "<=")
optimum <- lp(direction="max", objective.in, const.mat,
              const.dir, const.rhs)
```

- Optimal values of $x_1$ and $x_2$

```r
optimum$solution
```

```
## [1] 45 75
```

- Objective at minimum

```r
optimum$objval
```

```
## [1] 2625
```

# Outline

# Quadratic Programming

## Mathematical specification

1. Compact form

$$\min_{\boldsymbol{x}} \frac{1}{2}\boldsymbol{x}^T D\boldsymbol{x} - \boldsymbol{d}^T\boldsymbol{x} \text{ subject to } A^T\boldsymbol{x} \geq \boldsymbol{b}$$

2. Matrix notation

$$\min_{x} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}^T \begin{bmatrix} d_{11} & d_{12} & \dots & d_{1n} \\ d_{21} & d_{22} & \dots & d_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ d_{m1} & d_{m2} & \dots & d_{mn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} - \begin{bmatrix} d_1 \\ d_2 \\ \vdots \\ d_n \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} \text{ s.t. } \begin{bmatrix} a_{11} & a_{12} & \dots \\ a_{21} & a_{22} & \dots \\ \vdots & \vdots & \ddots \\ a_{m1} & a_{m2} & \dots \end{bmatrix}$$

## Quadratic Programming

- Parameter mapping in R
  - Quadratic coefficients $D$ are mapped to `Dmat`
  - Linear coefficients $d$ are mapped to `dvec`
  - Constraints matrix $A$ is mapped to `Amat`
  - Constraint equalities or inequalities $b$ are provided in `bvec`
  - Parameter `meq=` $n$ sets the firs $n$ entries as equality constraints; all further constraints are inequality
- Function call with package `quadprog`

```r
require(quadprog)
solve.QP(Qmat, dvec, Amat, bvec, meq)
```

- Many problems can formulated in quadratic form, e.g., portfolio optimization, circus tent problem, demand response, ...

# Example Circus Tent

**Question**

How to bring this into quadratic form?

## Example Circus Tent

- How to calculate the height of the tent at every point?
- Tent height at each grid point $(x, y)$ is given by $u(x, y)$
- Tent sheet settles into minimal energy state $E[u]$ for each height $u$
- Use the Dirichlet energy to estimate $E[u]$ of $u$
- We discretize the energy and ultimately come up with

$$E[u] \approx \frac{h_x h_y}{2} \boldsymbol{u}^T L \boldsymbol{u} \tag{1}$$

which is quadratic

**Full description**

http://blog.ryanwalker.us/2014/04/the-circus-tent-problem-with-rs-quadprog.html

# Outline

# Overview: Non-Linear Optimization

| | | | | |
|---|---|---|---|---|
| **Dimensionality** | **One-dimensional** | **Multi-dimensional** | | |
| **Category** | **Non-gradient based** | **Gradient based** | **Hessian based** | **Non-gradient based** |
| **Algorithms** | Golden Section Search | Gradient descent methods | Newton and quasi-Newton methods | Golden Section Search, Nelder-Mead |
| **Package** | stats | optimx | | |
| **Functions** | optimize() | CG | BFGS<br>L-BFGS-B | Nelder-Mead |

## One-Dimensional Non-linear Programming

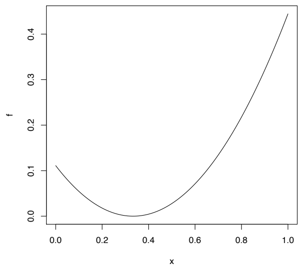
- Golden Section Search can be used to solve one-dimensional non-linear problems
- Basic steps:
  1. Golden Ratio defined as $\varphi = \frac{\sqrt{5}-1}{2} = 0.618$
  2. Pick an interval [a, b] containing the optimum
  3. Evaluate $f(x_1)$ at $x_1 = a + (1-\varphi)(b-a)$ and compare with $f(x_2)$ at $x_2 = a + \varphi(b-a)$
  4. If $f(x_1) < f(x_2)$, continue the search in the interval $[a, x_1]$, else $[x_2, b]$
- Implementation in R with built-in packages

```r
optimize(f = , interval = ,  ...,
         tol = .Machine$double.eps^0.25)
```

## Golden Section Search Iterations

- Minimize $f(x) = (x - \frac{1}{3})^2$ with `optimize`
- Use `print` to show steps of $x$

