BUSINESS OPTIMIZATION AND SIMULATION

Module 4

Nonlinear optimization

STRUCTURE OF THE MODULE

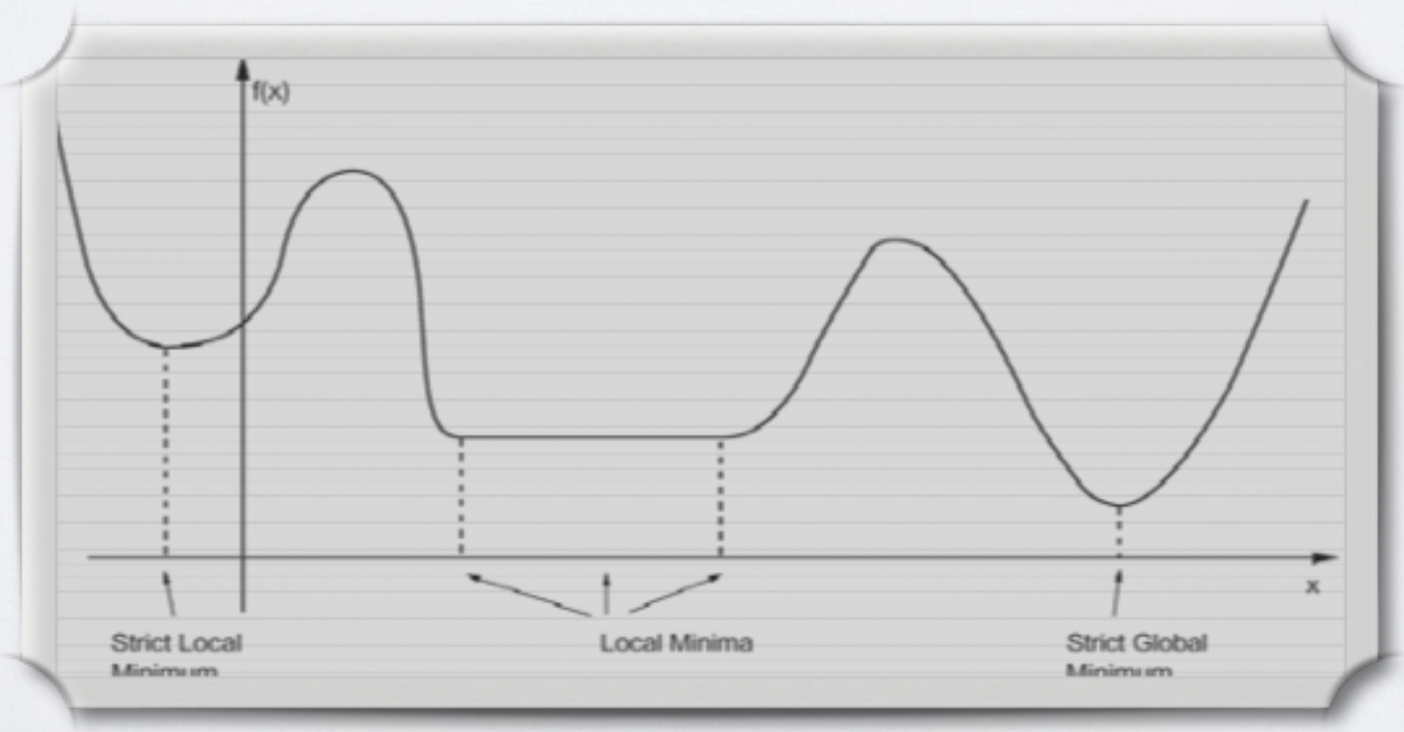
- Sessions:
  - The unconstrained case: formulation, examples
  - Optimality conditions y methods
  - Constrained nonlinear optimization problems
  - Solving constrained problems

UNCONSTRAINED PROBLEMS

- Consider the case of optimization problems with no constraints on the variables and a nonlinear objective function

$$\min_x f(x)$$

  - Local solutions: cannot be improved by values close to the solution
  - Global solutions: the best of all local solutions



