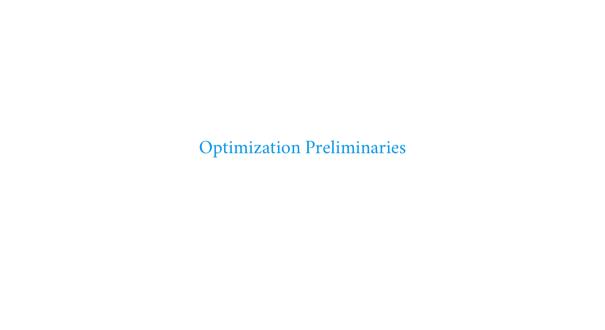
Introduction to Matlab

Lesson 03 — Optimization

Rafael Serrano-Quintero

Department of Economics University of Barcelona



Optimization Preliminaries

- Agents optimize is the foundational assumption of economic theory.
 - Firms minimize costs / maximize profits.
 - Consumers maximize utility / minimize expenditures.
- Not only in theory ... Econometricians use
 - o Maximum likelihood, least squares, method of moments ...
 - All optimization problems.
- We will learn the basics of how to state and solve this type of problems in Matlab.

Optimization Preliminaries — Definition of the Problem

The most general definition of an optimization problem (Note that $\max f(x) = \min -f(x)$)

$$\min_{x \in \mathbb{R}^n} f(x)$$
 (Objective Function)
s.t. $g(x) = 0$ (Equality Constraints)
 $h(x) \leq 0$ (Inequality Constraints)

where

- the Objective Function $f: \mathbb{R}^n \mapsto \mathbb{R}$
- the *m* Equality Constraints $g: \mathbb{R}^n \mapsto \mathbb{R}^m$
- the *l* Inequality Constraints $h: \mathbb{R}^n \mapsto \mathbb{R}^l$

Optimization Preliminaries — Definitions

Let $f: \mathcal{D} \subseteq \mathbb{R}^n \mapsto \mathbb{R}$.

Definition 1

A critical point
$$x^* \in \mathcal{D}$$
 of f satisfies $\nabla f(x^*) \equiv \left(\frac{\partial f}{\partial x_1}(x^*), \dots, \frac{\partial f}{\partial x_n}(x^*)\right) = 0$.

Definition 2

A point $x^* \in \mathcal{D}$ is a **min** of f on \mathcal{D} if $f(x^*) \leq f(x) \forall x \in \mathcal{D}$. It is a **strict min** if $f(x^*) < f(x) \forall x \neq x^* \in \mathcal{D}$.

Definition 3

A point $x^* \in \mathcal{D}$ is a **local (or relative or weak) min** of f on \mathcal{D} if there is a ball $B_r(x^*)$ such that $f(x^*) \leq f(x) \forall x \in B_r(x^*) \cap \mathcal{D}$. It is a **strict local (or relative or weak) min** if $f(x^*) < f(x) \forall x \neq x^* \in B_r(x^*) \cap \mathcal{D}$

Optimization Preliminaries — Definitions

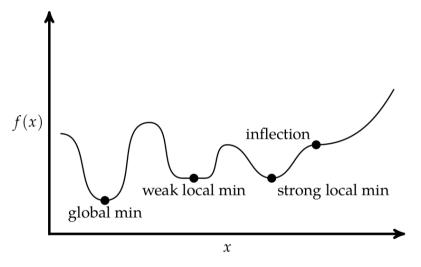


Figure 1: Classification of Critical Points. See Kochenderfer and Wheeler 2019

Optimization Preliminaries — First Order Conditions

- All points **need** that $f'(x^*) = 0$. Notice this is a **necessary condition** but not sufficient.
- \circ The inflection point also has $f'(x^*)=0$ (An inflection point is where the sign of the second derivative changes).

Theorem 1

Let $f: \mathcal{D} \subseteq \mathbb{R}^n \mapsto \mathbb{R}$ be a \mathcal{C}^1 function. If x^* is a local min or max of f in \mathcal{D} and x^* is an interior point of \mathcal{D} , then

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

Optimization Preliminaries — Second Order Conditions

Theorem 2

Let $f: \mathcal{D} \subseteq \mathbb{R}^n \mapsto \mathbb{R}$ be a C^2 function. Suppose x^* is a critical point of f.

