Nonlinear Programming

- Basic Notions of Nonlinear Programming
- Necessary Conditions of Optimality
- Interpretation of Lagrange Multipliers
- Minimal Primer on Algorithms for NLPs
- Computation of Derivatives

Contents

Nonlinear Program (NLP)

Problem formulation:

$$\min_{x \in \mathbb{R}^{n_x}} \quad f(x) \quad \text{subject to} \quad \begin{cases} h(x) = 0 \\ g(x) \leq 0 \end{cases}$$

- Objective $f : \mathbb{R}^{n_x} \to \mathbb{R}$;
- Equality constraints $h(x) : \mathbb{R}^{n_x} \to \mathbb{R}^{n_h}$, $h(x) = [h_1(x), ..., h_{n_h}(x)]^\top$;
- Inequality constraints $g(x) : \mathbb{R}^{n_x} \to \mathbb{R}^{n_g}$, $g(x) = [g_1(x), ..., g_{n_g}(x)]^\top$.

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Why discuss NLPs in this course?

- Nonlinear Programming = optimization in Euclidian space
- Optimal Control (OC) = optimization in a function space
- NLP techniques are used to solve Optimal Control Problems (OCP)
  - Discrete-time optimal control $\equiv$ NLP

$$\min_{\{x_k\},\{u_k\}} \sum_{k=0}^{N-1} \ell(x_k, u_k) \quad \text{subject to} \begin{cases} \forall\, k \in \{0, \dots, N-1\} \\ x_{k+1} - f(x_k, u_k) = 0 \\ x_0 - \bar{x} = 0 \\ g(x_k, u_k) \le 0 \end{cases}$$

  - Continuous-time dynamics $\rightarrow$ approximate solution obtained via NLPs

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  - Continuous-time dynamics $\rightarrow$ approximate solution obtained via NLPs

Example – Nonlinear Program

$$\min_{x \in \mathbb{R}^2} (x_1 - 3)^2 + (x_2 - 2)^2$$

subject to

$$g_1(x) = x_1^2 - x_2 - 3 \leq 0$$

$$g_2(x) = x_2 - 1 \leq 0$$

$$g_3(x) = -x_1 \leq 0$$

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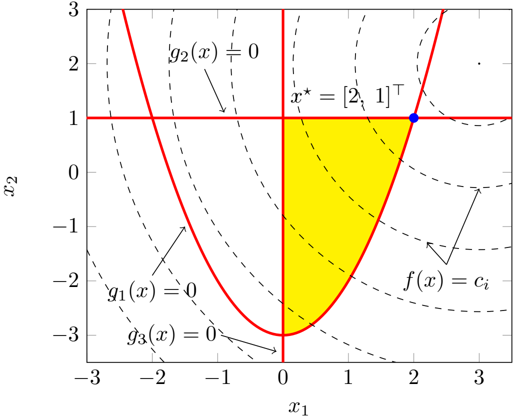

Feasibility

Definition (Feasible Set)

$$\mathbb{S} := \{x \in \mathbb{R}^{n_x} \,|h(x) = 0 \text{ and } g(x) \leq 0\}$$

- Consider NLP

$$\min_{x \in \mathbb{S}} \quad f(x)$$

with feasible set $\mathbb{S} \subseteq \mathbb{R}^{n_x}$.

$$\mathbb{S} \neq \emptyset \Longleftrightarrow \text{NLP is feasible.}$$

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Definition of Optimality – Infimum

Definition (Infimum)

The infimum of a partially ordered set $\mathbb{S}$, denoted as $\inf \mathbb{S}$, provided it exists, is the greatest lower bound for $z \in \mathbb{S}$, i.e., a real number α satisfying

1. $z \geq \alpha, \forall z \in \mathbb{S}$;
2. $\forall \bar{\alpha} > \alpha, \exists z \in \mathbb{S}$ such that $z < \bar{\alpha}$.

Definition of Optimality – Minimum

Definition

A point $x^* \in \mathbb{S}$ is said to be a (global) *minimizer* of f on $\mathbb{S} \subseteq \mathbb{R}^{n_x}$ if

$$f(x) \geq f(x^*), \quad \forall x \in \mathbb{S},$$

and $f(x^*)$ is called (global) minimum of f on $\mathbb{S}$.

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It is said to be a strict (global) minimizer of f on $\mathbb{S} \subseteq \mathbb{R}^{n_x}$ if

$$f(x) > f(x^*), \quad \forall x \in \mathbb{S},\ x \neq x^*,$$

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Definition of Optimality – Local Minimum

ϵ-ball around $\bar{x}$ (or ϵ-neighborhood):

$$\mathbb{B}_\epsilon(\bar{x}) := \{x \in \mathbb{R}^{n_x} \,|\, \|x - \bar{x}\| \leq \epsilon\} \subset \mathbb{R}^{n_x}$$

Definition (Local minimum)

A point $x^* \in \mathbb{S}$ is said to be local minimizer of f, if

$$\exists\, \epsilon > 0,\ \forall\, x \in \mathbb{B}_\epsilon(x^*) \cap \mathbb{S},\quad f(x) \geq f(x^*).$$

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Existence of Minima and Maxima

Theorem (Extreme value theorem)

Let $\mathbb{S}$ *be nonempty and compact and let* f *be continuous on* $\mathbb{S}$*.*

Then, the following problem has a minimizer in $\mathbb{S}$*,*

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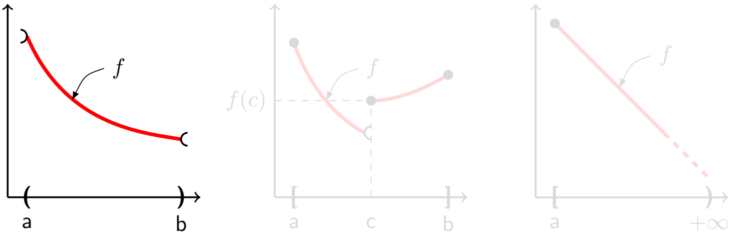

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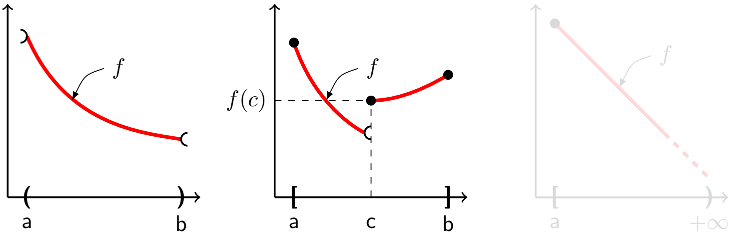