OPTIMIZING UNCONSTRAINED PROBLEMS

- Ideal outcome: compute a global solution
  - In general, it is not possible to find one in a reasonable amount of time
- Two alternatives:
  - Accept a quick local solution
  - Attempt to compute a heuristic approximation to a global solution
    - Or one based on deterministic algorithms if the dimension of the problem is not large
  - In general, basic versions of optimization solvers are only able to find local solutions
    - Global solutions only found when some conditions are satisfied:
      - Convexity: local optimizers = global optimizers

OPTIMIZING UNCONSTRAINED PROBLEMS

- Advanced solvers use heuristics to compute approximations to the global optimizers under general conditions
  - Without imposing requirements on differentiability, convexity, etc.
- In practice:
  - If we maximize and the function is concave, we may obtain the maximizer in a reasonable amount of time
  - If we minimize and the function is convex, we may compute the minimizer in a reasonable amount of time

EXAMPLE 1: SMARTPHONE MARKETING

- Description:
  - A company wishes to sell a smartphone to compete with other high-end products
    - It has invested one million euros to develop this product
    - The success of the product will depend on the investment on the marketing campaign and the final price of the phone
  - Two important decisions:
    - a : amount to invest in the marketing campaign
    - p : price of the smartphone

EXAMPLE 1: SMARTPHONE MARKETING

- Description:
  - Formula used by the marketing department to estimate the sales of the new product during the coming year:

$$S = 20000 + 5\sqrt{a} - 60p$$

    - The production cost of the phone is 100 euros/unit
- How could the company maximize its profits for the coming year?

EXAMPLE 1: SMARTPHONE MARKETING

- Model:
  - Profits from sales:

$$\boxed{(20000 + 5\sqrt{a} - 60p)p}$$

  - Total production costs:

$$\boxed{(20000 + 5\sqrt{a} - 60p)100}$$

  - Development costs:

$$\boxed{1000000}$$

  - Marketing costs:

$$\boxed{a}$$

  - Total profit: $\boxed{(20000 + 5\sqrt{a} - 60p)(p - 100) - 1000000 - a}$

EXAMPLE 1: SMARTPHONE MARKETING

- Optimal strategy?
  - Maximize profit
- Constraints?
  - Nonnegative values for the variables
    - Do you need to include them?
- Initial iterate:
  - What happens if the initial values are negative?
  - What if they are large and positive?
  - Small and positive?
- Is the problem convex?
  - Does the problem have more than one local solution?
  - Can you compute the global solution?

EXAMPLE 2: DATA FITTING

- Regression problems
  - How to fit a model to some available data
  - Different approaches: criteria to define what is best
    - Least squares:

$$\boxed{\text{minimize}_\beta \quad \frac{1}{2}\sum_i (y_i - x_i^T\beta)^2}$$

    - Nonlinear least squares:

$$\boxed{\text{minimize}_\beta \quad \frac{1}{2}\sum_i (y_i - F_i(\beta; x_i))^2}$$

    - Minimum absolute deviation:

$$\boxed{\text{minimize}_\beta \quad \sum_i |y_i - x_i^T\beta|}$$

EXAMPLE 2: DATA FITTING

- An specific example: exponential or logit regression
  - For example, it may be of interest to study the relationship between the growth rate of a person and his/her age
    - This relationship is nonlinear
    - The rate is high in the first years of life and then it stabilizes
  - A model could be

$$\text{rate} = \beta_0 + \beta_1 \exp(\beta_2 \text{ age}) + \text{error}$$

UNCONSTRAINED OPTIMALITY CONDITIONS

- When solving practical problems:
  - We may fail to obtain a solution
    - We need good estimates for the initial values of the variables
  - Even if we find a solution, in many cases we have no information about other possible solutions
    - Try with different starting points
- How can we obtain better information about the solutions?
  - Theoretical properties
    - Study the conditions satisfied at a solution
      - Check if they are satisfied
      - Or use them to find other candidate solutions