```
f <- function(x) (print(x) - 1/3)^2
xmin <- optimize(f,
                 interval = c(0, 1),
                 tol = 0.0001)

## [1] 0.381966
## [1] 0.618034
## [1] 0.236068
## [1] 0.3333333
## [1] 0.3333
## [1] 0.3333667
## [1] 0.3333333

xmin

## $minimum
## [1] 0.3333333
##
## $objective
## [1] 0
```



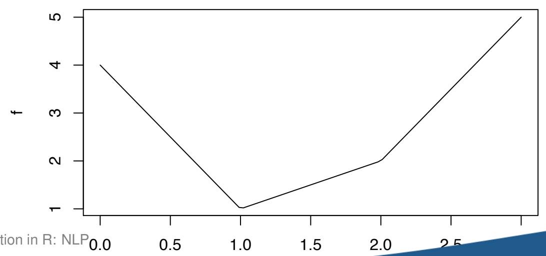
## Example: Non-differentiable function with optimx()

- Does not require differentiability, e.g., $f(x) = |x-2| + 2|x-1|$

```
f <- function(x) return(abs(x-2) + 2*abs(x-1))
xmin <- optimize(f, interval = c(0, 3), tol = 0.0001)
xmin
```

```
## $minimum
## [1] 1.000009
##
## $objective
## [1] 1.000009
```

```
plot(f, 0, 3)
```



## Non-Linear Multi-Dimensional Programming

- Collection of non-linear methods in package `optimx`

```
require(optimx)
optimx(par, fn, gr=Null, Hess=Null, lower=inf,
       upper=inf, method='', itnmax=Null, ...)
```

- Multiple optimization algorithms possible
  - Gradient based: Gradient descent methods ('CG')
  - Hessian based: Newton and quasi-Newton methods ('BFGS', 'L-BFGS-B')
  - Non-gradient based: Golden section search, Nelder-Mead, ... ('Nelder-Mead')
- The default method of `optimx` is "Nelder-Mead"; if constraints are provided, "L-BFGS-B" is used

## Optimx parameters

- Important input parameters

| | |
|---|---|
| `par` | Initial values for the parameters (vector) |
| `fn` | Objective function with minimization parameters as input |
| `method` | Search method (possible values: 'Nelder-Mead', 'BFGS', 'CG', 'L-BFGS-B', 'nlm', 'nlminb', 'spg', 'ucminf', 'newuoa', 'bobyqa', 'nmkb', 'hjkb', 'Rcgmin', or 'Rvmmin) |
| `control` | List of control parameters |

- Important output parameters

| | |
|---|---|
| `pn` | Optimal set of parameters |
| `value` | Minimum value of `fn` |
| `fevals` | Number of calls to `fn` |
| `gevals` | Number of calls to the gradient calculation |
| `xtimes` | Execution time in seconds |

# Himmelblau's function

- Definition

$$f(x,y) = (x^2 + y - 11)^2 + (x + y^2 - 7)^2 \tag{2}$$

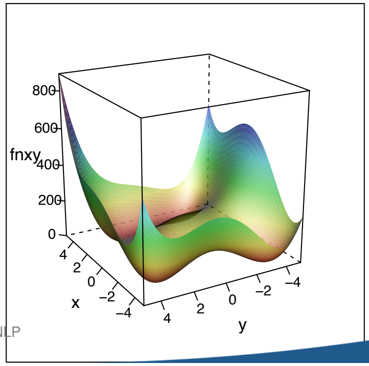
- Himmelblau's function (Zimmermann 2007) is a popular multi-modal function to benchmark optimization algorithms
- Four equivalent minima are located at $f(-3.7793; -3.2832) = 0$, $f(-2.8051; 3.1313) = 0$, $f(3; 2) = 0$ and $f(3{,}5844; -1{,}8481) = 0$.

## Implementation of Himmelblau's function

