Computing Unit 6: Optimization and Root Finding

WIRTSCHAFTS UNIVERSITÄT WIEN VIENNA UNIVERSITY OF ECONOMICS AND BUSINESS

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Outline

- Basics
- Root finding
- Optimization

Basics

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Simplest case where max/min are attained: life can be more complicated.

If $X = \mathbb{R}^n$: unconstrained optimization problem.

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Note that the f for optimization always is a *scalar* function!

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- Find roots of polynomials: `polyroot()`.
- Find roots of continuous univariate functions: `uniroot()`.
  This is based on the *bisection method*.
- Already encountered Newton’s method for root finding, which is a *fixed-point iteration* method.
  Interestingly, no function for this in base R.

Bisection method

Suppose f is continuous with a sign change in $[a, b]$ (i.e., $f(a)$ and $f(b)$ have opposite signs).

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Can be found by the following iteration: Starting with $a_0 = a$ and $b_0 = b$,

- Take the current interval $[a_n, b_n]$.
- If $b_n - a_n$ is small enough; done. Otherwise, compute the midpoint $x_n = (a_n + b_n)/2$.
- If f has a sign change in $[a_n, x_n]$, take this as the next interval; otherwise take $[x_n, b_n]$.

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In each step, halves the interval (length).

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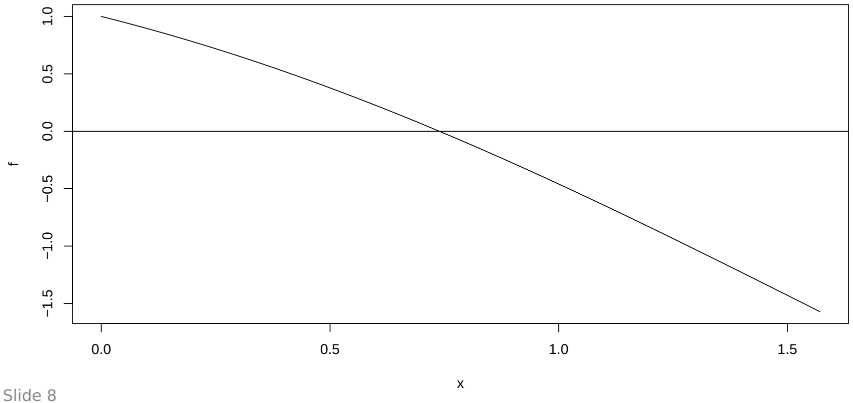
Hence the computational complexity is *logarithmic* in the precision (interval length) sought.

Example

The function $f(x) = \cos(x) - x$ has a root in $[0, \pi/2]$:

```
R> f <- function(x) cos(x) - x
R> plot(f, 0, pi / 2); abline(h = 0)
```



Example

```
R> uniroot(f, c(0, pi / 2))

$root
[1] 0.7390839

$f.root
[1] 2.059443e-06

$iter
[1] 5

$init.it
[1] NA

$estim.prec
[1] 6.103516e-05
```

Fixed-point iteration

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$$x_{n+1} = g(x_n)$$

gives a sequence x_n with (finite) limit x^*. What can we say about x^*?

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By continuity,

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Can use to find roots of f via fixed points of $g(x) = x + f(x)$? Not quite so simple . . .

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If g is smooth about x^*,

$$x_{n+1} - x^* = g(x_n) - g(x^*) \approx g'(x^*)(x_n - x^*),$$

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Otherwise, the approximation error $x_n - x^*$ would not get reduced.

In the attractive case, approximation errors go to zero exponentially fast.

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Prime example: Newton's method. This uses

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Clearly,

$$x = g(x) \Rightarrow \frac{f(x)}{f'(x)} = 0 \Rightarrow f(x) = 0.$$

Also,

$$g'(x) = 1 - \frac{f'(x)^2 - f(x)f''(x)}{f'(x)^2} = \frac{f(x)f''(x)}{f'(x)^2}.$$

Fixed-point iteration

Hence, if x^* is a fixed point of g: $g'(x^*) = 0$!