UNCONSTRAINED OPTIMALITY CONDITIONS

- Unconstrained optimization problem: $\boxed{\text{minimize}_x \quad f(x)}$

- If we wish to maximize the objective function, we could also solve

$$\boxed{\text{minimize}_x \quad -f(x)}$$

- A point (or a decision) x* is a local solution if there is no better alternative close to it

$$\boxed{\exists \epsilon > 0,\ f(x^*) \leq f(x) \quad \forall x : \|x - x^*\| < \epsilon}$$

- A point (or a decision) x* is a global solution if there is no better point (in all the space)

$$\boxed{f(x^*) \leq f(x) \quad \forall x}$$

OPTIMALITY CONDITIONS

- Necessary conditions:
  - Univariate case:

$$f'(x) = 0, \qquad f''(x) \geq 0$$

  - Extension to the multivariate case
    - First-order conditions:
      - If x^* is a local minimizer, then

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

    - Second-order conditions:
      - If x^* is a local minimizer, then

$$\nabla^2 f(x^*) \succeq 0$$

OPTIMALITY CONDITIONS

- Sufficient conditions:
  - Univariate case: $$\boxed{f'(x) = 0, \quad f''(x) > 0}$$
  - Extension to the multivariate case
    - If the following conditions hold at *x**, it is a local minimizer:

$$\boxed{\begin{aligned} \nabla f(x^*) &= 0 \\ \nabla^2 f(x^*) &\succ 0 \end{aligned}}$$

OPTIMALITY CONDITIONS

- Example:
  - Consider the unconstrained problem:

$$\min_x \; f(x), \qquad f(x_1, x_2) \equiv \tfrac{1}{3}x_1^3 + \tfrac{1}{2}x_1^2 + 2x_1x_2 + \tfrac{1}{2}x_2^2 - x_2 + 9$$

  - Necessary conditions:

$$\nabla f(x) = \begin{pmatrix} x_1^2 + x_1 + 2x_2 \\ 2x_1 + x_2 - 1 \end{pmatrix} = 0$$

    - There exist two stationary points (minimizer candidates):

$$x_a = \begin{pmatrix} 1 \\ -1 \end{pmatrix} \quad \text{and} \quad x_b = \begin{pmatrix} 2 \\ -3 \end{pmatrix}$$

OPTIMALITY CONDITIONS

- Example:
  - Sufficient condition

$$\nabla^2 f(x) = \begin{pmatrix} 2x_1 + 1 & 2 \\ 2 & 1 \end{pmatrix} \quad \Rightarrow$$

$$\nabla^2 f(x_a) = \begin{pmatrix} 3 & 2 \\ 2 & 1 \end{pmatrix} \quad \text{and} \quad \nabla^2 f(x_b) = \begin{pmatrix} 5 & 2 \\ 2 & 1 \end{pmatrix}$$

    - Thus,
      - $\nabla^2 f(x_b)$ is positive definite $\Rightarrow$ x_b local minimizer
      - $\nabla^2 f(x_a)$ is indefinite, and x_a is neither a local minimizer nor a local maximizer

EXAMPLE 1: SMARTPHONE MARKETING

- A company wishes to sell a smartphone to compete with other high-end products
  - Optimization model:

$$\boxed{(20000 + 5\sqrt{a} - 60p)(p - 100) - 1000000 - a}$$

  - First-order conditions:

$$\boxed{\nabla f = \begin{pmatrix} 5(p-100)\frac{1}{2\sqrt{a}} - 1 \\ 20000 + 5\sqrt{a} - 120p + 6000 \end{pmatrix} = 0}$$

    - One solution: $a = 106003.245$, $p = 230.233$

  - Second-order condition: Hessian matrix

$$\boxed{\nabla^2 f = \begin{pmatrix} -\frac{5}{4}(p-100)a^{-3/2} & \frac{5}{2}a^{-1/2} \\ \frac{5}{2}a^{-1/2} & -120 \end{pmatrix}}$$

OPTIMALITY CONDITIONS

- What happens if a minimizer does not satisfy the sufficient conditions?

$$f_1(x) = x^3, \quad f_2(x) = x^4, \quad f_3(x) = -x^4$$

- For all these functions it holds that $\nabla f(0) = \nabla^2 f(0) = 0$
- Thus, $x = 0$ is a candidate for a local minimizer in all cases
  - But while f_2 has a local minimum at $x = 0$
  - f_1 has a saddle point at that point
  - f_3 has a local maximum at the point
- The points satisfying these conditions are known as singular points