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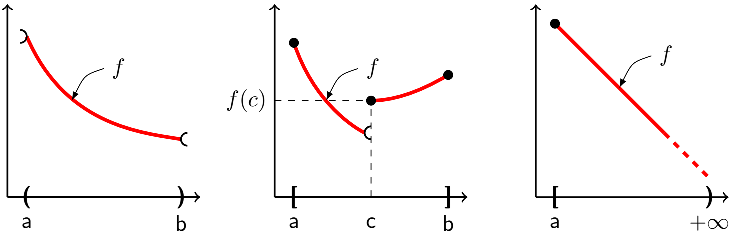

Convex Analysis

Definition (Convex set)

A set $\mathbb{C} \subset \mathbb{R}^{n_x}$ is said to be convex if

$$\forall\, x, y \in \mathbb{C},\ \forall\, \lambda \in [0,1]: \quad z = \lambda x + (1-\lambda) y \in \mathbb{C}.$$

Definition (Convex function)

A function $f : \mathbb{C} \to \mathbb{R}$ is said to be convex on $\mathbb{C}$ if its domain $\mathbb{C}$ is aconvex set and if

$$\forall\, x, y \in \mathbb{C},\ \forall\, \lambda \in [0,1]: \quad f(\lambda x + (1-\lambda) y) \leq \lambda f(x) + (1-\lambda) f(y).$$

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Let $\mathbb{C}$ be a nonempty convex set, and let f be convex on $\mathbb{C}$. NLP

$$\min_{x \in \mathbb{C}} \quad f(x)$$

is called a convex program or convex optimization problem.

Theorem

Let x^* be a local minimizer of a convex program, then x^* is a also a global minimizer.

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Exercises

Given a convex function $f : \mathbb{R}^{n_x} \to \mathbb{R}$ and a non-empty compact set $\mathcal{S} \subseteq \mathbb{R}^{n_x}$. Let $\partial\mathcal{S}$ denote the boundary of the set $\mathcal{S}$.

Which of the following statements are correct? Justify your answers.

a) The minimum of f on $\mathcal{S}$ is unique.

b) The minimizer of f on $\mathcal{S}$ is unique.

c)

$$\arg\min_{x\in\mathcal{S}} f(x) \quad \cap \quad \partial\mathcal{S} \neq \emptyset$$

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Exercises

Given are the following for optimization problems:

a1)

$$\min_{x \in \mathbb{R}} c \cdot x \quad \text{subject to } 0 < x \leq 1$$

with $c \in \mathbb{R}$ arbitrary.

a1) Solution:

- If $c > 0$, the minimizer does not exist.
- If $c = 0$, any x satisfying $0 < x \leq 1$ is a minimizer.
- If $c < 0$, the minimizer is $x = 1$.

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Given are the following for optimization problems:

a2)

$$\inf_{x \in \mathbb{R}} c \cdot x \quad \text{subject to } 0 < x \leq 1$$

with $c \in \mathbb{R}$ arbitrary.

a2) Solution:

- If $c > 0$, the infimum is 0 and $x \to 0$.
- If $c = 0$, the infimum is 0 with any x satisfying $0 < x \leq 1$.
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Contents

Notation: Gradients and Partial Derivatives

Consider a function $f : \mathbb{R}^{n_x} \to \mathbb{R}$,

- Partial derivative (the Jacobian) of f

$$\frac{\partial f}{\partial x} = \begin{bmatrix} \frac{\partial f}{\partial x_1} & \frac{\partial f}{\partial x_2} & \dots & \frac{\partial f}{\partial x_{n_x}} \end{bmatrix} \in \mathbb{R}^{1 \times n_x}$$

- Gradient of f

$$\nabla f = \left(\frac{\partial f}{\partial x} \right)^\top \in \mathbb{R}^{n_x}$$

- $f \in \mathcal{C}^n$: f is n-times continuously differentiable on $\mathbb{R}^{n_x}$

Equality Constrained Problem

Consider NLP

$$\mathscr{P}_{\text{eq}}: \quad \min_{x \in \mathbb{R}^{n_x}} \; f(x) \quad \text{subject to } \; h_i(x) = 0, \; i \in \mathcal{E} := \{1, ..., n_h\}$$

Definition (Regular point)

Consider $\mathbb{S} := \{x \in \mathbb{R}^{n_x} \, | h_i(x) = 0, \; i \in \mathcal{E}\}$ with continuously differentiable $h_i : \mathbb{R}^{n_x} \to \mathbb{R}$, $i \in \mathcal{E}$ on $\mathbb{R}^{n_x}$.

A vector $\bar{x} \in \mathbb{S}$ is said to be a regular point if the gradient $\nabla h_i(\bar{x})$, $i \in \mathcal{E}$ are linearly independent, i.e.,

$$\frac{\partial h}{\partial x} \in \mathbb{R}^{n_h \times n_x} \text{ is full row rank.}$$

This is also called linear independence constraint qualification (LICQ).

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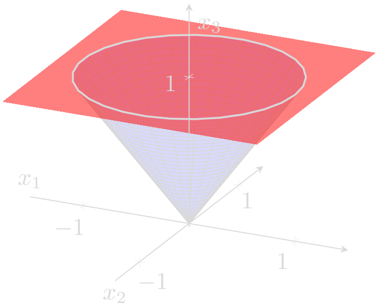
Equality Constraints – Example

$$\mathbb{S} = \left\{ x \in \mathbb{R}^3 : h_i(x) = 0,\ i \in \{1, 2\} \right\}$$

$$h_1(x) = x_3 - (x_1^2 + x_2^2)$$

$$h_2(x) = x_3 - 1$$



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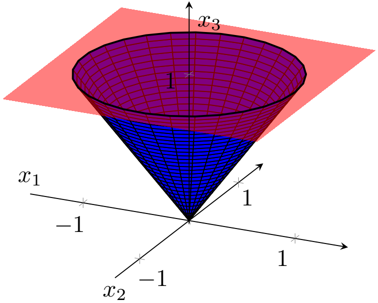

Necessary Condition of Optimality

Theorem (1st order optimality condition)

Consider Problem $\mathscr{P}_{\mathrm{eq}}$ *and let* $f : \mathbb{R}^{n_x} \to \mathbb{R}$, $h_i : \mathbb{R}^{n_x} \to \mathbb{R}$, $i \in \mathcal{E}$ *be continuously differentiable on* $\mathbb{R}^{n_x}$*.*

If a local minimizer x^* *is a regular point of the constraints, then there exists a unique vector* $\lambda^* \in \mathbb{R}^{n_h}$ *such that*

$$\nabla f(x^*) + \nabla h(x^*)\lambda^* = 0.$$

Active Constraints and Active Set

Consider generic NLP

$$\mathscr{P}_{\text{ieq}}: \quad \begin{aligned} &\min_{x \in \mathbb{R}^{n_x}} \quad f(x) \\ &\text{subject to} \begin{cases} h_i(x) = 0, \ i \in \mathcal{E} := \{1, ..., n_h\} \\ g_i(x) \leq 0, \ i \in \mathcal{I} := \{1, ..., n_g\} \end{cases} \end{aligned}$$

Definition (Active Constraint)

A constraint g_i is said to be active at $\bar{x}$, if $g_i(\bar{x}) = 0$.

