AA 203
Optimal and Learning-Based Control
Nonlinear optimization theory

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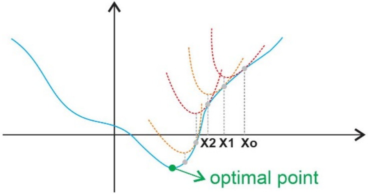
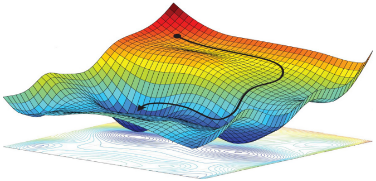
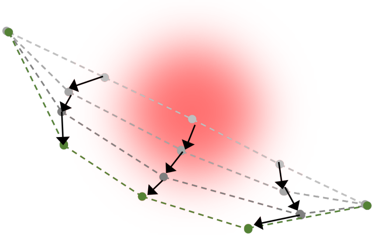
Optimization in many dimensions



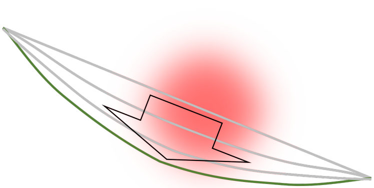
1-D



2-D



N-D



∞-D

Agenda

1. Unconstrained optimization
2. Descent methods for unconstrained problems
3. Equality-constrained optimization
4. Inequality-constrained optimization

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Unconstrained optimization

Given an objective function $f : \mathbb{R}^n \to \mathbb{R}$, we denote an *unconstrained nonlinear program* with the notation

$$\underset{x \in \mathbb{R}^n}{\text{minimize}}\, f(x).$$

We usually assume either $f \in \mathcal{C}^1$ (i.e., "continuously differentiable") or $f \in \mathcal{C}^2$ (i.e., "twice continuously differentiable").

A solution candidate $x^* \in \mathbb{R}^n$ can be a:

local minimum $\exists \varepsilon > 0 : f(x^*) \leq f(x), \ \forall x : \|x - x^*\| \leq \varepsilon$

global minimum $f(x^*) \leq f(x), \ \forall x \in \mathbb{R}^n$

If the inequality is strict, i.e., "$<$", then x^* is a strict unconstrained local/global minimum. Any (strict) global minimum is also a (strict) local minimum.

There can be many minima, or none at all!

First-order necessary optimality condition

Let x^* be a local minimum.

Suppose $f \in \mathcal{C}^1$. Then near x^* we have must have

$$f(x^* + \Delta x) - f(x^*) \approx \nabla f(x^*)^\mathsf{T} \Delta x \geq 0$$

For each i, take $\Delta x = \delta e^{(i)}$ and $\Delta x_i = -\delta e^{(i)}$ for small $\delta > 0$, where

$$e^{(i)} \coloneqq (\underbrace{0, \dots 0}_{i-1}, 1, 0, \dots 0) \in \{0, 1\}^n.$$

Then we get

$$\frac{\partial f}{\partial x_i}(x^*)\delta \geq 0, \ -\frac{\partial f}{\partial x_i}(x^*)\delta \geq 0 \iff \frac{\partial f}{\partial x_i}(x^*) = 0.$$

Overall, we have $\nabla f(x^*) = 0$, i.e., x^* must be a *stationary point*.

Second-order necessary optimality condition

Let x^* be a local minimum.

Suppose $f \in \mathcal{C}^2$. Then near x^* we have must have

$$f(x^* + \Delta x) - f(x^*) \approx \nabla f(x^*)^\mathsf{T} \Delta x + \frac{1}{2} \Delta x^\mathsf{T} \nabla^2 f(x^*) \Delta x \geq 0$$

We know $\nabla f(x^*) = 0$, so we must have

$$\frac{1}{2} \Delta x^\mathsf{T} \nabla^2 f(x^*) \Delta x \geq 0.$$

Since we can choose Δx arbitrarily within an ε-sized ball around x^*, we must have $\nabla^2 f(x^*) \succeq 0$, i.e., the Hessian of f at x^* is a *positive semi-definite* matrix.