```r
fn <- function(para){ # Vector of the parameters
    matrix.A <- matrix(para, ncol=2)
    x <- matrix.A[,1]
    y <- matrix.A[,2]
    f.x <- (x^2+y-11)^2+(x+y^2-7)^2
    return(f.x)
}
par <- c(1,1)
```

## Plot of Himmelblau's function

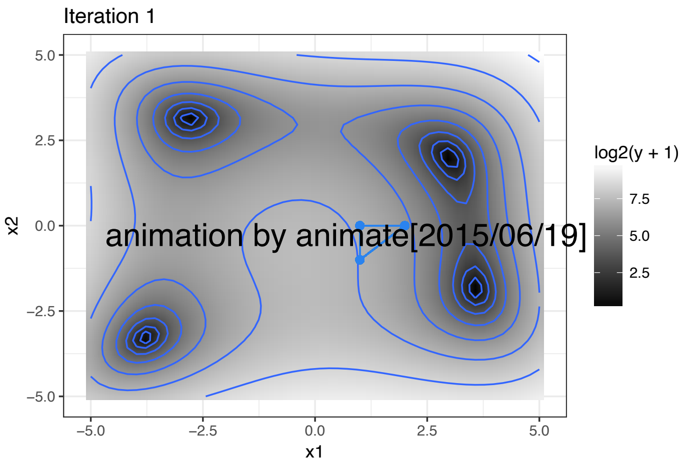
```r
xy <- as.matrix(expand.grid(seq(-5,5,length = 101),
                            seq(-5,5,length = 101)))
colnames(xy) <- c("x", "y")
df <- data.frame(fnxy = fn(xy), xy)