- 1. If $H_f(x)$ is positive (negative) definite, then x^* is a strict local min (max) of f.
- 2. If $H_f(x)$ is indefinite, then x^* is neither a local min or max of f.

Definition 4

Let $f: \mathcal{D} \subseteq \mathbb{R}^n \mapsto \mathbb{R}$ be a \mathcal{C}^2 function. The Hessian matrix H_f is a square $n \times n$ matrix whose (i,j)—th entry is defined by $(H_f)_{i,j} = \frac{\partial^2 f}{\partial x_i \partial x_j}$.

Optimization Preliminaries — Recap

- This has been a very brief recap on basic optimization.
- For a refresher, you can take a look at Simon and Blume 1994, Chapters 17-19.
- We will cover the very basics of optimization and implementation in Matlab.
- All numerical optimization methods:
 - Search for feasible choices
 - Generate a sequence of guesses
 - Try to make the sequence **converge** to the true solution.

Pretty similar to root finding algorithms...right?

Optimization in One Dimension

The Simplest Optimization Problem

The simplest optimization problem is unconstrained optimization in one dimension

$$\min_{x \in \mathbb{R}} f(x)$$

where $f : \mathbb{R} \to \mathbb{R}$. Why focusing on one dimension?

- 1. Illustrate techniques in a clear way.
- 2. Many multivariate methods boil down to solving a sequence of one-dimensional problems.

Optimization Methods — Categories

Four general categories for optimization methods:

1. Use derivatives.

- 2. Do not use derivatives.
- 3. Mixed methods.

4. Simulation-based methods.

We will look at basic methods in the first two categories.



Bracketing Method — The Intuition

- Suppose $f : \mathbb{R} \mapsto \mathbb{R}$ is unimodal.
- Let $a < b < c \in \mathbb{R}$ be three points such that

$$f(a), f(c) > f(b) \tag{1}$$

• Then, we know a minimum exists in [a, c].

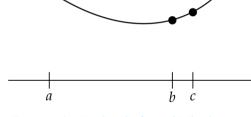
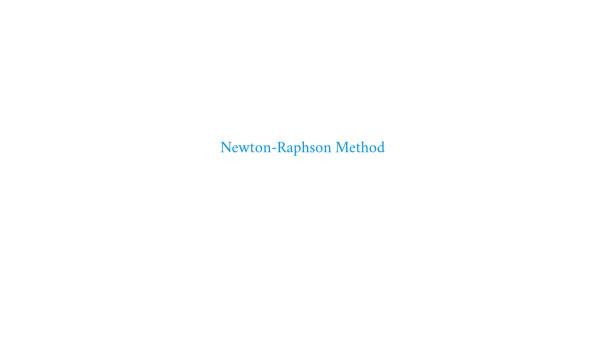


Figure 2: See Kochenderfer and Wheeler 2019

• How to find the optimum?

Bracketing Method — Remarks

- Slow. Similar to bisection.
- The stopping criterion is clear. If the length of the interval [a, c] is sufficiently small, for practical terms, we have found the optimum.
- The method finds a **local minimum**, depending on the starting triplet (a, b, c) the method will converge to one minimum or another. This is a fairly common problem in many methods.
- If we know there is only one solution, the method always converges.
- Note we need three points in each iteration, depending on how costly it is to compute f
 this might be a problem.



Newton-Raphson Method

- Familiar? Yes! It is very closely related to the root finding algorithm!
- Given an initial x_0 , compute a second order Taylor expansion around x_0 :

$$f(x) \approx f(x_0) + f'(x_0)(x - x_0) + \frac{f''(x_0)}{2}(x - x_0)^2$$

• Minimizing this approximation, the FOC we get is

$$f'(x_0) + f''(x_0)(x^* - x_0) = 0$$

solving for x^*

$$x^* = x_0 - \frac{f'(x_0)}{f''(x_0)}$$

• Which is the **same iteration scheme** that we saw previously!