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Convergence to x^* is actually “locally quadratic” in the sense that

$$|x_{n+1} - x^*| \le \text{const}\, |x_n - x^*|^2.$$

(Note the confusing terminology: approximation errors go to zero faster than exponentially fast!).

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Optimization with base R

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Optimization with base R

- `optimize()` optimizes a univariate function based on golden section search.
- `nlm()` optimizes functions via Newton-type algorithms (i.e., via finding critical points)
- `optim()` provides several optimization methods: Nelder-Mead, quasi-Newton and conjugate-gradient algorithms, and simulated annealing.
- `nls()` solves non-linear least squares problems
- `constrOptim()` minimizes a function subject to linear inequality constraints using an adaptive barrier algorithm.

Much more in add-on packages . . . and other courses.

Here, we really only show the tip of the iceberg, and some basics.

Golden section search

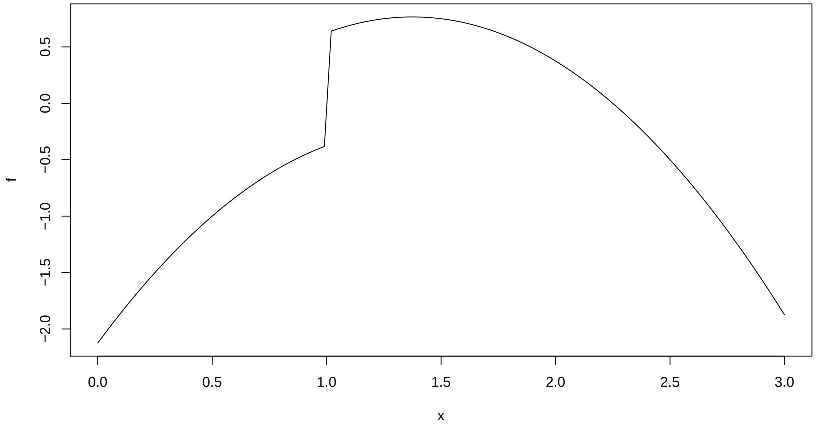
A function f is *unimodal* (over some interval $[a, b]$) if there is an m in the interval such that

$$f \text{ is increasing for } a \leq x < m \text{ and decreasing for } m < x \leq b.$$

In this case, clearly f has its maximum at m, and no local maxima.

f does not have to be continuous. Example:

Golden section search



Golden section search

Golden section search is based on “trisection”.

One starts with an interval $[a, b]$ containing the maximum, and adds two more points x_1 and x_2 to cut into three subintervals:

$$a < x_1 < x_2 < b.$$

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If $f(x_1) > f(x_2)$, the max cannot be in $[x_2, b]$, and the new interval is $[a, x_2]$.

If $f(x_1) < f(x_2)$, the max cannot be in $[a, x_1]$, and the new interval is $[x_1, b]$.

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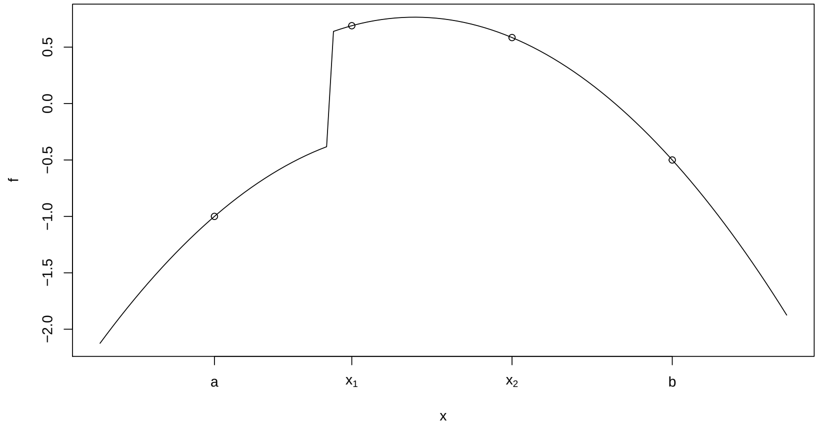

Golden section search

Golden section search is based on the following idea:

- Intervals are always partitioned in constant proportions:

$$x_1 = a + \gamma_1(b - a), \qquad x_2 = a + \gamma_2(b - a)$$

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  The γ_i are chosen in a way that one of the previous x_i points (and hence its function value $f(x_i)$) can be re-used.