library(lattice)
wireframe(fnxy ~ x*y, data = df, shade = TRUE, drape=FALSE,
          scales = list(arrows = FALSE),
          screen = list(z=-240, x=-70, y=0))
```



## Gradient-Free Method: Nelder-Mead

- Nelder Mead solves multi-dimensional equations using function values
- Works also with non-differentiable functions
- Basic steps:
  1. Choose a simplex consisting of $n+1$ points $p_1, p_2, \ldots p_{n+1}$ are chosen with n being the number of variables
  2. Calculate $f(p_i)$ and sort by size, e.g., $f(p_1) \leq f(p_2) \leq f(p_{n+1})$
  3. Check if the best value is good enough, if so, stop
  4. Drop the point with highest $f(p_i)$ from the simplex
  5. Choose a new point to be added to the simplex
  6. Continue with step 2
- Different options and implementations to choose new point, often these are combined:
  - Reflection to the center of gravity of the simplex formed by the other points and further expansion in the same direction
  - Contraction of the 'worst' point towards the center of the simplex
  - Compression, e.g., contraction of all points towards the 'best' point
  - Usage of the gradient to determine direction of next point

# Nelder mead search

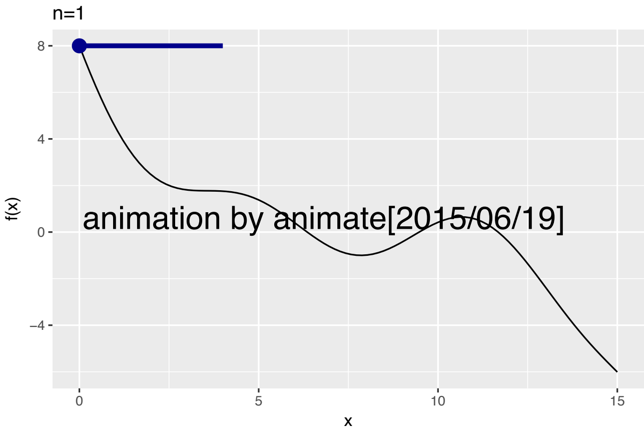


## Gradient-Based: Conjugate Gradients

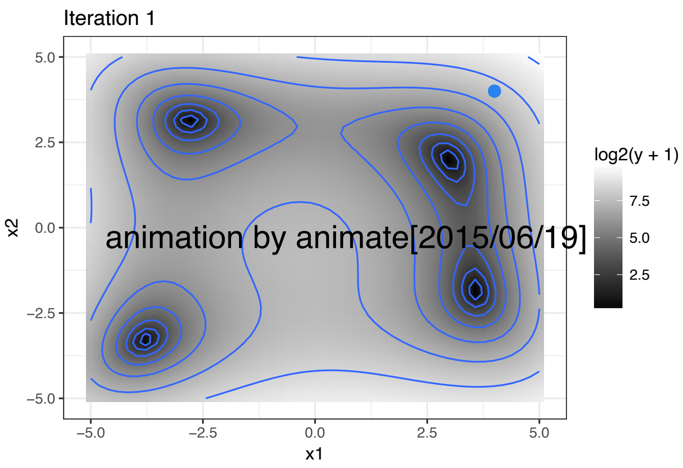
- Use the first derivative to obtain gradient for the search direction
- Search direction $s_n$ of the next point results from the negative gradient of the last point
- Basic steps
  1. Calculate search direction $s_n = -\Delta f(x_n)$
  2. Pick next point $x_{n+1}$ by moving with step size $a_n$ in the search direction; step size $a$ can be fixed or variable
  3. Repeat until $\Delta f(x_n) = 0$ or another stopping criterion
- Results in a "zig-zagging" movement towards the minimum

## One Dimensional CG

- Find minima of the function $f(x) = -sin(x) - (.25x - 2)^3$



# Gradient descent search path



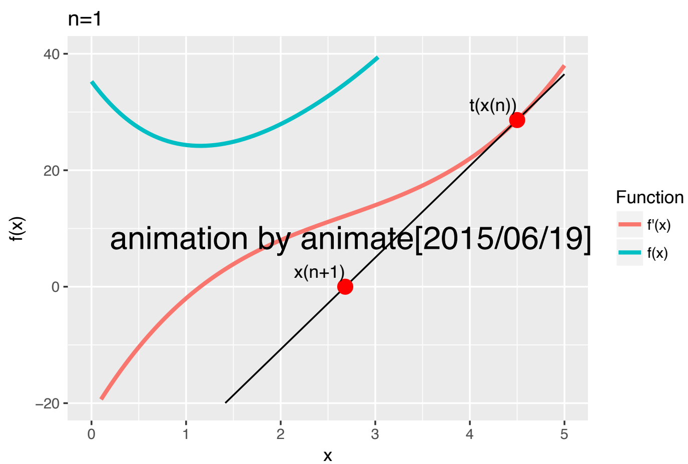

- $a_n$ for gradient descent is fixed at 0.01
- The algorithm stops when its within 0.1 of a zero

# Newton-Raphson

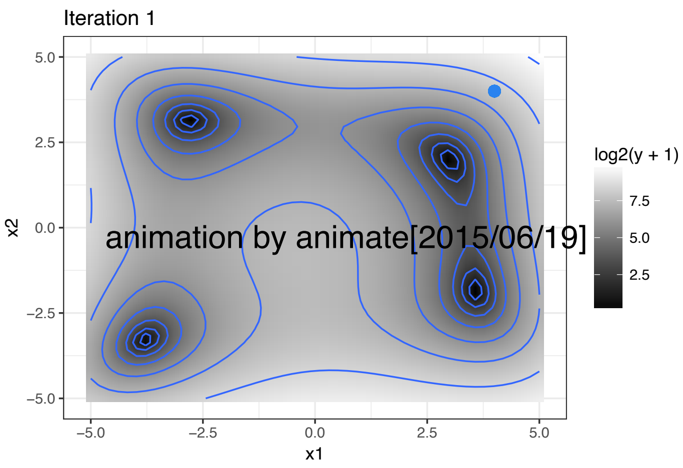
- Newton's method is often used to find the zeros of a function
- Minima fulfill the conditions $f'(x^*) = 0$ and $f''(x^*) > 0$, so Newton can be used to find the zeros of the first derivative
- Basic steps
  1. Approximate the function at the starting point with a linear tangent (e.g., second order Taylor series) $t(x) \approx f'(x_0) + (x - x_0)f''(x_0)$
  2. Find the intersect $t(x_i) = 0$ as an approximation for $f'(x^*) = 0$
  3. Use the intersect as new starting point
  4. Finally, the algorithm $x_{n+1} = x_n - \frac{f'(x_n)}{f''(x_n)}$ is repeated until $f'(x_n)$ is close enough to 0.

# Visualization of Newton-Raphson Search

- Find minima of $f(x) = \frac{1}{4}(x-3)^4 + \frac{1}{3}x^3 + 5x + 15$



# Newton Raphson search paths

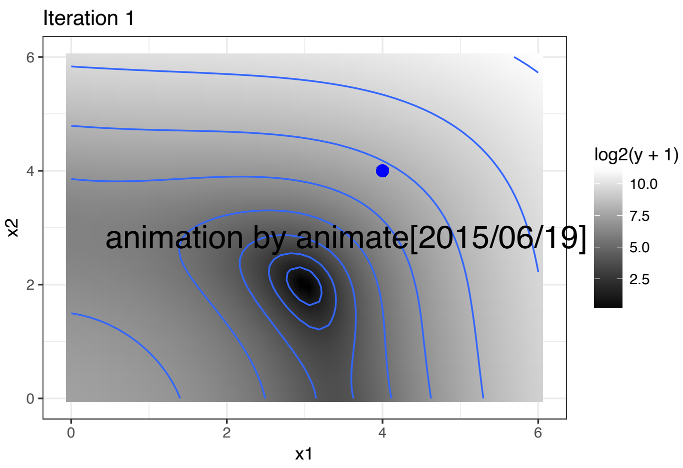



- The algorithm stops when its within 0.1 of a zero

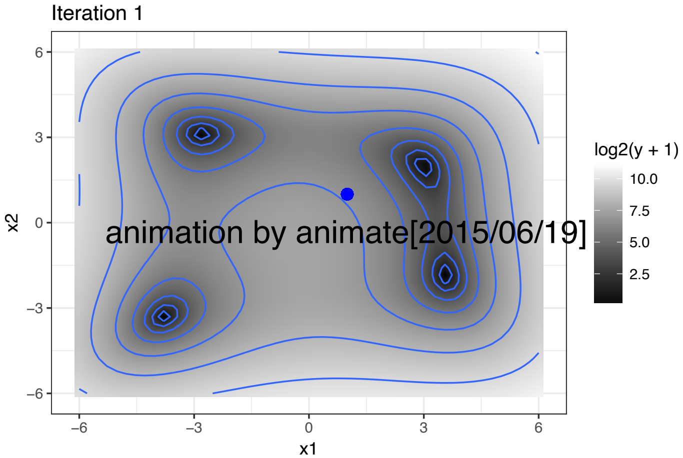
## Hessian-Based: BFGS and L-BFGS-B

- Broyden-Fletcher-Goldfarb-Shanno (BFGS) algorithm builds on the idea of Newton's method to take gradient information into account
- Gradient information comes from an approximation of the Hessian matrix
- No guaranteed conversion; expecially problematic if Taylor expansion does not fit well
- L-BFGS-B stands for limited-memory-BFGS-box
  - Extension of BFGS
  - Memory efficient implementation
  - Additionally handles box constraints

# Comparison Newton and Gradient Descent



# Comparison Newton and Gradient Descent




- $a_n$ for gradient descent is fixed at 0.01
- Both algorithm stop if they are within 0.01 of a zero

# Method Comparison with optimx()

- Optimization comparison requires `optimx` package