OPTIMALITY CONDITIONS

- Summary:
  - A point is stationary if $\nabla f(x^*) = 0$
  - For these points:
    - $\nabla^2 f(x^*) > 0 \;\Rightarrow\;$ minimizer
    - $\nabla^2 f(x^*) < 0 \;\Rightarrow\;$ maximizer
    - $\nabla^2 f(x^*)$ indefinite $\;\Rightarrow\;$ saddle point
    - $\nabla^2 f(x^*)$ singular $\;\Rightarrow\;$ any of the above

NEWTON'S METHOD

- Computing a (local) solution:
  - Most algorithms are iterative and descending
    - They compute points with decreasing values of the objective function

$$x_0, x_1, x_2, \ldots \quad \text{such that} \quad f(x_{k+1}) < f(x_k), \;\; k = 0, 1, 2, \ldots$$

      - The main step is to compute a search direction, p_k, to take us from x_k to x_{k+1}
      - Newton's method. The iterations take the form:

$$x_{k+1} = x_k + p_k, \qquad p_k = -(\nabla^2 f(x_k))^{-1} \nabla f(x_k)$$

CONSTRAINED PROBLEMS

- If we allow constraints on the variables, the problem is now

$$\boxed{\begin{aligned} \min_{x} \quad & f(x) \\ \text{s.t.} \quad & c(x) \geq 0 \end{aligned}}$$

- We consider the case when either the objective function or the constraints are nonlinear functions
  - The optimizers may have significantly different properties than those corresponding to unconstrained problems
    - Local solution: belongs to the feasible region and it cannot be improved in a feasible neighborhood of the solution
    - Global solution: belongs to the feasible region, and is the best of all local solutions

CONSTRAINED PROBLEMS

- Solution properties:
  - Differences with unconstrained problems
    - Identifying the active constraints at the solution can be as important as finding points with good gradient values
  - Differences with linear problems
    - Solutions do not need to be at vertices
  - Finding a local solution. Either
    - Transform the problem to one without inequality constraints, or
    - Find the correct active constraints at a solution
      - Efficient trial and error procedures

CONSTRAINED PROBLEMS

- Practical difficulties:
  - Local solutions
    - If the problem is not convex, the solution found by the Solver may only be a local solution (not a global one)
      - Very difficult to check formally
      - Heuristic: You can try to solve the problem from different starting points
  - Ill-defined functions
    - In some cases, the objective or constraint functions may not be defined in all points (square roots, power functions, logarithms)
      - Even if you add constraints to avoid these points, the algorithm may generate infeasible points in that region
      - Heuristic: start close enough to a solution

EXAMPLE 1: PORTFOLIO OPTIMIZATION

- The problem:
  - You have n assets in which you can invest a certain amount of money
    - To simplify the formulation, we will assume this amount to be 1
  - The random variable R_i represents the return rate associated to each asset
  - Your goal is to find the proportions x_i to invest in each of the assets
    - To maximize your return (after one period)
    - And to minimize your investment risk

EXAMPLE 1: PORTFOLIO OPTIMIZATION

- The model:
  - We wish to solve:

$$\begin{array}{ll} \text{maximize}_x & \sum_i R_i x_i \\ \text{subject to} & \sum x_i = 1 \end{array}$$

    - Is this problem well-defined?
    - A well-defined version:

$$\begin{array}{lll} \text{maximize}_x & \sum_i r_i x_i, & r_i \equiv \mathbb{E}[R_i] \\ \text{subject to} & \sum x_i = 1, & x_i \geq 0 \end{array}$$

    - But, is this reasonable?