Definition (Active Set)

The active set $\mathcal{A}(\bar{x})$ at any feasible $\bar{x}$ of $\mathscr{P}_{\text{ineq}}$ is denoted by

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Regular Points of General NLPs

Definition

Let h_i, $i \in \mathcal{E}$ and g_i, $i \in \mathcal{I}$ be continuously differentiable on $\mathbb{R}^{n_x}$ and let

$$\nabla g_{\mathcal{A}}(\bar{x}) := [\nabla g_i(\bar{x})],\ i \in \mathcal{I} \cap \mathcal{A}(\bar{x})$$

with a feasible point $\bar{x}$ of $\mathscr{P}_{\text{ieq}}$. Then, $\bar{x}$ is said to be a regular point if

$$\operatorname{rank}([\nabla h(\bar{x}),\ \nabla g_{\mathcal{A}}(\bar{x})]^{\top}) = |\mathcal{A}(\bar{x})|.$$

Karush-Kuhn-Tucker (KKT) Conditions

Definition (KKT point)

Let f, h_i, $i \in \mathcal{E}$ and g_i, $i \in \mathcal{I}$ be continuously differentiable on $\mathbb{R}^{n_x}$. Consider Problem $\mathscr{P}_{\text{ieq}}$, any pair (x, λ, κ) with $x \in \mathbb{R}^{n_x}$, $\lambda \in \mathbb{R}^{n_h}$ and $\kappa \in \mathbb{R}^{n_g}$ satisfying

$$
\begin{aligned}
\textsc{Stationarity} \quad & 0 = \nabla f(x) + \sum_{i \in \mathcal{E}} \lambda_i \nabla h_i(x) + \sum_{i \in \mathcal{I}} \kappa_i \nabla g_i(x) \\
\textsc{Primal feasibility} \quad & 0 = h_i(x),\ i \in \mathcal{E},\ 0 \geq g_i(x),\ i \in \mathcal{I} \\
\textsc{Dual feasibility} \quad & 0 \leq \kappa_i,\ i \in \mathcal{I} \\
\textsc{Complementarity} \quad & 0 = \kappa_i g_i(x),\ i \in \mathcal{I}
\end{aligned}
$$

is called a KKT point of $\mathscr{P}_{\text{ieq}}$.

KKT Necessary Conditions of Optimality

Theorem

Consider Problem $\mathscr{P}_{\text{ieq}}$ *and let* f, h_i, $i \in \mathcal{E}$ *and* g_i, $i \in \mathcal{I}$ *be continuously differentiable on* $\mathbb{R}^{n_x}$. *If*

- x^* *is a (local) minimizer of* $\mathscr{P}_{\text{ieq}}$ *and*
- x^* *is a regular point,*

then there exist $\lambda^* \in \mathbb{R}^{n_h}$ *and* $\kappa^* \in \mathbb{R}^{n_g}$ *such that* $(x^*, \lambda^*, \kappa^*)$ *is a KKT point of* $\mathscr{P}_{\text{ieq}}$.

Exercises

Consider NLP

$$\min_{x \in \mathbb{R}^2} \quad \left(x_1 - \frac{3}{2}\right)^2 + (x_2 - t)^4 \quad \text{subject to} \begin{cases} x_1 + x_2 - 1 \leq 0 \\ x_1 - x_2 - 1 \leq 0 \\ -x_1 + x_2 - 1 \leq 0 \\ -x_1 - x_2 - 1 \leq 0 \end{cases}$$

For what value of t does $x^* = [1, 0]^\top$ satisfy the KKT condition?

Exercises

Consider NLP

$$\min_{x \in \mathbb{R}^2} \quad -2x_1 + x_2 \quad \text{subject to} \begin{cases} x_2 - (1 - x_1)^3 \leq 0 \\ 1 - 0.25x_1^2 - x_2 \leq 0 \end{cases}$$

the optimal solution is $x^* = [0, 1]^\top$, questions:

a) Is x^* a regular point?

b) Are the KKT conidtions satisfied?

Contents

Equality Constrained NLP

Consider NLP

$$\min_{x \in \mathbb{R}^{n_x}} \quad f(x) \quad \text{subject to} \;\; h(x) = 0$$

Necessary condition of optimality:

$$\nabla f(x^*) + \nabla h(x^*)\lambda^* = 0$$
$$h(x^*) = 0$$

Question: how does the minimum $f(x^*)$ change for varying constraints $h(x) = c$?

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Interpretation of Lagrangian Multipliers

Perturbed problem

$$\mathscr{P}_c: \qquad \min_{x \in \mathbb{R}^{n_x}} \quad f(x) \quad \text{subject to} \quad h(x) = c$$

Assumption

For each c, $\mathscr{P}_c$ has a unique regular solution, i.e.,

$$\xi^\star(c) = \arg\min_x \quad f(x) \quad \textit{subject to} \quad h(x) = c$$

$$\phi^\star(c) = \min_x \quad f(x) \quad \textit{subject to} \quad h(x) = c$$

with $\xi^\star(0) = x^*$ and $\phi^\star(0) = f(x^*)$.

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$$h(\xi^\star(c)) = c \;\Rightarrow\; \nabla_x h(\xi^\star(c))^\top \nabla_c \xi^\star(c)^\top = \mathrm{I}$$

$$\begin{aligned}
\nabla_c \phi^\star(c)\Big|_{c=0} &= \nabla_c \xi^\star(0)^\top \nabla_x f(x^*) \\
&= -\underbrace{\nabla_c \xi^\star(0)^\top \nabla_x h(\xi^\star(0))^\top}_{\mathrm{I}} \lambda^* \\
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Interpretation of Lagrangian Multipliers

- The Lagrange multiplier λ^* can be interpreted as the sensitivity of the optimal objective function with respect to changes in the constraint $h(x) = 0$.
- In Economics Lagrange multipliers are used to characterize *marginal values* or *shadow prices*.
- Can be extended to general NLPs with inequality constraints $g(x) \leq c$: multipliers $\kappa^* \approx$ sensitivity of $f(x^*)$ with respect to c.
- Inactive inequality constraints $\kappa_i^* = 0$, $i \in \mathcal{I} \backslash (\mathcal{I} \cap \mathcal{A}(x^*)) \Rightarrow$ no change of optimum for small perturbations.
- Active inequality constraints $\kappa_i^* \geq 0$, $i \in \mathcal{I} \cap \mathcal{A}(x^*) \Rightarrow$ enlarged feasible region, optimal cost cannot increase.