Newton-Raphson Method — Remarks

- Newton-Raphson's method tries to find critical points.
- We **must check** $f''(x^*)$ to check what we have found.
- Problems:
 - Convergence is not ensured.
 - o f''(x) might be difficult to compute. If we rely on finite difference methods, we will be adding errors.
 - Very sensitive to initial conditions.
- From Fernández-Villaverde's slides: If you do not know where you're going, at least go slowly.

Newton-Raphson Method — An Example

Example 1

Apply the Newton-Raphson method to solve

$$\min_{x \in \mathbb{R}^n} f(x) = \frac{x^2}{2} - \log(x^2)$$

- The true solution is $x^* = \pm \sqrt{2} \approx \pm 1.4142...$
- \circ Your choice of starting point x_0 will determine to which minimum you converge.

Newton-Raphson Method — An Example

Solution 1

First, we need the first and second derivatives of f(x) which are

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

We define the functions as anonymous functions as

```
fun = Q(x) (x.^2)./2 - \log(x.^2);

fpr = Q(x) x - (2./x);

fppr = Q(x) 1 + 2./(x.^2);
```

Finally, we need to set up a standard loop checking for terminal conditions and use the iteration scheme

```
x1 = x0 - fpr(x0)./fppr(x0);
```





Unconstrained Optimization in Matlab

- We have covered two basic methods of unconstrained optimization.
- We are going to see now how to solve **(un)constrained optimization** problems using Matlab's routines.

- We start with the unconstrained optimization routine fminunc.
- This solves unconstrained multivariate optimization problems.
- It can use two types of algorithms. Both based on Newton-Raphson methods.
 - BFGS which is a quasi-Newton method.
 - Trust-region methods. Approximates the objective function in a subset, if this
 approximates well the function, it extends the region, otherwise, it contracts the region.

Unconstrained Optimization — fminunc

The basic syntax of fminunc takes as inputs a function fun and an initial point x0

```
[x, fval] = fminunc(fun,x0)
```

The basic output is x^* and $f(x^*)$

- This computes the derivatives numerically
- You can also supply the gradient and the Hessian.
- To supply gradient and Hessian, you need to write it in the function script.

Unconstrained Optimization — fminunc Example

Example 2

Let's solve previous example

$$\min_{x \in \mathbb{R}^n} f(x) = \frac{x^2}{2} - \log(x^2)$$

- The true solution is $x^* = \pm \sqrt{2} \approx \pm 1.4142...$
- Using fminunc the initial choice will crucially determine which optimum we achieve.

Unconstrained Optimization — fminunc Example

Solution 2

Since it is a simple function, we will use an anonymous function to optimize it.

```
fmin = @(x) (x.^2 ./ 2) - log(x.^2)

% Find the minimum
x0 = 1;
[xmin1, fval1] = fminunc(@(x) fmin(x), x0);

% Changing the initial guess, will change the minimum
x0 = -1
[xmin2, fval2] = fminunc(@(x) fmin(x), x0);
```

Example 3

Let's move to multivariate optimization and minimize the Rosenbrock function.

$$f(x_1, x_2) = 100 (x_2 - x_1^2)^2 + (1 - x_1)^2$$

The gradient is

$$\nabla f(x) = \begin{pmatrix} -400(x_2 - x_1^2)x_1 - 2(1 - x_1) \\ 200(x_2 - x_1^2) \end{pmatrix}$$

We will write $f(x_1, x_2)$ as a function script that will give as outputs the value of f and the value of the gradient. Check out nargout and nargin

• The function script

```
function [f, fgrad] = rosenbrock(x)
  % Not necessary, but for clarity we unpack the two inputs
x1 = x(1);
  x2 = x(2);
   % Compute f
   f = 100.*(x2 - x1.^2).^2 + (1 - x_1).^2;
   % Compute gradient (if necessary)
   if nargout > 1
10
       % Notice this is a vector, and the order MATTERS!
11
       fgrad = [-400*(x2 - x1.^2).*x1 - 2*(1 - x1);
12
       200*(x2 - x1.^2);
13
14
  end
15 end
```

• The optimization call

```
1 % Initial point
2 x0 = [14, 4];
3 % Optimization call
4 [x, fval] = fminunc(@(x)rosenbrock(x),x0);
```

- This **does not** tell fminunc that we must use the gradient.
- We need to use an options parser. Check out optimoptions.