Why? Function evaluation can be very expensive.

Golden section search

If $f(x_1) > f(x_2)$, the new interval is $[a' = a, b' = x_2]$, and the new x points are

$$x'_1 = a + \gamma_1(x_2 - a), \qquad x'_2 = a + \gamma_2(x_2 - a)$$

One of these must be x_1, and clearly $x'_1 < x_1$, so we must have $x'_2 = x_1$.

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Thus,

$$a + \gamma_1(b - a) = x_1 = x'_2 = a + \gamma_2(x_2 - a) = a + \gamma_2^2(b - a)$$

from which $\gamma_1 = \gamma_2^2$.

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$$x'_1 = x_1 + \gamma_1(b - x_1), \qquad x'_2 = x_1 + \gamma_2(b - x_1)$$

One of these must be $x_2 = (1-\gamma_2)a + \gamma_2 b$. As clearly $x'_2 = (1-\gamma_2)x_1 + \gamma_2 b > x_2$, we must have $x_2 = x'_1$. Thus:

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$$\begin{aligned} a + \gamma_2(b - a) &= x_1 + \gamma_1(b - x_1) \\ &= (1 - \gamma_1)x_1 + \gamma_1 b \\ &= a + (1 - \gamma_1)(x_1 - a) + \gamma_1(b - a) \\ &= a + (1 - \gamma_1)\gamma_1(b - a) + \gamma_1(b - a) \end{aligned}$$

from which $\gamma_2 = 2\gamma_1 - \gamma_1^2$.

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As $\gamma_1 < \gamma_2$ and $\gamma_2^2 - \gamma_1^2 = (\gamma_2 - \gamma_1)(\gamma_2 + \gamma_1)$, we get

$$\gamma_2 + \gamma_1 = 1.$$

Golden section search

Substituting now gives $\gamma_2^2 = \gamma_1 = 1 - \gamma_2$, so that γ_2 solves

$$\gamma_2^2 + \gamma_2 - 1 = 0.$$

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Roots are $-1/2 \pm \sqrt{5/4}$, so that

$$\gamma_2 = \frac{\sqrt{5}-1}{2} = \frac{\sqrt{5}-1}{2}\frac{\sqrt{5}+1}{\sqrt{5}+1} = \frac{2}{\sqrt{5}+1} = \frac{1}{\phi} \approx 0.61803$$

is the reciprocal value of the golden ratio ϕ!

Similarly,

$$\gamma_1 = 1 - \gamma_2 = 1 - \frac{1}{\phi} = 1 - (\phi - 1) = 2 - \phi \approx 0.38197.$$

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With the function we used as example:

```
R> f <- function(x) - (x - 0.5) * (x - 2.25) + ifelse(x < 1, -1, 0)
```

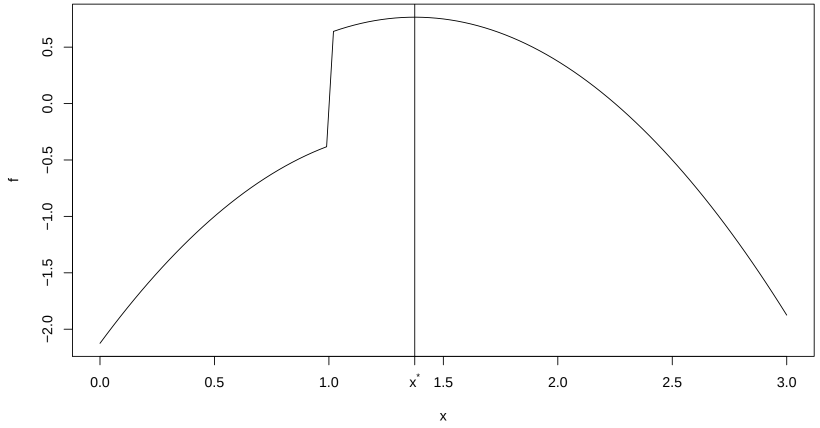
Golden section search

```
R> optimize(f, c(0, 3), maximum = TRUE)

$maximum
[1] 1.375

$objective
[1] 0.765625
```

