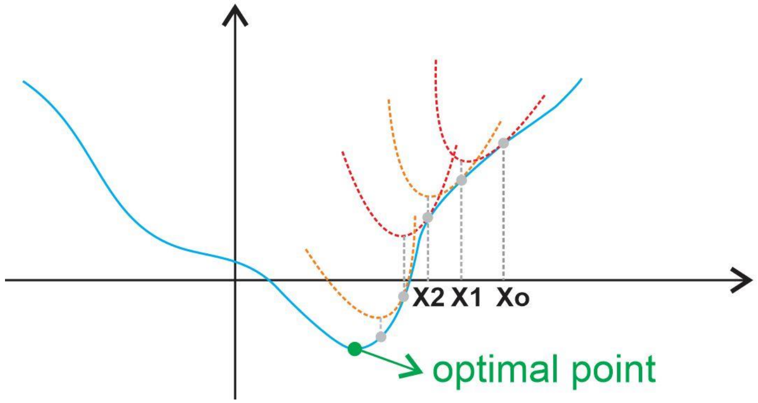
AA203
Optimal and Learning-based Control

Optimization theory

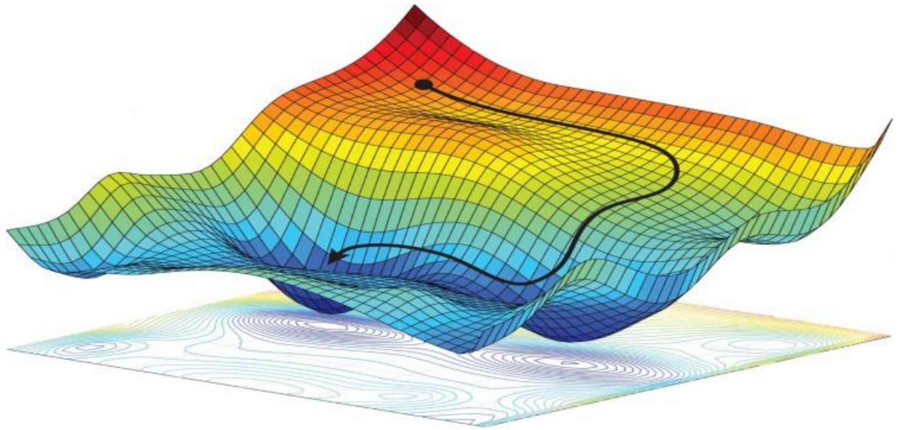
Stanford University

Autonomous Systems Lab

Optimization in many dimensions

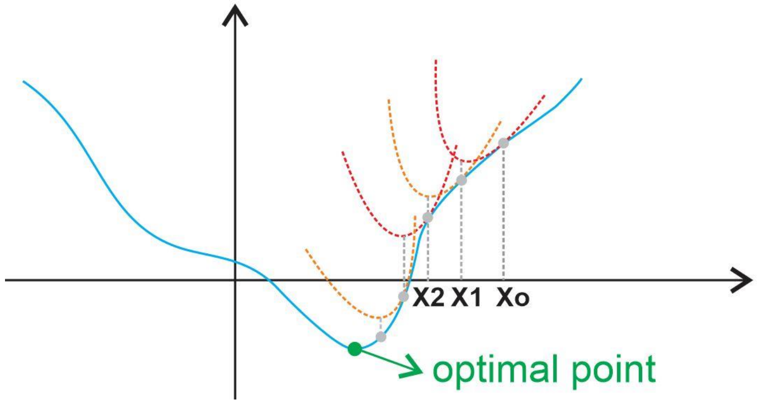


1-D

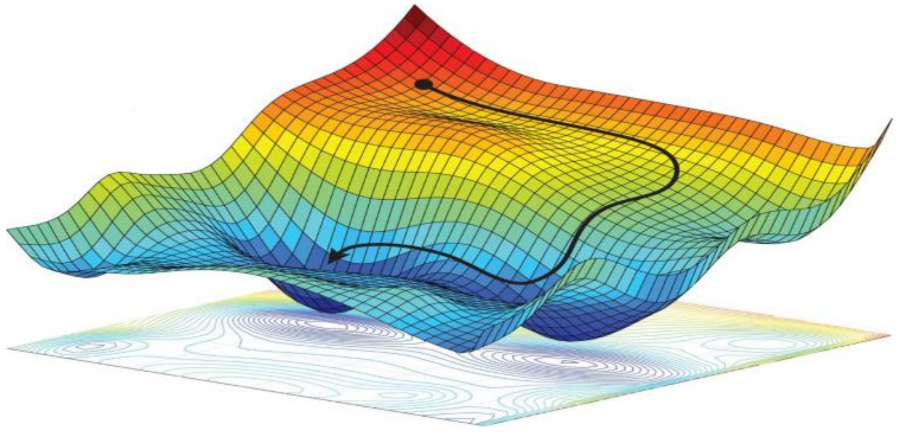


2-D

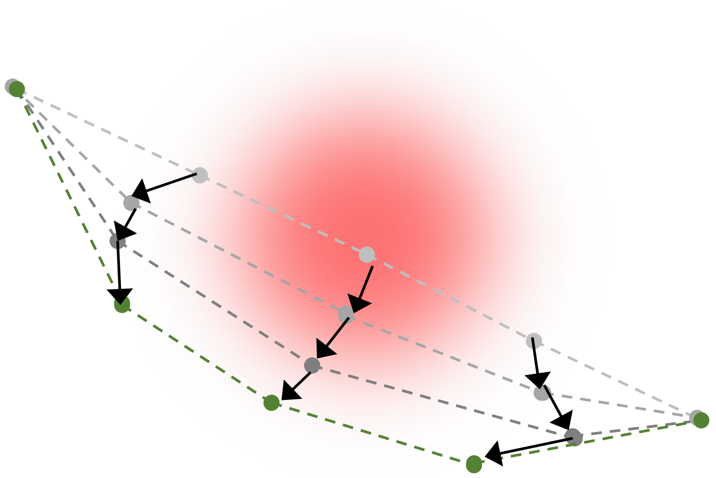
Optimization in many dimensions



1-D

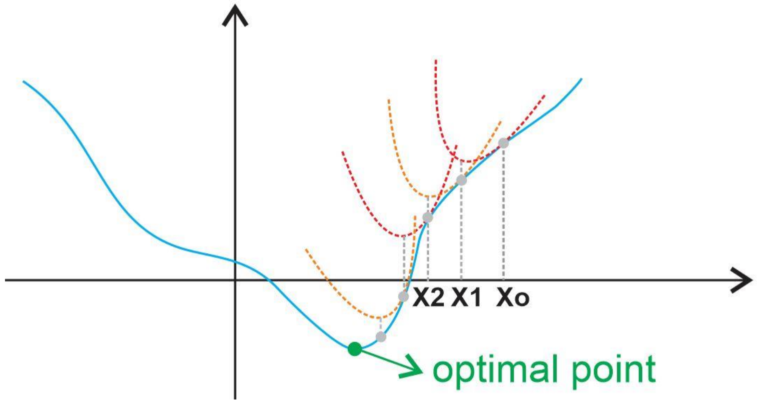


2-D

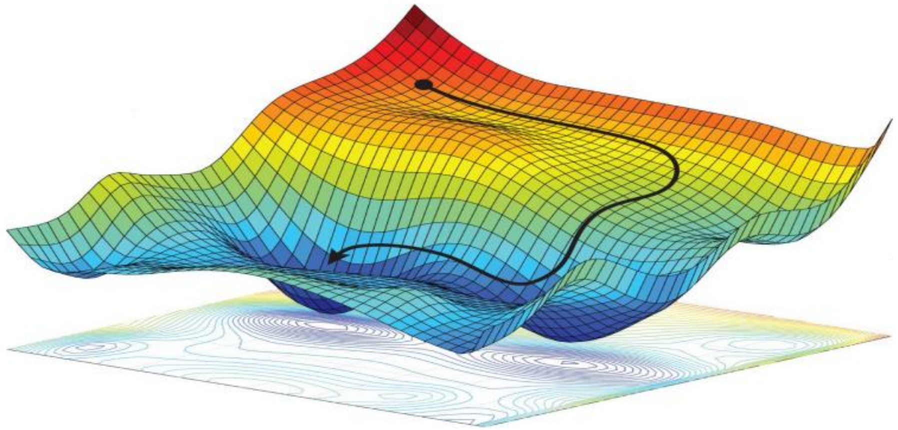


10-D

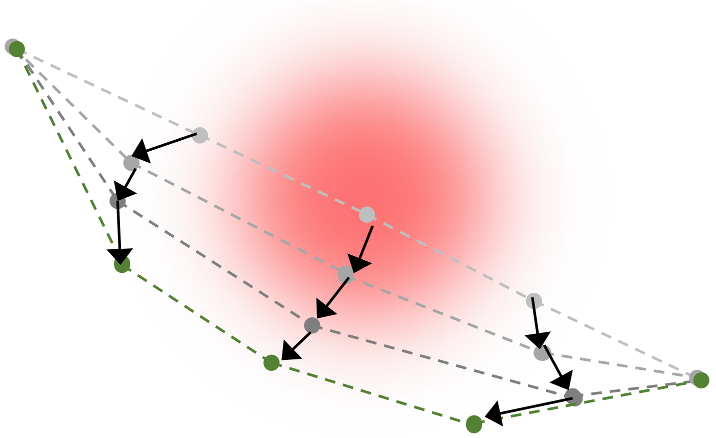
Optimization in many dimensions



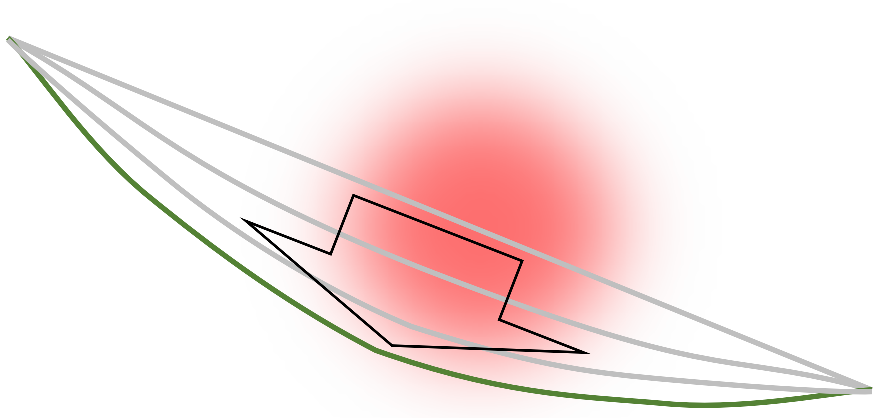
1-D



2-D



10-D



∞-D

Outline

1. Unconstrained optimization
2. Computational methods for unconstrained optimization
3. Optimization with equality constraints
4. Optimization with inequality constraints

Unconstrained optimization

Unconstrained non-linear program