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Algorithm Concepts

Algorithm:

- Given an initial point x^0 compute a sequence $\{x^k\}$ by repeated application of an algorithmic rule.
- Objective: make $\{x^k\}$ converge to a point $\bar{x}$.

Why do we talk about algorithms for NLPs?

- Solvers usually require initial guess and termination criteria $\Rightarrow$ basic understanding of solution algorithms necessary to use solvers.
- Solvers often terminate prematurely $\Rightarrow$ understand and diagnose reasons?

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Global and Local Convergence

Definition (Global convergence)

An algorithm is said to be *globally convergent* if, for any initial point x^0, it generates a sequence of points that converges to a point $\bar{x}$ in the solution set.

Definition (Local convergence)

An algorithm is said to be *locally convergent* if there exists $\rho > 0$ such that for any initial point x^0 with $\|x^0 - \bar{x}\| < \rho$, it generates a sequence of points that converges to a point $\bar{x}$ in the solution set.

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Order of Convergence

Definition

The *order of convergence* of a sequence $\{x^k\}$, with $\lim_{k \to \infty} x^k = \bar{x}$, is the largest non-negative number p such that

$$\lim_{k \to \infty} \frac{\|x^{k+1} - \bar{x}\|}{\|x^k - \bar{x}\|^p} = \beta < \infty.$$

- $p = 1$ and $\beta < 1 \Rightarrow$ linear convergence
- $p = 1$ and $\beta = 0 \Rightarrow$ superlinear convergence
- $p = 1$ and $\beta = 1 \Rightarrow$ sublinear convergence
- $p = 2 \Rightarrow$ quadratic convergence

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Example:

$$x^k = 1 + 0.5^k$$

$$x^k = 1 + k^{-k}$$

$$x^k = 1 + 0.5^{2^k}$$

Newton's Methd for Nonlinear Equations

Given a function $F : \mathbb{R}^n \to \mathbb{R}^n$, search for solutions of the nonlinear equation

$$F(x) = 0 \text{ with } F \in \mathbb{C}^1.$$

Main idea:

- Start with x_0 and solve linear equations

$$F(x^k) + M(x^k)(x^{k+1} - x^k) = 0,\ k \in \{1, 2, \ldots\}.$$

- Matrix $M(x)_k \in \mathbb{R}^{n_x \times n_x}$ chosen in such a way that

$$F(x^k) + M(x^k)(x - x^k) \approx F(x)$$

  is an approximation of F.

- $M(x^k) = \partial F(x^k)$ corresponds to the so called Newton method.

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Newton's Method for Nonlinear Equations

If $M(x^k)$ is invertible, the method can be written in the form

$$x^{k+1} = x^k - M(x^k)^{-1} F(x^k),\ k \in \{1, 2, ...\}.$$

- In practice, we usually work with approximations $M(x^k) \approx \partial F(x^k)$.
- If $M(x^k)$ is independent of x^k, we only need to decompose M once (e.g., using LR or QR decomposition).
- Some methods try to update M at every step without re-computing the Jacobian (e.g., BFGS update).

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Scaling Properties of Newton's Method

- $F(x^*) = 0 \Rightarrow S \cdot F(x^*) = 0$ with $S \in \mathbb{R}^{n_x \times n_x}$ any (invertible) scaling matrix.
- Applying Newton's method to solve scaled equation

$$\widetilde{F}(x) = S \cdot F(x) = 0$$

  yields iteration $x^{k+1} = x^k - M(x^k)^{-1} S \cdot F(x^k)$.
- Using exact Jacobian $M(x^k) = \partial \widetilde{F}(x^k)$, we have

$$x^{k+1} = x^k - \partial F(x^k)^{-1} F(x^k).$$

- Newton's methods with exact Jacobians is invariant under scaling.

Local Convergence of Newton's Method

Assumption

- *There exists a point x^* with $F(x^*) = 0$.*
- *The initial point x^0 is already in a small neighborhood of x^*.*
- *Matrix $M(x^k)^{-1}\partial F(x)$ is Lipschitz continuous w.r.t. x in a neighborhood of x^* with constant $\omega \geq 0$.*

The basic idea is to estimate the distance of the iterates to x^*:

$$
\begin{aligned}
& \left\| x^{k+1} - x^* \right\| = \left\| x^k - x^* - M(x^k)^{-1} F(x^k) \right\| \\
= \quad & \left\| x^k - x^* - M(x^k)^{-1} \int_0^1 \partial F(x^* + s(x^k - x^*))(x^k - x^*) ds \right\| \\
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Local Convergence of Newton's Method

In summary, we have the estimate

$$\left\|x^{k+1} - x^*\right\| \leq \eta \left\|x^k - x^*\right\| + \frac{\omega}{2} \left\|x^k - x^*\right\|^2$$

as long as $\left\|\mathrm{I} - M(x^k)^{-1} \partial F(x^k)\right\| \leq \eta$. Here, η can be interpreted as a bound on the accuracy of the Jacobian approximation M.

If we have $\eta < 1$ and $\|x^0 - x^*\| < \frac{2}{\omega}(1 - \eta)$, the iterates contract and we have

$$\lim_{k \to \infty} x^k \to x^*.$$

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Convergence of Newton's Method

The convergence rate estimate

$$\left\|x^{k+1} - x^*\right\| \leq \eta \left\|x^k - x^*\right\| + \frac{\omega}{2} \left\|x^k - x^*\right\|^2$$

implies that

- if we have $0 < \eta < 1$, the convergence rate is linear.
- if we choose $M(x^k) = \partial F(x^k)$, we have $\eta = 0$ and

$$\left\|x^{k+1} - x^*\right\| \leq \frac{\omega}{2} \left\|x^k - x^*\right\|^2 .$$

  In this case, the convergence rate is quadratic.

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Exercises

Let scalar function $f : \mathbb{R} \to \mathbb{R}$ be three times continuously differentiable with bounded third-order derivative. The first and second derivative of f are denoted by f' and f'', respectively. We additionally assume:

- $f(x^*) = 0$ and $f''(x^*) = 0$ at a point $x^* \in \mathbb{R}$;
- $f'(x^*) \neq 0$.