Necessary optimality conditions (NOCs) for unconstrained problems

Theorem (NOCs for unconstrained problems)

Suppose $x^* \in \mathbb{R}^n$ *is an unconstrained local minimum of* $f : \mathbb{R}^n \to \mathbb{R}$.

- *If* $f \in \mathcal{C}^1$ *on an open set* $\mathcal{X} \subseteq \mathbb{R}^n$ *containing* x^*, *then* $\nabla f(x^*) = 0$.
- *If* $f \in \mathcal{C}^2$ *on* $\mathcal{X}$, *then* $\nabla^2 f(x^*) \succeq 0$.

Sufficient optimality conditions (SOCs) for unconstrained problems

If $\nabla f(x^*) = 0$ and $\nabla^2 f(x^*) \succ 0$, then

$$f(x^* + \Delta x) - f(x^*) \approx \frac{1}{2}\Delta x^\mathsf{T} \nabla^2 f(x^*)\Delta x > 0$$

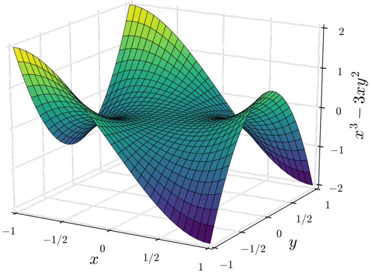
for small Δx.

Theorem (SOCs for unconstrained problems)

Suppose $f \in \mathcal{C}^2(\mathcal{X}, \mathbb{R})$ on some open set $\mathcal{X} \subseteq \mathbb{R}^n$. If $x^* \in \mathcal{X}$ satisfies

$$\nabla f(x^*) = 0, \quad \nabla^2 f(x^*) \succ 0,$$

then x^* is an unconstrained strict local minimum of f.



We cannot just use $\nabla^2 f(x^*) \succeq 0$ due to saddle points.

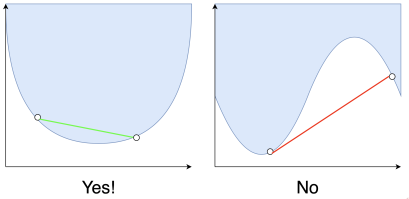
Convex sets and convex functions

A set $\mathcal{X} \subseteq \mathbb{R}^n$ is *convex* if

$$\alpha x + (1-\alpha)y \in \mathcal{X}, \ \forall x, y \in \mathcal{X}, \ \forall \alpha \in [0,1].$$

A function $f : \mathcal{X} \to \mathbb{R}^n$ is *convex* on $\mathcal{X}$ if

$$f(\alpha x + (1-\alpha)y) \leq \alpha f(x) + (1-\alpha) f(y), \quad \forall x, y \in \mathcal{X}, \ \forall \alpha \in [0,1].$$



If the inequality is strict, then f is *strictly convex*.

A function $f \in \mathcal{C}^2$ is convex on $\mathcal{X}$ if and only if $\nabla^2 f(x) \succeq 0$ for all $x \in \mathcal{X}$. If $\nabla^2 f(x) \succ 0$ for all $x \in \mathcal{X}$, then f is strictly convex.

Important examples of convex functions for this course are:

Quadratic $f(x) = x^\mathsf{T} Q x$ (where $Q \succeq 0$)

Affine $f(x) = Ax + b$ (both convex and concave)

Unconstrained convex problems

Theorem (NOCs are SOCs for unconstrained convex problems)

Let $f : \mathcal{X} \to \mathbb{R}$ be a convex function over a convex set $\mathcal{X} \in \mathbb{R}^n$.