- The optimization without gradient yields $f(x_1, x_2) = 1.4045$
- The optimization with gradient yields $f(x_1, x_2) = 1.459 \times 10^{-11}$. Quite a change!
- Note however the initial guess is pretty bad x = (14, 4) when it should be close to (1, 1).
- Improving the guess reduces the differences. Numerical derivatives work well in this
 case.

A derivative free solver for unconstrained optimization is **fminsearch**.



Constrained Optimization

- Matlab offers several options.
- fminbnd Finds a minimum of a single-variable function f(x) in a given interval. The constraints are of the type $a \le x \le b$.
- fmincon It is a multivariate constrained optimization command. It accepts constraints of the type $g(x) \le 0$ and h(x) = 0.
- There are others that you can check out here.

Constrained Optimization — fmincon

- Let's focus on fmincon which is quite general for the type of problems you will most likely encounter.
- The general declaration of the function is

```
x = fmincon(fun, x0, A, b, Aeq, beq, lb, ub, nonlcon, options)
```

- We know options, fun, and x0 from before.
- A and b are a matrix and a vector respectively denoting linear constraints such as $Ax \le b$. Aeq and beq denote Ax = b.
- 1b and ub are lower and upper bounds respectively for each variable (i.e. $a \le x \le b$).

Constrained Optimization — fmincon

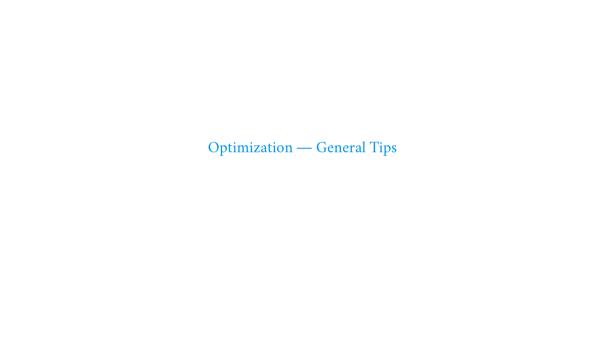
- o nonlcon are the nonlinear constraints that are supplied in function scripts. These should take the form h(x) = 0.
- To optimize the Rosenbrock function in a unit circle, we add the constraint $(x_1 1)^2 + (x_2 1)^2 1 = 0$.
- The arugment nonlcon must be

```
ucircle = @(x) c = (x(1)-1)^2 + (x(2)-1)^2 - 1;

[x, fval] = fmincon(@(x)rosenbrock(x), x0

,[],[],[],[],[],@ucircle);
```

• The empty brackets [] denote empty arguments.



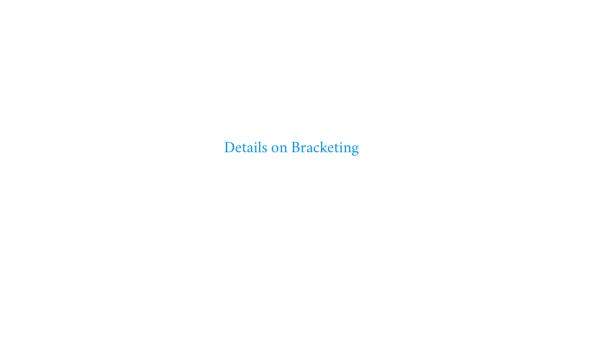
Optimization — General Tips I

- $g(x) \le 0$ is easier to solve than g(x) = 0. Recall tolerances.
- A good initial guess is extremely important when optimizing nonlinear functions.
- o Normalize variables, unit free problems are typically easier.
- o Simplify the computations as much as you can.

Optimization — General Tips II

- Good approaches to solving complex problems:
 - Solve an easier version of the problem to get a good guess.
 - Change of variables.
 - Combine local and global solution methods.

Details on Optimization Methods



Bracketing Method — The Algorithm

1. Define h as the step size, a constant $\alpha > 1$, and a given initial x_0 and compute

$$f(x_0), f(x_0 \pm \alpha h), f(x_0 \pm \alpha^2 h), \dots$$

until we find a triplet satisfying (1). Choose a stopping criterion ε .