$$\min_{\mathbf{x}\in\mathbb{R}^n} \; f(\mathbf{x})$$

- f usually assumed continuously differentiable (and often twice continuously differentiable)

Local and global minima

- A vector $\mathbf{x}^*$ is said to be an unconstrained *local* minimum if $\exists \epsilon > 0$ such that

$$f(\mathbf{x}^*) \leq f(\mathbf{x}), \qquad \forall \mathbf{x} \,\big|\, \|\mathbf{x} - \mathbf{x}^*\| < \epsilon$$

- A vector $\mathbf{x}^*$ is said to be an unconstrained *global* minimum if

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

- $\mathbf{x}^*$ is a strict local/global minimum if the inequality is strict

Necessary conditions for optimality

Key idea: compare cost of a vector with cost of its close neighbors

- Assume $f \in C^1$, by using Taylor series expansion

$$f(\mathbf{x}^* + \Delta\mathbf{x}) - f(\mathbf{x}^*) \approx \nabla f(\mathbf{x}^*)'\Delta\mathbf{x}$$

- If $f \in C^2$

$$f(\mathbf{x}^* + \Delta\mathbf{x}) - f(\mathbf{x}^*) \approx \nabla f(\mathbf{x}^*)'\Delta\mathbf{x} + \frac{1}{2}\Delta\mathbf{x}'\nabla^2 f(\mathbf{x}^*)\Delta\mathbf{x}$$

Necessary conditions for optimality

- We expect that if $\mathbf{x}^*$ is an unconstrained local minimum, the first order cost variation due to a small variation $\Delta\mathbf{x}$ is nonnegative, i.e.,

$$\nabla f(\mathbf{x}^*)'\Delta\mathbf{x} = \sum_{i=1}^{n} \frac{\partial f(\mathbf{x}^*)}{\partial x_i}\Delta x_i \geq 0$$

- By taking $\Delta\mathbf{x}$ to be positive and negative multiples of the unit coordinate vectors, we obtain conditions of the type

$$\frac{\partial f(\mathbf{x}^*)}{\partial x_i} \geq 0, \quad \text{and} \quad \frac{\partial f(\mathbf{x}^*)}{\partial x_i} \leq 0$$

- Equivalently we have the necessary condition

$$\boxed{\nabla f(\mathbf{x}^*) = 0} \qquad (\mathbf{x}^* \text{ is said a stationary point})$$