EXAMPLE 1: PORTFOLIO OPTIMIZATION

- A reasonable version (Markowitz model):

$$\begin{array}{ll} \text{maximize}_x & r^T x - \frac{1}{2}\,\gamma\, x^T S x \\ \text{subject to} & \sum_i x_i = 1 \end{array}$$

where $S = \mathrm{Var}(R)$ and γ is a risk-aversion coefficient

- This model allows the construction of an efficient frontier (policies that, for a given return, have minimum variance)
  - It is a quadratic problem

EXAMPLE 1: PORTFOLIO OPTIMIZATION

- Another reasonable alternative:

$$\begin{array}{ll} \text{minimize}_x & \mathrm{VaR}_\beta \left(-(R_1 x_1 + \cdots + R_n x_n)\right) \\ \text{subject to} & \sum x_i = 1 \end{array}$$

where VaR_β is the Value-at-Risk (percentile) corresponding to a given $0 \leq \beta \leq 1$

- This is a nonlinear, nonconvex problem
  - How can you compute a solution?
  - Advanced techniques of nonlinear optimization

SOLVING CONSTRAINED PROBLEMS

- Studying local solutions for a constrained problem:

$$
\begin{array}{ll}
\text{minimize} & f(x) \\
\text{subject to} & c_{\mathcal{E}}(x) = 0 \\
& c_{\mathcal{I}}(x) \geq 0
\end{array}
$$

- Use the optimality conditions to obtain additional information
  - Form of the optimality conditions in the constrained case

$$
\begin{array}{rr}
\nabla_x f(x^*) - \nabla_x c(x^*)\lambda^* = 0 & \text{stationarity} \\
c_{\mathcal{I}}(x^*) \geq 0 \text{ and } c_{\mathcal{E}}(x^*) = 0 & \text{feasibility} \\
c_{\mathcal{I}}(x^*)^T \lambda_{\mathcal{I}}^* = 0 & \text{complementarity} \\
\lambda_{\mathcal{I}}^* \geq 0 & \text{multiplier sign}
\end{array}
$$

  - We say that x^* is a stationary point if they hold for some λ^*

SOLVING CONSTRAINED PROBLEMS

- The preceding conditions are necessary but not sufficient
  - First-order optimality conditions (no second derivatives)
    - The vector $\boldsymbol{\lambda}$ is known as the vector of Lagrange multipliers
    - Part of the Karush-Kuhn-Tucker (KKT) conditions
  - Second-order condition:

$$L(x, \lambda) \equiv f(x) - \sum_j \lambda_j c_j(x)$$

Z matrix with columns forming a basis for $\{d : \nabla \hat{c}(x) d = 0\}$

where $\hat{c}$ denotes the active constraints, $\hat{c}(x) = 0$

$$Z^T \nabla^2_{xx} L(x, \lambda) Z \succeq 0$$

OPTIMALITY CONDITIONS

- Example:

$$
\begin{aligned}
&\text{minimize}_x \quad f(x) = (x_1 - 3/2)^2 + (x_2 - 5/4)^2 \\
&\text{subject to} \quad c(x) = \begin{pmatrix} 1 - x_1 - x_2 \\ 1 - x_1 + x_2 \\ 1 + x_1 - x_2 \\ 1 + x_1 + x_2 \end{pmatrix} \geq 0
\end{aligned}
$$

- Check that the point (1,0) satisfies the necessary conditions

OPTIMALITY CONDITIONS

- The multiplier vector $\boldsymbol{\lambda}^* = (3/4, 1/4, 0, 0)$ satisfies

$$\begin{pmatrix} -1 \\ -0.5 \end{pmatrix} - \begin{pmatrix} -1 & -1 & 1 & 1 \\ -1 & 1 & -1 & 1 \end{pmatrix} \begin{pmatrix} \lambda_1^* \\ \lambda_2^* \\ \lambda_3^* \\ \lambda_4^* \end{pmatrix} = 0$$

$$\begin{pmatrix} 1 - 1 - 0 \\ 1 - 1 + 0 \\ 1 + 1 - 0 \\ 1 + 1 + 0 \end{pmatrix} \geq 0$$

$$\begin{pmatrix} 0 \\ 0 \\ 2 \\ 2 \end{pmatrix} \circ \begin{pmatrix} \lambda_1^* \\ \lambda_2^* \\ \lambda_3^* \\ \lambda_4^* \end{pmatrix} = 0$$

$$\lambda^* \geq 0$$