Prove that the iterates of the exact Newton method, $x^{k+1} = x^k - \frac{f(x^k)}{f'(x^k)}$, converge locally with cubic convergence rate, i.e.,

$$\left|x^{k+1} - x^*\right| \leq \gamma \left|x^k - x^*\right|^3, \;\; \gamma < \infty.$$

Exercises

Solution:

1. Locally, we have

$$\left|x^{k+1}-x^*\right| = \left|x^k - x^* - \frac{f(x^k)}{f'(x^k)}\right| = \left|x^k - x^* - \frac{1}{f'(x^k)}\int_{x^*}^{x^k} f'(z)dz\right|$$

2. For the integral above, we can substitute the Taylor expansion,

$$\begin{aligned} f'(z) =& f'(x^k) + f''(x^k)(z-x^k) + \mathbf{O}(|z-x^k|^2) \\ =& f'(x^k) + \mathbf{O}(|x^k-x^*||z-x^k|) + \mathbf{O}(|z-x^k|^2) \end{aligned}$$

3. Thus, we have

$$\begin{aligned} \left|x^{k+1}-x^*\right| \le& \left|x^k - x^* - \frac{1}{f'(x^k)}\int_{x^*}^{x^k} f'(x^k)dz\right| + \mathbf{O}(|x^k-x^*|^3) \\ =& \mathbf{O}(|x^k-x^*|^3) \end{aligned}$$

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Newton's Method for Unconstrained Optimization

Problem formulation:

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

Remark

- *If f is twice Lipschitz-continuously differentiable, a minimizer can be founded by applying Newton's method to*

$$\nabla f(x) = 0.$$

- *If a solution x^* satisfies $\nabla^2 f(x) \succ 0$, it must a local minimizer.*

Newton's Method for Unconstrained Optimization

Newton-type iteration for unconstrained optimization problem

$$x^{k+1} = x^k - M(x^k)^{-1}\nabla f(x^k)$$

with $M(x^k) \approx \nabla^2 f(x^k)$ a suitable Hessian approximation.

- In practice, we often choose a symmetric M.
- If $M(x^k)$ is symmetric and positive definite, the iterate x^{k+1} is the minimizer of the quadratic function

  $$\min_{x^{k+1}} \; f(x^k) + \nabla f(x^k)^\top (x^{k+1} - x^k) + \frac{1}{2}(x^{k+1} - x^k)^\top M(x^k)(x^{k+1} - x^k),$$

  which can be interpreted as a quadratic model of f.

Line Search Methods

So far, we have only analyzed the local convergence properties of Newton-type methods. If we start far from a local solution, Newton type methods are often take "too big" steps and are divergent.

One way to fix this problem is to first compute a step-direction by

$$\Delta x^k = -M(x^k)^{-1} \nabla f(x^k)$$

and update the iterate as

$$x^{k+1} = x^k + \alpha^k \Delta x^k .$$

Here, $\alpha^k \in (0, 1]$ is a so-called step size, which is found by (approximately) solving the scalar optimization problem

$$\min_{\alpha^k \in (0,1]} \quad f(x^k + \alpha^k \Delta x^k).$$

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and update the iterate as

$$x^{k+1} = x^k + \alpha^k \Delta x^k .$$

Here, $\alpha^k \in (0, 1]$ is a so-called step size, which is found by (approximately) solving the scalar optimization problem

$$\min_{\alpha^k \in (0,1]} \quad f(x^k + \alpha^k \Delta x^k).$$

Line Search Methods

So far, we have only analyzed the local convergence properties of Newton-type methods. If we start far from a local solution, Newton type methods are often take "too big" steps and are divergent.

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Armijo Linear Search Conditions

In practice the line search optimization

$$\min_{\alpha^k \in (0,1]} \quad f(x^k + \alpha^k \Delta x^k).$$

is not solved exactly (too expensive), but only approximately.

One way to implement this is by using back-tracking until the Armijo condition

$$f(x^k + \alpha^k \Delta x^k) \leq f(x^k) + c \cdot \alpha^k \quad \underbrace{\nabla f(x^k)^\top \Delta x^k}_{\text{DIRECTIONAL DERIVATIVE}}$$

for a constant $c \ll 1$ is satisfied. This condition ensures that the line search parameter is not excessively large, although it is not sufficient to prove convergence in general.

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Quasi-Newton Methods – Preliminaries

One way to represent invertible matrices is by considering matrices of the form

$$A = \underbrace{B}_{\text{EASY-TO-STORE}} + \underbrace{UV^\top}_{\text{LOW RANK}}$$

with $B \in \mathbb{R}^{n\times n}$ and $U, V \in \mathbb{R}^{n\times m}$, $m \ll n$.

If B is easy to invert or B^{-1} is already known, we have A^{-1} as

$$(B + UV)^{-1} = B^{-1} - B^{-1}U(I + V^\top B^{-1}U)^{-1}V^\top B^{-1},$$

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Quasi-Newton Methods – Broyden's Updates

The Newton-type iterates

$$x^k = x^{k-1} - M(x^{k-1})^{-1}\nabla f(x^{k-1}),\ x^{k+1} = x^k - M(x^k)^{-1}\nabla f(x^k), \ldots$$

We have to compute the gradient ∇f at each iteration such that we can obtain the directional estimate

$$\nabla^2 f(x^{k+1})(x^{k+1} - x^k) \approx \nabla f(x^{k+1}) - \nabla f(x^k).$$

Questions: can we use this relation to improve our next Hessian approximation $M(x^{k+1}) \approx \nabla^2 f(x^{k+1})$?

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Define $d^k = x^{k+1} - x^k$ and $y^k = \nabla f(x^{k+1}) - \nabla f(x^k)$, the relation

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motivates to improve our current estimate of $\nabla^2 f$ constructing M^+ by solving

$$\min_{M^+} \ \frac{1}{2} \left\| M^+ - M(x^k) \right\|_F^2 \quad \text{subject to} \ M^+ d^k = y^k$$

with $\| \cdot \|_F$ the Frobenius norms ($\|X\|_F^2 = \mathrm{Tr}(XX^\top)$).

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$$M^+ = M(x^k) - \frac{(M(x^k)d^k - y^k)(d^k)^\top}{\|d^k\|_2^2}$$

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$$(M^+)^{-1} = M(x^k)^{-1} + \frac{(d^k - M(x^k)^{-1}y^k)(d^k)^\top M(x^k)^{-1}}{(d^k)^\top M(x^k)^{-1}y^k}$$

Remarks:

- both update are rank-1 update.
- we don't need to compute any second order derivatives.
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But: M^+ may be non-symmetric even if $M(x^k)$ was symmetric.