Golden section search



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- Golden section search is only guaranteed to work if f is unimodal (for max).
- By default, `optimize` does minimization and not maximization.
- `optimize` only works for functions $f : \mathbb{R} \to \mathbb{R}$. Does not need derivatives: blessing or curse?

Example: MLE for the Poisson distribution

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We'll learn how to do this in the Statistics 2 course.

Example: MLE for the Poisson distribution

The preferred method is *maximum likelihood estimation* (MLE): one forms the likelihood function

$$L(\lambda|x_1,\ldots,x_n) = \prod_{i=1}^{n} \frac{\lambda^{x_i}}{x_i!} e^{-\lambda}$$

and maximizes this over λ.

Usually, one actually takes the log-likelihood because this is more convenient to work with.

Example: MLE for the Poisson distribution

Up to an additive constant, the log-likelihood is

$$LL(\lambda|x_1,\dots,x_n) = \sum_{i=1}^{n}(x_i \log(\lambda) - \lambda) = s(x_1,\dots,x_n)\log(\lambda) - n\lambda$$

with $s(x_1,\dots,x_n) = \sum_{i=1}^{n} x_i$.

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So for the MLE we have to find $\max_{\lambda>0} s\log(\lambda) - n\lambda$.

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The MLE is obviously given by $\hat{\lambda} = s/n = \bar{x}$.

Nice as we can do math to find a simple formula.

Example: MLE for the Poisson distribution

Numerically, we can simply do

```
R> mle_pois <- function(x) {
+     LL <- function(lambda) {
+         sum(x) * log(lambda) - length(x) * lambda
+     }
+     optimize(LL, lower = 0, upper = max(x), maximum = TRUE)
+ }
```

(Some finite upper bound is needed.)

Example: MLE for the Poisson distribution

To illustrate:

```
R> x <- rpois(100, 3.2)
R> mle_pois(x)

$maximum
[1] 3.660001

$objective
[1] 108.8715

R> ## Compare to
R> mean(x)

[1] 3.66
```

Multivariate optimization

Newton-type algorithms use the following idea.

Suppose $f : X \to \mathbb{R}$ with $X \subseteq \mathbb{R}^n$ is twice continuously differentiable on the interior of X and attains its max there at some x^*.

Then x^* must be a critical point:

$$\nabla f(x^*) = 0,$$

where

$$\nabla f(x) = \left[\frac{\partial f}{\partial \xi_1}(x), \ldots, \frac{\partial f}{\partial \xi_n}(x) \right]', \qquad x = (\xi_1, \ldots, \xi_n)'$$

is the gradient (and the prime denotes transposition).

Multivariate optimization

We can try finding roots of the gradient using a multivariate version of Newton's method.

First, close to x_n we have

$$\nabla f(x) \approx L_n(x) = \nabla f(x_n) + H_f(x_n)(x - x_n),$$

where

$$H_f(x) = \left[\frac{\partial^2 f}{\partial \xi_i \partial \xi_j}(x) \right]_{1 \le i,j \le n}$$

is the *Hessian* of f at x, i.e., the matrix of all second partial derivatives of f.

Details in the math course.

Multivariate optimization

Now solve $L_n(x) = 0$. Mathematically, this gives the linear system

$$H_f(x_n)(x - x_n) = -\nabla f(x_n)$$

which has solution

$$x - x_n = -H_f(x_n)^{-1}\nabla f(x_n).$$

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That's the basic idea. Things are really more complicated, but fortunately we can simply use functions like `optim()` or `nlm()`.