- *If $x^* \in \mathcal{X}$ is local minimum of f, then it is also a global minimum over $\mathcal{X}$.*
- *If f is strictly convex, then there exists at most one global minimum of f over $\mathcal{X}$.*
- *Suppose additionally that $\mathcal{X}$ is open and $f \in \mathcal{C}^1(\mathcal{X}, \mathbb{R})$. Then $\nabla f(x^*) = 0$ if and only if x^* is a global minimum of f over $\mathcal{X}$.*

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Descent methods for unconstrained problems

Iterative descent methods start at an initial guess $x^{(0)}$, and try to successively generate vectors $\{x^{(1)}, x^{(2)}, \dots\}$ such that the objective decreases at each iteration, i.e.,

$$f(x^{(k+1)}) \leq f(x^{(k)}),\ \forall k \in \{0, 1, 2, \dots\}.$$

The hope is that we can decrease f all the way to a minimum.

Consider the update rule

$$x^{(k+1)} = x^{(k)} + \alpha^{(k)} d^{(k)},$$

where $\alpha^{(k)} > 0$ is the *step-size* and $d^{(k)} \in \mathbb{R}^n$ is the *descent direction*. Then

$$f(x^{(k+1)}) \approx f(x^{(k)}) + \alpha^{(k)}\, \nabla f(x^{(k)})^\mathsf{T} d^{(k)}.$$

The goal is to choose $\alpha^{(k)} > 0$ and $d^{(k)} \in \mathbb{R}^n$ such that this approximation is appropriate and $\nabla f(x^{(k)})^\mathsf{T} d^{(k)} < 0$.

Gradient descent directions

Let $d^{(k)} = -D^{(k)} \nabla f(x^k)$, where $D^{(k)} \succ 0$. Then

$$\begin{aligned} f(x^{(k+1)}) &\approx f(x^{(k)}) + \alpha^{(k)} \nabla f(x^{(k)})^\mathsf{T} d^{(k)} \\ &= f(x^{(k)}) - \alpha^{(k)} \nabla f(x^{(k)})^\mathsf{T} D^{(k)} \nabla f(x^{(k)}) \end{aligned}.$$

Since $D^{(k)} \succ 0$, we have that $f(x^{(k+1)}) \leq f(x^{(k)})$ for small enough $\alpha^{(k)} > 0$.

Popular choices for the descent scaling $D^{(k)}$ are

steepest $D^{(k)} = I$.

Newton $D^{(k)} = \nabla^2 f(x^{(k)})^{-1}$, provided that the inverse exists.

The Newton descent direction analytically minimizes the quadratic approximation

$$f(x^{(k+1)}) \approx f(x^{(k)}) + \nabla f(x^{(k)})^\mathsf{T} d^{(k)} + \frac{1}{2} d^{(k)\mathsf{T}} \nabla^2 f(x^{(k)}) d^{(k)}$$

at each iteration k, assuming $\nabla^2 f(x^{(k)})$ is invertible.

Selecting the step-size

Constant Choose $\alpha^{(k)} \equiv \alpha > 0$. Convergence can be slow, or the iterates could diverge if α is too large.

Diminishing Ensure $\alpha^{(k)} \to 0$ and $\sum_{k=0}^{\infty} \alpha^{(k)} = \infty$. This does not guarantee descent at each iteration, but it can avoid diverging iterates.

Line search Given the current iterate $x^{(k)}$ and a descent direction $d^{(k)}$, compute

$$\alpha^{(k)} = \arg\min_{\alpha > 0} f(x^{(k)} + \alpha d^{(k)})$$

exactly if possible. Otherwise, do *backtracking line search*

initialize $\alpha^{(k)} = 1$
while $f(x^{(k)} + \alpha d^{(k)}) > f(x^{(k)}) + \gamma \alpha^{(k)} \nabla f(x^{(k)})^{\mathsf{T}} d^{(k)}$
$\quad \alpha^{(k)} \leftarrow \beta \alpha^{(k)}$

where $\gamma \in (0, 0.5)$ and $\beta \in (0, 1)$ are hyperparameters.