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Quasi-Newton Methods – BFGS Updates

Broyden-Fletcher-Goldfarb-Shanno Updates

The idea is to maintain the symmetry of the updates by solving

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with $\left\|M^+ - M(x^k)\right\|^2 := \left\|W^{\frac{1}{2}}(M^+ - M(x^k))W^{\frac{1}{2}}\right\|_{\mathrm{F}}^2 =$

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Here, the norm is (mainly for computational reasons) a weighted Frobenius norm by W any symmetric positive definite weighting matrix satisfying

$$Wy^k = d^k.$$

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Algorithms for Constrained NLPs

Nonlinear program

$$\min_{x \in \mathbb{R}^{n_x}} \quad f(x) \quad \text{subject to} \begin{cases} h_i(x) = 0, \ i \in \mathcal{E} := \{1, ..., n_h\} \\ g_i(x) \leq 0, \ i \in \mathcal{I} := \{1, ..., n_g\} \end{cases}$$

Convert into unconstrained problem:

- Penalty function method;
- Interior point method.

Solve necessary conditions of optimality:

- Newton-like methods;
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Exterior Penalty Function Methods

Penalty function

$$\Phi(x) = \sum_{i \in \mathcal{E}} \psi(h_i(x)) + \sum_{i \in \mathcal{I}} \phi(g_i(x)),\ \psi, \phi \in \mathbb{C}^0$$

$$\text{with } \begin{cases} \psi(z) = 0 & \text{if } z = 0 \\ \psi(z) > 0 & \text{else} \end{cases} \text{ and } \begin{cases} \phi(z) = 0 & \text{if } z \leq 0 \\ \phi(z) > 0 & \text{else} \end{cases}$$

Typical choice: $\psi(z) = |z|^p$, $p \in \mathbb{N}_{>0}$ and $\phi(z) = (\max\{0, z\})^p$.

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Unconstrained optimization problem

$$\min_{x \in \mathbb{R}^{n_x}} \quad f(x) + \mu \cdot \Phi(x) \;\; \text{with} \;\; \mu > 0.$$

Remark

- *recovering solution of the original problem $\mu \to \infty$.*
- *ill-conditioned for large μ.*

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Sequential Unconstrained Optimization

Main idea:

- Start at an initial x^0, update x^k by solving

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- *Iterates x^k are typically infeasible.*
- *Remedy? $\rightarrow$ interior point methods.*

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Barrier Method

Inequality constrained NLPs

$$\min_{x \in \mathbb{R}^{n_x}} \quad f(x) \quad \text{subject to} \ \ g_i(x) \leq 0, \ i \in \mathcal{I} := \{1, ..., n_g\}$$

Barrier function

$$b(x) = \sum_{i \in \mathcal{I}} \phi(g_i(x)) \ \text{ with} \begin{cases} \phi(z) \geq 0 \ \text{ if } z \leq 0 \\ \lim_{z \to 0^-} = \infty \end{cases}$$

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KKT condition:

$$\begin{aligned} \nabla f(x) + \nabla g(x)\kappa &= 0 \\ g(x) &\leq 0 \\ \kappa &\geq 0 \\ \kappa_i \cdot g_i(x) &= 0, \; i \in \mathcal{I} \end{aligned}$$

Perturbed KKT condition:

$$\begin{aligned} \nabla f(x) + \nabla g(x)\kappa &= 0 \\ \kappa_i \cdot g_i(x) &= \mu, \; i \in \mathcal{I} \end{aligned}$$

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Interior Point Method

Main Idea:

- Apply Newton's method to deal with nonlinear equations

$$F_\mu(x,\kappa) = \begin{bmatrix} \nabla f(x) + \nabla g(x)\kappa \\ \mathrm{diag}(\kappa) g(x) - \mu \cdot \mathbf{1}_{n_g} \end{bmatrix} = 0$$

- Update μ with $\mu \to 0$, ref. [Chapter 19.3, NW06]
- Linear search is necessary, ref. [Chapter 19.4, NW06]

Remark

Log-barrier based unconstrained problem $\min_x \quad f(x) + \mu \cdot b(x)$ *has KKT conditions equivalent to the perturbed KKT, i.e.,*

$$\nabla f(x) + \sum_{i \in \mathcal{I}} \frac{\mu}{g_i(x)} \nabla g_i(x) = 0 \;\Rightarrow\; \kappa_i = \frac{\mu}{g_i(x)}$$

[NW06] J. Nocedal and S. Wright, Numerical optimization. 2006.

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Sequential Quadratic Programming (SQP)

Equality constrained NLP

$$\min_{x\in\mathbb{R}^{n_x}} \quad f(x) \quad \text{subject to} \;\; h(x) = 0$$

1st order optimality conditions

$$F(y) = \begin{bmatrix} \nabla f(x) + \nabla h(x)\lambda \\ h(x) \end{bmatrix} = 0 \;\; \text{with} \;\; y = \begin{pmatrix} x \\ \lambda \end{pmatrix}$$

Main idea: applying Newton's method to solve $F(y) = 0$, i.e.,

$$\begin{bmatrix} H(x) & A(x)^\top \\ A(x) & \end{bmatrix} \begin{bmatrix} \Delta x \\ \Delta \lambda \end{bmatrix} = - \begin{bmatrix} \nabla f(x) + \nabla h(x)\lambda \\ h(x) \end{bmatrix}$$

with $H(x) = \nabla_{xx} \left\{ f(x) + \lambda^\top h(x) \right\}$ and $A = \nabla h(x)^\top$.

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$$F(y) = \begin{bmatrix} \nabla f(x) + \nabla h(x)\lambda \\ h(x) \end{bmatrix} = 0 \;\; \text{with} \;\; y = \begin{pmatrix} x \\ \lambda \end{pmatrix}$$

Main idea: applying Newton's method to solve $F(y) = 0$, i.e.,

$$\begin{bmatrix} H(x) & A(x)^\top \\ A(x) & \end{bmatrix} \begin{bmatrix} \Delta x \\ \Delta \lambda \end{bmatrix} = - \begin{bmatrix} \nabla f(x) + \nabla h(x)\lambda \\ h(x) \end{bmatrix}$$

with $H(x) = \nabla_{xx} \left\{ f(x) + \lambda^\top h(x) \right\}$ and $A = \nabla h(x)^\top$.

Sequential Quadratic Programming (SQP)

Equality constrained NLP

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1st order optimality conditions

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Globalization

How do we measure progress towards a solution?

Recall: in unconstrained minimization, the main idea was to accept the next iterate x^{k+1} if $f(x^{k+1})$ is sufficiently smaller than $f(x^k)$.