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- This needs f smooth and the first and second partials of f. We can either provide these in addition to f, or have R approximate these numerically.
- This can only find some local optimum of f, which may not be the global one.
- Things will always be fine if we maximize a concave function.

Example: MLE for the normal distribution

The density of the normal distribution with parameters μ and σ^2 at x is given by

$$\frac{1}{\sqrt{2\pi}\sigma}\exp\left(\frac{(x-\mu)^2}{2\sigma^2}\right)$$

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Suppose we observe a sample $x_1, \ldots, x_n$ from a normal distribution with unknown μ and σ^2. How can we estimate μ and σ^2 from that sample?

Example: MLE for the normal distribution

The likelihood of a sample $x_1, \ldots, x_n$ is

$$L(\mu, \sigma^2 | x_1, \ldots, x_n) = \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi}\sigma} \exp\left(\frac{(x_i - \mu)^2}{2\sigma^2} \right)$$

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This has partials

$$\frac{\partial LL}{\partial \mu} = \frac{1}{\sigma^2} \sum_{i=1}^{n} (x_i - \mu), \qquad \frac{\partial LL}{\partial \sigma^2} = -\frac{n}{2} \frac{1}{\sigma^2} + \frac{1}{2\sigma^4} \sum_{i=1}^{n} (x_i - \mu)^2.$$

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This has a unique critical point given by

$$\hat{\mu} = \bar{x}, \qquad \hat{\sigma}^2 = \frac{1}{n}\sum_{i=1}^{n}(x_i - \bar{x})^2$$

where $\bar{x}$ is the mean of x, which thus gives the MLEs.

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Nice as we can do math to find a simple formula.

Example: MLE for the normal distribution

Numerically, we can simply minimize twice the negative log-likelihood:

```
R> mle_norm <- function(x, p0) {
+     nLL <- function(p) {
+         mu <- p[1]
+         sigmasq <- p[2]
+         length(x) * log(sigmasq) + sum((x - mu) ^ 2) / sigmasq
+     }
+     optim(p0, nLL)
+ }
```

This needs some initial estimate of (μ, σ^2).

Example: MLE for the normal distribution I

To illustrate (note that in R the normal distribution is parametrized by the standard deviation σ and not the variance σ^2):

```
R> x <- rnorm(100, 0.5, 2)
R> mle_norm(x, c(0, 1))

$par
[1] 0.6005534 4.5651644

$value
[1] 251.826

$counts
function gradient
      53       NA

$convergence
```

Example: MLE for the normal distribution II

```
[1] 0

$message
NULL

R> ## Compare to
R> c(mean(x), (1 - 1 / length(x)) * var(x))

[1] 0.6003242 4.5642757
```

Example: MLE for the normal distribution

By default, this actually uses Nelder-Mead, which

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> *uses only function values and is robust but relatively slow. It will work reasonably well for non-differentiable functions.*

Could also do quasi-Newton: `optim(method = "BFGS")`, which

> *uses function values and gradients to build up a picture of the surface to be optimized.*

(No explicit computation of second partials.)

Example: MLE for the normal distribution

Alternatively, we can use `nlm()` which employs a Newton-type method (and always minimizes), without explicitly providing gradients and Hessians):

```
R> nLL2 <- function(p, x) {
+     mu <- p[1]
+     sigmasq <- p[2]
+     length(x) * log(sigmasq) + sum((x - mu) ^ 2) / sigmasq
+ }
```

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+ }
```

Starting from $(0, 1)$ again:

Example: MLE for the normal distribution

```
R> nlm(nLL2, c(0, 1), x)

$minimum
[1] 251.826

$estimate
[1] 0.6003227 4.5642620

$gradient
[1] -4.237677e-05 -5.506546e-05

$code
[1] 1

$iterations
[1] 15
```