Further topics to explore

There is a wealth of mathematical analyses of descent methods involving:

- guarantees for convergence to a stationary point
- good convergence criteria (e.g., $\|x^{(k)} - x^{(k-1)}\| < \varepsilon$, $|f(x^{(k)}) - f(x^{(k-1)})| < \varepsilon$, $\|\nabla f(x^{(k)})\| < \varepsilon$)
- convergence rates (e.g., $f(x^{(k)}) - f(x^*) \lesssim \frac{1}{k}\|x^{(0)} - x^*\|_2^2$)

There are other descent methods that can be implemented “derivative-free”, such as

- coordinate descent
- Nelder-Mead algorithms

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Equality-constrained optimization

Given an objective function $f : \mathbb{R}^n \to \mathbb{R}$ and a *constraint function* $h : \mathbb{R}^n \to \mathbb{R}^m$, we denote an *equality-constrained nonlinear program* with the notation

$$\begin{aligned} \underset{x \in \mathbb{R}^n}{\text{minimize}} \; & f(x) \\ \text{subject to} \; & h(x) = 0 \end{aligned}$$

We assume $f \in \mathcal{C}^1(\mathbb{R}^n, \mathbb{R})$ and $h \in \mathcal{C}^1(\mathbb{R}^n, \mathbb{R}^m)$.

Lagrange multipliers for equality-constrained problems

Define the *Lagrangian* function

$$L(x,\lambda) \coloneqq f(x) + \lambda^\mathsf{T} h(x) = f(x) + \sum_{i=1}^{m} \lambda_i h_i(x),$$

where $\lambda \in \mathbb{R}^m$ is a vector of *Lagrange multipliers*.

Theorem (First-order NOC for equality-constrained problems)

Suppose $x^* \in \mathbb{R}^n$ is a local minimum of $f \in \mathcal{C}^1(\mathbb{R}^n, \mathbb{R})$ subject to $h(x^*) = 0$ with $h \in \mathcal{C}^1(\mathbb{R}^n, \mathbb{R}^m)$. Moreover, assume $\{\nabla h_i(x^*)\}_{i=1}^m$ are linearly independent. Then there exists a unique $\lambda^* \in \mathbb{R}^m$ such that

$$\nabla_x L(x^*, \lambda^*) = \nabla f(x^*) + \sum_{i=1}^{m} \lambda_i^* \nabla h_i(x^*) = 0.$$

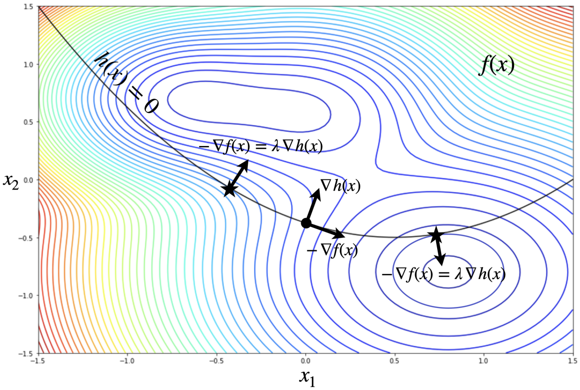
Second-order NOCs and SOCs for constrained problems are discussed in AA203-Notes and (Bertsekas, 2016).

First-order NOC visualized

Re-arrange $\nabla_x L(x^*, \lambda^*) = 0$ to get

$$-\nabla f(x^*) = \sum_{i=1}^{m} \lambda_i^* \nabla h_i(x^*).$$

Further reduction of the objective value would produce a change in the constraint function, thereby violating $h(x) = 0$.



Regularity conditions for equality-constrained problems

The first-order NOC required that x^* is a *regular* point, i.e., that $\{\nabla h_i(x^*)\}_{i=1}^m$ are linearly independent vectors. Since $\nabla h_i(x^*) \in \mathbb{R}^n$, this implicitly requires $m \leq n$ (i.e., you cannot find more than n linearly independent vectors in $\mathbb{R}^n$).

Solving $\min_{x\,:\,h(x)=0} f(x)$ can be viewed as solving for n variables subject to m constraints.