In equality constrained optimization we need to measure two things:

1. The objective value $f(x)$ and
2. the constraint violation $\|h(x)\|$

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2. the constraint violation $\|h(x)\|$

L1-Penalty Functions

One way to measure progress towards a solution is to introduce the L1-penalty function

$$\Psi(x) = f(x) + \sum_{i \in \mathcal{E}} \bar{\lambda}_i |h_i(x)|$$

with $\bar{\lambda}_i$ being sufficiently large constants.

An important property of the function $\Psi(x)$ is that (under mild conditions) we have

$$\Psi(x^*) = f(x^*) \quad \text{but also} \quad \Psi(x) \geq f(x)$$

for all $x \in \mathbb{X}$ within a compact subset $\mathbb{X} \subseteq \mathbb{R}^{n_x}$ and $\bar{\lambda}_i$ are sufficiently large

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Armijo Line Search Conditions

Similar to unconstrained optimization, the line search parameter α^k can be found by using back-tracking until the Armijo condition

$$\Psi(x^k + \alpha^k \Delta x^k) \leq \Psi(x^k) + c \cdot \alpha^k D(\Psi(x^k), \Delta x^k)$$

for a constant $c \ll 1$ is satisfied. Here, $D(\Psi(x^k), \Delta x^k)$ denotes the directional derivative

$$D(\Psi(x^k), \Delta x^k) = \left\| h(x^k) + \nabla h(x^k)^\top \Delta x^k \right\|_1$$

SQP for Equality Constrained NLP

1. Choose initial guesses $x^0 \in \mathbb{R}^{n_x}$ and $\lambda^0 \in \mathbb{R}^{n_h}$, tolerance $\epsilon > 0$.
2. **Repeat:**

   2.1 Choose Hessian approximation $M(x^k) \approx \nabla_{xx} \left\{ f(x^k) + (\lambda^k)^\top h(x^k) \right\}$ and $A(x^k) = \nabla h(x^k)$.

   2.2 Solve subQP

$$\begin{aligned} \min_{\Delta x^k \in \mathbb{R}^{n_x}} \quad & \frac{1}{2}(\Delta x^k)^\top H(x^k) \Delta x^k + \nabla f(x^k)^\top \Delta x^k \\ \text{subject to} \quad & h(x^k) + A(x^k)^\top \Delta x^k = 0 \qquad \mid \lambda^{\mathrm{QP}} \end{aligned}$$

   2.3 Terminate if $\left| \nabla f(x^k)^\top \Delta x^k \right| + \sum_{i \in \mathcal{E}} |\lambda_i| \, |h_i(x)| \leq \epsilon$.

   2.4 Choose a line-search parameter $\alpha^k \in (0, 1]$ and set $x^{k+1} = x^k + \alpha^k \Delta x^k$ and $\lambda^{k+1} = \lambda^k + \alpha^k (\lambda^{\mathrm{QP}} - \lambda^k)$.

SQP for Inequality Constrained NLP

- Include linearized inequality constraints in subQPs, i.e.,

$$\begin{aligned}\min_{\Delta x^k \in \mathbb{R}^{n_x}} \quad & \frac{1}{2}(\Delta x^k)^\top H(x^k)\Delta x^k + \nabla f(x^k)^\top \Delta x^k \\ \text{subject to} \quad & h(x^k) + A(x^k)^\top \Delta x^k = 0 \\ & g(x^k) + B(x^k)^\top \Delta x^k \leq 0\end{aligned}$$

  with $B(x^k) = \nabla g(x^k)$.

- Use the following L1-penalty function for linear search

$$\Psi(x) = f(x) + \sum_{i\in\mathcal{E}} |\bar{\lambda}_i||h_i(x)| + \sum_{i\in\mathcal{I}} |\bar{\kappa}_i|(\max\{0, g_i(x)\})$$

  with sufficiently large $\bar{\lambda}_i$ and $\bar{\kappa}_i$.

Numerical Implementation

- SubQP infeasible $\Rightarrow$ relax the constraints
- Hessian regularization, e.g., $M(x^k) = \nabla_{xx}\{f(x) + \lambda^\top h(x)\} + \sigma \mathrm{I} \succ 0$.
- Rank-deficient constraints $\Rightarrow$ reformulated the constraints, e.g.,

$$\min_x \ x \quad \text{subject to} \ x^2 = 0$$

  with $x^* = 0$ but we cannot find a λ^* since

$$0 = \nabla f(x^*) + \nabla h(x^*)\lambda^* = 1$$

  is wrong. Replacing $x^2 = 0$ by $x = 0$ can avoid this degeneracy.
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Motivation

$$\min_{x \in \mathbb{R}^{n_x}} \quad f(x) \quad \text{subject to} \begin{cases} h(x) = 0 \\ g(x) \leq 0 \end{cases}$$

- Derivatives of objectives and constraints (gradients);
- Sensitivities of ODE or DAEs (needed later);
- Jacobians to solve implicit equations (e.g. implicit ODEs, DAEs, ...).

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- Numerical differentiation
- Algorithmic differentiation

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Numerical Differentiation – Finite Differences

The derivative of a twice continuously differentiable function $f : \mathbb{R} \to \mathbb{R}$ can be approximated by finite differences:

$$\frac{df(x)}{dx} \approx \frac{f(x+h) - f(x)}{h}$$

- The mathematical approximation error, given by

$$\left| \frac{f(x+h) - f(x)}{h} - \frac{df(x)}{dx} \right| \approx \frac{h}{2} \left| \frac{d^2 f(x)}{dx^2} \right| = \mathbf{O}(h)$$

  tends to 0 with $h \to 0$.

- How to choose increment h?

$$h = \sqrt{\text{eps}} \quad \Rightarrow \quad \textbf{Limited accuracy} \sqrt{\text{eps}}$$

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In order to reduce the mathematical approximation error, we can use central differences:

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$$\frac{df(x)}{dx} \approx \frac{\mathrm{Im}(f(x + i \cdot h))}{h}, \; i^2 = -1.$$

- The mathematical approximation error is same as central differences, i.e.,

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  but the computation is cheap.

- Sketch Proof:

$$f(x + i \cdot h) = f(x) + i \cdot \frac{df(x)}{dx} h - \frac{1}{2} \frac{d^2 f(x)}{dx^2} h^2 - \mathbf{O}(i \cdot h^3)$$

- Easy to implement in `Matlab`

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Factorable Functions

Many (but not all) functions of our interest can be composed into a finite list of atom operations from a given library L, e.g., $L = \{+, -, *, \sin, \cos, \exp, ...\}$.