- 2. If b a < c b, set d = (b + c)/2, otherwise, d = (a + b)/2. Compute f(d).
- 3. If d < b and f(d) > f(b), replace (a,b,c) with (d,b,c). If d < b and f(d) < f(b), replace (a,b,c) with (a,d,b). If d > b and f(d) < f(b), replace (a,b,c) with (b,d,c). Otherwise, replace (a,b,c) with (a,b,d).
- 4. If $c a < \varepsilon$, stop. Otherwise, go to step 2.

Bracketing Method — An Example

Let's minimize

$$f(x) = \frac{x^2}{2} - x$$

- The function has a global minimum in x = 1.
- Let us divide the code into two blocks:
 - 1. Initial bracketing.
 - 2. Refining given the bracketing.

- 1. Start from guess x_0 and compute $x_1 = x_0 + \alpha h$.
- 2. Evaluate $f(x_0)$ and $f(x_1)$. If $f(x_1) < f(x_0)$ keep increasing until $f(x_2) > f(x_1)$
- 3. Otherwise, change direction and increase interval until $f(x_2) > f(x_0)$.
- 4. Increase α in each step to make the interval larger.

• Start from guess $x_0 = -5$ (why not?) and compute increment.

```
1 % Parameters of bracketing method
h = 1e-2:
alp = 1.1;
5 % Step 1 - Initial bracketing
6 	 x0 = -5:
fx0 = fun(x0);
 x1 = x0 + alp*h; 
fx1 = fun(x1):
10 % If function is increasing in this direction, change
      direction
if fx1 > fx0
h = -h;
13 end
```

• Stablish the outer loop.

• Suppose h < 0

• Suppose h > 0

```
x2 = x1 + alp*h;
fx2 = fun(x2);
% We found the function increases!
if fx2 > fx1
a = x0;
b = x1;
c = x2;
condition = false;
end
```

• If we have not found the function increases, update α

```
alp = alp*2;
```

• Then, simply put all together in nested if-else statements.

Bracketing Method — Refining Bracketing

Initiallize loop

```
while (difference > tol) && (it < maxit)
% Stuff goes here
end</pre>
```

• Define d and compute f(d)

```
% Step 2: define d and compute f(d)
if (b - a) > (c - b)
d = (a + b)/2;
else
d = (b + c)/2;
end
fd = fun(d);
```

Bracketing Method — Refining Bracketing

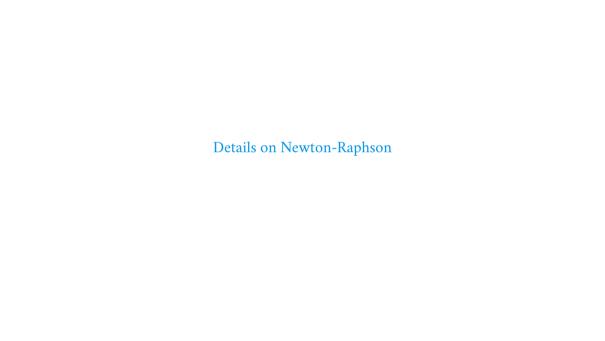
• Refine the interval if d < b

```
1 % Step 3: refine the
  interval
_2 if d < b
if fd > fb
 a1 = d:
b1 = b;
 c1 = c;
7 else
a1 = a;
 b1 = d;
   c1 = b;
10
11 end
12 else
```

• Refine the interval if d > b

```
1 % Step 3: refine the
 interval
2 else
if fb < fd
a1 = a;
b1 = b;
c1 = d;
7 else
a1 = b;
b1 = d;
c1 = c;
11 end
12 end
```

Rename a1 by a, compute (c - a), and update iteration counter.



Newton-Raphson Method — The Algorithm

- 1. Choose initial guess x_0 and stopping parameters δ , $\varepsilon > 0$.
- 2. Use the iteration scheme

$$x_{k+1} = x_k - \frac{f'(x_k)}{f''(x_k)}$$

$$\frac{|x_k - x_{k+1}|}{1 + |x_k|} < \varepsilon \text{ and } |f'(x_k)| < \delta$$

stop. Otherwise, go to step 1.