The proof of the first-order NOC relies on eliminating m variables to arrive at an unconstrained problem in $n - m$ variables, which in turn relies on $\{\nabla h_i(x^*)\}_{i=1}^m$ being linearly independent to apply the implicit function theorem.

See (Bertsekas, 2016, §4.1.2) for further details.

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Inequality-constrained optimization

Given an objective function $f : \mathbb{R}^n \to \mathbb{R}$ and *constraint functions* $h : \mathbb{R}^n \to \mathbb{R}^m$ and $g : \mathbb{R}^n \to \mathbb{R}^r$, we denote an *inequality-constrained nonlinear program* with the notation

$$\begin{aligned} \underset{x \in \mathbb{R}^n}{\text{minimize}} \;& f(x) \\ \text{subject to } & h(x) = 0 \\ & g(x) \preceq 0 \end{aligned}$$

We assume $f \in \mathcal{C}^1(\mathbb{R}^n, \mathbb{R})$, $h \in \mathcal{C}^1(\mathbb{R}^n, \mathbb{R}^m)$, and $g \in \mathcal{C}^1(\mathbb{R}^n, \mathbb{R}^r)$. We use "$\preceq$" to denote element-wise inequality in this scenario.

For any feasible point x, i.e., such that $h(x) = 0$ and $g(x) \preceq 0$, define the set of *active inequality constraints* by

$$\mathcal{A}_g(x) \coloneqq \{j \in \{1, 2, \ldots, r\} \mid g_j(x) = 0\}.$$

Karush-Kuhn-Tucker (KKT) NOC conditions

With Lagrangian multipliers $\lambda \in \mathbb{R}^m$ and $\mu \in \mathbb{R}^r$, define the Lagrangian

$$L(x, \lambda, \mu) := f(x) + \lambda^\mathsf{T} h(x) + \mu^\mathsf{T} g(x) = f(x) + \sum_{i=1}^{m} \lambda_i h_i(x) + \sum_{j=1}^{r} \mu_j g_j(x).$$

Theorem (First-order NOC for inequality-constrained problems)

Suppose $x^* \in \mathbb{R}^n$ is a local minimum of $f \in \mathcal{C}^1(\mathbb{R}^n, \mathbb{R})$ subject to $h(x^*) = 0$ and $g(x^*) \preceq 0$ with $h \in \mathcal{C}^1(\mathbb{R}^n, \mathbb{R}^m)$ and $g \in \mathcal{C}^1(\mathbb{R}^n, \mathbb{R}^r)$. Moreover, assume

$$\{\nabla h_i(x^*)\}_{i=1}^m \cup \{\nabla g_j(x^*)\}_{j \in \mathcal{A}_g(x^*)}$$

are linearly independent. Then there exist unique $\lambda^* \in \mathbb{R}^m$ and $\mu^* \in \mathbb{R}^r$ such that

$$\nabla_x L(x^*, \lambda^*, \mu^*) = 0, \qquad \mu^* \succeq 0, \qquad \mu_j^* = 0, \ \forall j \notin \mathcal{A}_g(x^*).$$

We can also write the last condition succinctly as ${\mu^*}^\mathsf{T} g(x^*) = 0$.

KKT conditions for convex problems

Consider when f is convex, each $g_j(x)$ is convex, and $h(x)$ is affine, i.e., $h(x) = Ax - b$. Then we have

$$\begin{aligned} \underset{x \in \mathbb{R}^n}{\text{minimize}} \ & f(x) \\ \text{subject to } & Ax = b \\ & g(x) \preceq 0 \end{aligned}$$

for which the feasible set $\mathcal{X} := \{x \in \mathbb{R}^n \mid Ax = b, \ g(x) \preceq 0\}$ is convex.