```
library(optimx)
```

- Nelder-Mead

```
optimx(par, fn, method = "Nelder-Mead")
```

```
##                   p1       p2       value fevals gevals niter convcode
## Nelder-Mead 2.999995 2.000183 5.56163e-07     67     NA    NA        0
##              kkt1 kkt2 xtimes
## Nelder-Mead FALSE TRUE      0
```

- Conjugate gradients

```
optimx(par, fn, method = "CG")
```

```
##    p1 p2        value fevals gevals niter convcode kkt1 kkt2 xtimes
## CG  3  2 1.081231e-12    119     31    NA        0 TRUE TRUE      0
```

- BFGS

```
optimx(par, fn, method = "BFGS")
```

```
##      p1 p2        value fevals gevals niter convcode kkt1 kkt2 xtimes
## BFGS  3  2 1.354193e-12     32     11    NA        0 TRUE TRUE      0
```

# Choosing Optimization Methods

- Many methods available, as problems vary in size and complexity
- Depending on the problem optimization methods have specific advantages
- optimx offers a great way to test and compare search methods

```
optimx(par, fn, method = c("Nelder-Mead", "CG", "BFGS", "spg", "nlm"))

##                   p1       p2        value fevals gevals niter convcode
## Nelder-Mead 2.999995 2.000183 5.561630e-07     67     NA    NA        0
## CG          3.000000 2.000000 1.081231e-12    119     31    NA        0
## BFGS        3.000000 2.000000 1.354193e-12     32     11    NA        0
## spg         3.000000 2.000000 2.239653e-13     15     NA    13        0
## nlm         3.000000 2.000000 1.450383e-14     NA     NA    10        0
##              kkt1 kkt2 xtimes
## Nelder-Mead FALSE TRUE   0.00
## CG           TRUE TRUE   0.00
## BFGS         TRUE TRUE   0.00
## spg          TRUE TRUE   0.08
## nlm          TRUE TRUE   0.00
```

## Control Object

- Control optimize allows to specify the optimization process

| | |
|---|---|
| `trace` | Non-negative integer to show iterative search information |
| `follow.on` | If `TRUE` and multiple methods, then later methods start the search where the previous method stopped (effectively a polyalgorithm implementation) |
| `maximize` | If `TRUE`, maximize the function (not possible for methods "nlm","nlminb" and "ucminf") |

- Example in R