Example

- The function $f(x) = \sin(x_1 * x_2) + \cos(x_1)$ will (internally) be evaluated as

$$\begin{aligned} x_3 &= x_1 * x_2 \\ x_4 &= \sin(x_3) \\ x_5 &= \cos(x_1) \\ x_6 &= x_4 + x_5 \\ f(x) &= x_6 \end{aligned}$$

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Consider a given factorable function $f : \mathbb{R}^n \to \mathbb{R}^m$, we define

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- augmented elementary function by $\Phi_i : \mathbb{R}^{n+i} \to \mathbb{R}^{n+i+1}$

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Algorithmic Differentiation – Forward Mode

- Recall: the representation of a factorable function $f : \mathbb{R}^n \to \mathbb{R}^m$,

$$f(x) = C \cdot \Phi_{m-1}(\Phi_{m-2}(\cdots \Phi_1(\Phi_0(x))))$$

The Jacobian $J_f = \frac{\partial f}{\partial x}$ can be written as

$$J_f = C \cdot J_{m-1} \cdot J_{m-2} \cdots J_1 \cdot J_0 \quad \text{with } J_i = \frac{\partial \Phi_i}{\partial s_i}$$

- Main idea: the directional derivative $J_f p$ with seed $p \in \mathbb{R}^n$ given by

$$J_f p = C \cdot (J_{m-1} \cdot (J_{m-2} \cdots (J_1 \cdot (J_0 p))))$$

we define $p = \tilde{s}_0 = [\tilde{x}_1, ..., \tilde{x}_n]^\top$ such that

$$\tilde{s}_{i+1} = J_i(s_i)\tilde{s}_i,\ i = 1, ..., m-1$$

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$x_4 = \sin(x_3)$	$\tilde{x}_4 = \cos(x_3)\tilde{x}_3$
$x_5 = \cos(x_1)$	$\tilde{x}_5 = -\sin(x_1)\tilde{x}_1$
$x_6 = x_4 + x_5$	$\tilde{x}_6 = \tilde{x}_4 + \tilde{x}_5$

Result: $\tilde{x}_6 = \tilde{s}_0^\top \nabla f(x)$.

$$\mathrm{Cost}(J_f) \text{ *in forward mode* } \leq 2n \cdot \mathrm{Cost}(f)$$

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$$\lambda^\top J_f = (((((\lambda^\top C) \cdot J_{m-1}) \cdot J_{m-2}) \cdots J_1) \cdot J_0)$$

we define $C^\top \lambda = \bar{s}_m$ such that

$$\bar{s}_i = J_i(s_i)^\top \bar{s}_{i+1},\ i = m-1, ..., 0$$

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Example: $f(x) = \sin(x_1 * x_2) + \cos(x_1)$:

$$\begin{aligned} x_3 &= x_1 * x_2 \\ x_4 &= \sin(x_3) \\ x_5 &= \cos(x_1) \\ x_6 &= x_4 + x_5 \end{aligned}$$

$$\begin{array}{lcl} \bar{x}_6 &=& 1,\ \bar{x}_i = 0,\ i = 1, ..., 5 \quad \text{define seed} \\ \hline \bar{x}_4 &=& \bar{x}_4 + \bar{x}_6 \\ \bar{x}_5 &=& \bar{x}_5 + \bar{x}_6 \\ \hline \bar{x}_1 &=& \bar{x}_1 - \sin(x_1)\bar{x}_5 \\ \hline \bar{x}_3 &=& \bar{x}_3 + \cos(x_3)\bar{x}_4 \\ \hline \bar{x}_1 &=& \bar{x}_1 + x_2 * \bar{x}_3 \\ \bar{x}_2 &=& \bar{x}_2 + x_1 * \bar{x}_3 \end{array}$$

Result: $\nabla f(x) = [\bar{x}_1, \bar{x}_2]^\top$.

$$\textit{Cost}(J_f) \textit{ in backward mode } \leq 3m \cdot \textit{Cost}(f)$$

Exercise

Consider function $f : \mathbb{R}^3 \to \mathbb{R}$,

$$f(x) = \sin(x_1 x_2) + \exp(x_1 x_2 x_3)$$

with $x = [x_1, x_2, x_3]^\top$. Write down

- its factorable form;
- the forward algorithmic differentiation;
- the backward algorithmic differentiation;

Exercise

Solution:

$$
\begin{array}{rcl|rcl}
x_4 & = & x_1 * x_2 & \tilde{x}_4 & = & x_1 * \tilde{x}_2 + \tilde{x}_1 * x_2 \\
x_5 & = & \sin(x_4) & \tilde{x}_5 & = & \cos(x_4)\tilde{x}_4 \\
x_6 & = & x_3 * x_4 & \tilde{x}_6 & = & x_3 * \tilde{x}_4 + \tilde{x}_3 * x_4 \\
x_7 & = & \exp(x_6) & \tilde{x}_7 & = & \exp(x_6)\tilde{x}_6 \\
x_8 & = & x_5 + x_7 & \tilde{x}_8 & = & \tilde{x}_5 + \tilde{x}_7
\end{array}
$$

Exercises

Solution:

INITIALIZE SEED

$\bar{x}_i = 0, \; i = 1, ..., 7$

$\bar{x}_8 = 1$

DIFFERENTIATION OF $x_8 = x_5 + x_7$

$\bar{x}_5 = \bar{x}_5 + \bar{x}_8$

$\bar{x}_7 = \bar{x}_7 + \bar{x}_8$

DIFFERENTIATION OF $x_7 = \exp(x_6)$

$\bar{x}_6 = \bar{x}_6 + \exp(x_6)\bar{x}_7$

DIFFERENTIATION OF $x_6 = x_3 * x_4$

$\bar{x}_3 = \bar{x}_3 + \bar{x}_4 * \bar{x}_6$

$\bar{x}_4 = \bar{x}_4 + \bar{x}_3 * \bar{x}_6$

DIFFERENTIATION OF $x_5 = \sin(x_4)$

$\bar{x}_4 = \bar{x}_4 + \cos(x_4)\bar{x}_5$

DIFFERENTIATION OF $x_4 = x_1 * x_2$

$\bar{x}_1 = \bar{x}_1 + x_2 * \bar{x}_4$

$\bar{x}_2 = \bar{x}_2 + x_1 * \bar{x}_4$

Summary

- Nonlinear programming = optimization in real-valued vector spaces.
- KKT-Conditions $\leftrightarrow$ first-order necessary conditions of optimality.
- Extendable to sufficient second-order conditions (not discussed here).
- Non-differentiable functions can cause numerical problems.
- Number of active constraints and correct identification of the active set is more important than the total number of constraints.

Initialization is key for solving non-convex problems.

Efficient derivative computation enables fast and reliable solutions.

Line search (and globalization) are crucial for global convergence.

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