Theorem (KKT conditions are NOCs and SOCs for convex problems)

Suppose $f \in \mathcal{C}^1(\mathbb{R}^n, \mathbb{R})$ and $g \in \mathcal{C}^1(\mathbb{R}^n, \mathbb{R}^r)$ are convex, and that there exists at least one strictly feasible point $x \in \mathcal{X}$, i.e., $Ax = b$ and $g(x) \prec 0$. Then (x^*, λ^*, μ^*) describe a global minimum if and only if

$$Ax^* = b, \quad g(x^*) \preceq 0, \quad \nabla_x L(x^*, \lambda^*, \mu^*) = 0, \quad \mu^* \succeq 0, \quad {\mu^*}^\mathsf{T} g(x^*) = 0.$$

Example: Maximal rectangle inside a circle

$$\text{maximize } x_1 + x_2$$
$$\text{subject to } x_1^2 + x_2^2 = r^2$$

We have $f(x) = -x_1 - x_2$ (for minimization) with $h(x) = x_1^2 + x_2^2 - r^2$, so

$$L(x, \lambda) = -x_1 - x_2 + \lambda(x_1^2 + x_2^2 - r^2).$$

The first-order NOC at a local minimum (x^*, λ^*) is

$$\nabla_x L(x^*, \lambda^*) = \begin{pmatrix} -1 + 2\lambda^* x_1^* \\ -1 + 2\lambda^* x_2^* \end{pmatrix} \stackrel{!}{=} 0 \iff x_1^* = x_2^* = \frac{1}{2\lambda^*}.$$

Substitute into ${x_1^*}^2 + {x_2^*}^2 = r^2$ to get $\lambda^* = \pm\frac{1}{\sqrt{2}r} \implies x_1^* = x_2^* = \pm\frac{1}{\sqrt{2}}r$.
Of the two possible solutions, $x_1^* = x_2^* = \frac{1}{\sqrt{2}}r$ is the global maximum (i.e., a square).

Optimality conditions in algorithm design

Why should we care about characterizing optimality conditions?

- Even just NOCs can form a filter for distilling local minima from feasible points.
- NOCs and SOCs can serve as a means for "measuring progress" towards optimality during an optimization procedure, particularly for convex problems.
- Problem structure (e.g., quadratic objective with linear constraints) coupled with convexity and the KKT conditions can be leveraged to implement efficient solvers with good convergence properties (Boyd and Vandenberghe, 2004).
- Even for non-convex problems, convex solvers can be used in iterative convex sub-problems that can converge to a local minimum.

Preview: Sequential Convex Programming (SCP)

Consider the non-convex problem

$$\begin{aligned} &\underset{x \in \mathbb{R}^n}{\text{minimize}} \ f(x) \\ &\text{subject to } h(x) = 0,\ g(x) \preceq 0 \end{aligned}$$

The basic idea of *sequential convex programming (SCP)* is to maintain an estimate $x^{(k)}$ and iteratively solve for $x^{(k+1)}$ via the convex sub-problem

$$\begin{aligned} &\underset{x \in \mathbb{R}^n}{\text{minimize}} \ \hat{f}^{(k)}(x) \\ &\text{subject to } \hat{h}^{(k)}(x) \coloneqq \hat{A}^{(k)}x - \hat{b}^{(k)} = 0,\ \hat{g}^{(k)}(x) \preceq 0,\ x \in \mathcal{T}^{(k)} \end{aligned}$$

where $(\hat{f}^{(k)}, \hat{g}^{(k)})$ and $\hat{h}^{(k)}$ are convex and affine, respectively, *approximations* of (f, g) and h, respectively, over a convex *trust region* constructed around $x^{(k)}$, e.g.,

$$\mathcal{T}^{(k)} \coloneqq \{x \mid \|x - x^{(k)}\|_\infty \leq \rho\},$$

for some $\rho > 0$.

Next class

Pontryagin's maximum principle and indirect methods for optimal control
(i.e., applying NOCs to optimal control problems)

References

D. Bertsekas. *Nonlinear Programming*. Athena Scientific, 3 edition, 2016.

S. Boyd and L. Vandenberghe. *Convex Optimization*. Cambridge University Press, 2004.