```r
optimx(par, fn, method = c("BFGS", "Nelder-Mead"),
    control = list(trace = 6, follow.on=TRUE, maximize=FALSE))
```

## Scaling

- Optimization treats all variables in the same way
- Sometimes, variables have strongly different scale
- Example, particle with speed $10^7 \ \frac{\mathrm{m}}{\mathrm{s}}$ and mass $10^{-27} \ \mathrm{kg}$
- Step size and error will be hugely different for the two variables
- Besides manual scaling, two options in `optimx`

| | |
|---|---|
| `fnscale` | Overall scaling to the function and gradient values |
| `parscale` | Vector scaling of parameters |

## Outline

# R Optimization Infrastructure (ROI)

- `ROI` is a package which provides a standardized interface to many R optimization packages
- Setup and installation

```
install.packages("ROI")
```

- The latest (non-stable) versions are on R-Forge, use the `repos` option to install these

```
install.packages("ROI",
                 repos="http://R-Forge.R-project.org")
```

- Currently supported solvers and corresponding plugins

```
require(ROI)
ROI_available_solvers()
              glpk                 quadprog                 symphony
 "ROI.plugin.glpk" "ROI.plugin.quadprog" "ROI.plugin.symphony"
```

- Implementation of many more solvers planned, overview
  `https://r-forge.r-project.org/R/?group_id=308`

# Installation of ROI plugins

- Solver plug-ins need to be installed separately

```r
install.packages("ROI.plugin.glpk")
install.packages("ROI.plugin.quadprog")
install.packages("ROI.plugin.symphony")
```

- Check solver plug-in installation

```r
library(ROI)
```

```r
ROI_installed_solvers()
```

```
##                  glpk              quadprog              symphony
##     "ROI.plugin.glpk" "ROI.plugin.quadprog" "ROI.plugin.symphony"
```

```r
ROI_registered_solvers()
```

```
##                nlminb                  glpk              quadprog
##   "ROI.plugin.nlminb"     "ROI.plugin.glpk" "ROI.plugin.quadprog"
##              symphony
## "ROI.plugin.symphony"
```

## Usage of ROI

- Package definition and function call

```r
require(ROI)
ROI_solve(x, solver, control = NULL, ...)
```

- Arguments of `ROI_solve`

| | |
|---|---|
| `x` | object with problem and constraint description |
| `solver` | solver to be used |
| `control` | list of additional control arguments |

# Solving optimization problems with ROI)

- linear 3-dimensional example

```
lp <- OP(objective = c(2, 4, 3),
         L_constraint(
             L = matrix(c(3, 2, 1, 4, 1, 3, 2, 2, 2),
                        nrow = 3),
             dir = c("<=", "<=", "<="),
             rhs = c(60, 40, 80)),
         maximum = TRUE)
lp
```

```
## ROI Optimization Problem:
##
## Maximize a linear objective function of length 3 with
## - 3 continuous objective variables,
##
## subject to
## - 3 constraints of type linear.
```

```
sol <- ROI_solve(lp, solver = "glpk")
sol
```

```
## Optimal solution found.
## The objective value is: 7.666667e+01
```

# Solving optimization problems with ROI)

- Quadratic problem with linear constraints

```
qp <- OP(
        Q_objective(Q = diag(1, 3),
                    L = c(0, -5, 0)),
        L_constraint(
            L = matrix(c(-4, -3, 0, 2, 1, 0, 0, -2, 1),
                       ncol = 3,
                       byrow = TRUE),
            dir = rep(">=", 3),
            rhs = c(-8, 2, 0)))
qp
```

```
## ROI Optimization Problem:
##
## Minimize a quadratic objective function of length 3 with
## - 3 continuous objective variables,
##
## subject to
## - 3 constraints of type linear.
```

```
sol <- ROI_solve(qp, solver = "quadprog")
sol
```

```
## Optimal solution found.
## The objective value is: -2.380952e+00
```

## Outline

## Optimization inside the LASSO

- Lasso (least absolute shrinkage and selection operator) is a popular method for predictions
- The underlying regression is solved by minimizing an error term, e.g., RSS (residual sum of squares) and a tuning parameter
- In case of the Lasso

$$\min_{\boldsymbol{\beta}} (\boldsymbol{y} - \boldsymbol{\beta}\boldsymbol{X})^2 \text{ subject to } \sum |\boldsymbol{\beta}| \leq s \tag{3}$$

- Regression part written out

$$\min_{\boldsymbol{\beta}} \boldsymbol{y}^T\boldsymbol{y} - 2\boldsymbol{y}^T\boldsymbol{X}\boldsymbol{\beta} + \boldsymbol{\beta}^T\boldsymbol{X}^T\boldsymbol{X}\boldsymbol{\beta} \tag{4}$$

- Variables for quadratic optimization $Dmat = \boldsymbol{X}^T\boldsymbol{X}$ and $dvec = \boldsymbol{y}^T\boldsymbol{X}$

# Comparison of regression and minimization

```r
# Sample data
n <- 100
x1 <- rnorm(n)
x2 <- rnorm(n)
y <- 1 + x1 + x2 + rnorm(n)
X <- cbind( rep(1,n), x1, x2 )

# Regression
r <- lm(y ~ x1 + x2)

# Optimization
library(quadprog)
s <- solve.QP( t(X) %*% X, t(y) %*% X, matrix(nr=3,nc=0), numeric(), 0 )

# Comparison
coef(r)

## (Intercept)          x1          x2
##   1.0645272   1.0802060   0.9807713

s$solution  # Identical

## [1] 1.0645272 1.0802060 0.9807713
```

## Optimization inside Quantile Regressions

- Basic problem, find the median such that

$$\min_{\mu} \sum_{i=0}^{N} |x_i - \mu| \tag{5}$$

- This can be written as a linear problem

$$\begin{aligned}
&\min_{\mu, a_i, b_i} \sum_{i=0}^{N} a_i + b_i && (6)\\
&\text{subject to } a_i \geq 0, && (7)\\
&\qquad b_i \geq 0 \text{ and} && (8)\\
&\qquad x_i - \mu = a_i - b_i && (9)
\end{aligned}$$

## Optimization inside Quantile Regressions

- Finding the median with a linear optimization

```
n <- 101  # Odd number for unique median
x <- rlnorm(n)
library(lpSolve)

# One constraint per row: a[i], b[i] >= 0
A1 <- cbind(diag(2*n),0)

# a[i] - b[i] = x[i] - mu
A2 <- cbind(diag(n), -diag(n), 1)

r <- lp("min",
        c(rep(1,2*n),0),
        rbind(A1, A2),
        c(rep(">=", 2*n), rep("=", n)),
        c(rep(0,2*n), x)
)

# Comparison
tail(r$solution,1)
## [1] 0.9890153
median(x)
## [1] 0.9890153
```

# Optimization inside Quantile Regressions

- Introducing $\tau = .3$ allows to calculate a quantile regression

```
require(lpSolve)
tau <- .3
n <- 100
x1 <- rnorm(n)
x2 <- rnorm(n)
y <- 1 + x1 + x2 + rnorm(n)
X <- cbind( rep(1,n), x1, x2 )
A1 <- cbind(diag(2*n), 0,0,0)  # a[i], b[i] >= 0
A2 <- cbind(diag(n), -diag(n), X) # a[i] - b[i] = (y - X %*% beta)[i]
r <- lp("min",
        c(rep(tau,n), rep(1-tau,n),0,0,0),
        rbind(A1, A2),
        c(rep(">=", 2*n), rep("=", n)),
        c(rep(0,2*n), y)
)
tail(r$solution,3)
```

```
## [1] 0.5827969 1.2125340 0.8054628
```

```
# Compare with quantreg
rq(y~x1+x2, tau=tau)
```

```
## Call:
## rq(formula = y ~ x1 + x2, tau = tau)
##
## Coefficients:
## (Intercept)          x1          x2
##   0.5827969   1.2125340   0.8054628
##
## Degrees of freedom: 100 total; 97 residual
```

# Outline

# Outlook

## Additional Material

- Short summary of Optimization with R $\longrightarrow$ Seminar Paper
- Further exercises as homework
- R Reference Card, will also be available during exam

## Future Exercises

R will be used to solve sample problems from Business Intelligence