Necessary conditions for optimality

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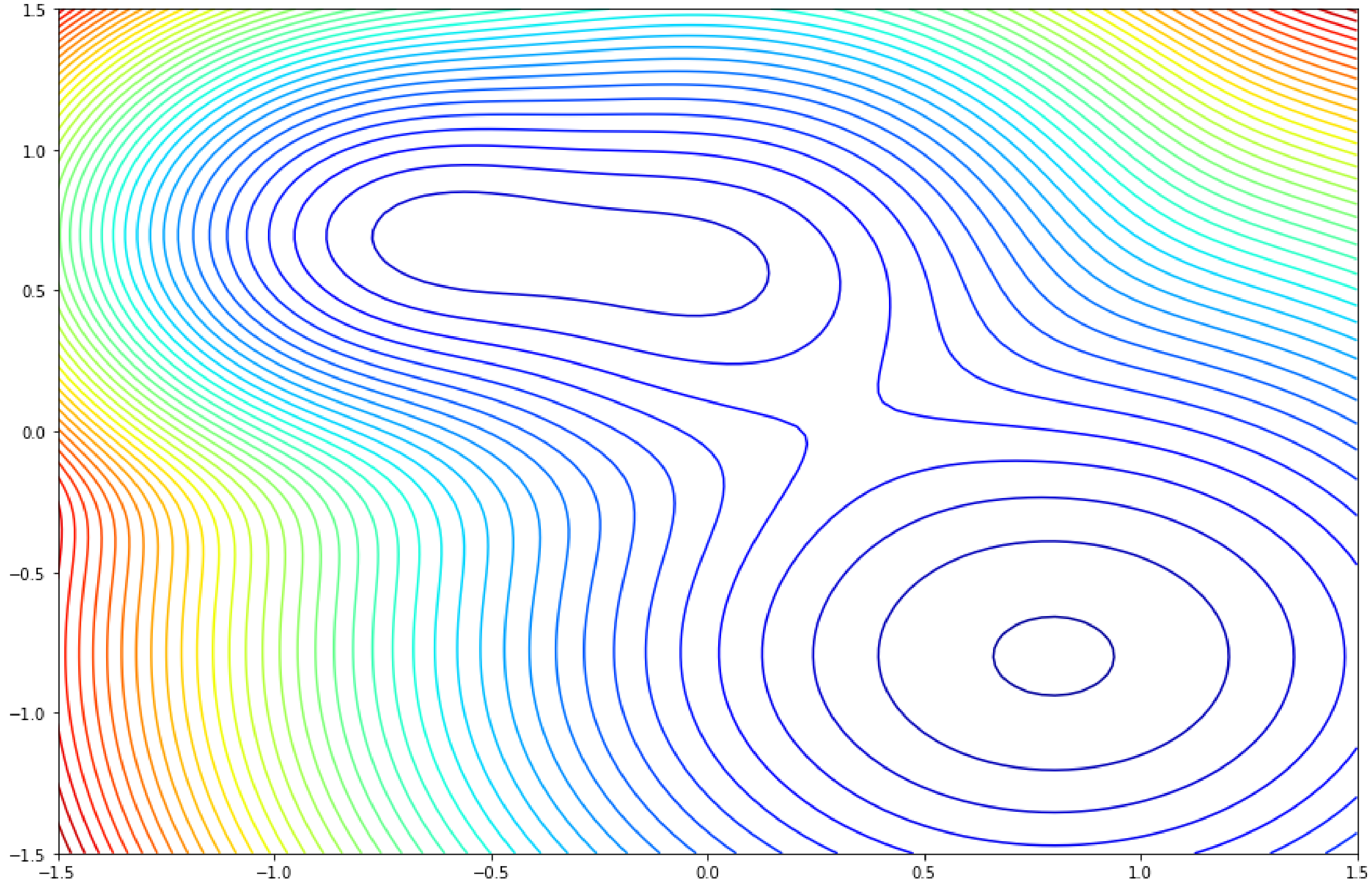

Necessary conditions for optimality

- Of course, also the second order cost variation due to a small variation $\Delta\mathbf{x}$ must be non-negative

$$\nabla f(\mathbf{x}^*)'\Delta\mathbf{x} + \frac{1}{2}\Delta\mathbf{x}'\nabla^2 f(\mathbf{x}^*)\Delta\mathbf{x} \geq 0$$

- Since $\nabla f(\mathbf{x}^*)'\Delta\mathbf{x}=0$, we obtain $\Delta\mathbf{x}'\nabla^2 f(\mathbf{x}^*)\Delta\mathbf{x} \geq 0$. Hence

$$\boxed{\nabla^2 f(\mathbf{x}^*) \text{ has to be positive semidefinite}}$$

Necessary conditions for optimality

Theorem: NOC

Let $\mathbf{x}^*$ be an unconstrained local minimum of $f: \mathbb{R}^n \mapsto \mathbb{R}$ and assume that f is C^1 in an open set S containing $\mathbf{x}^*$. Then

$$\nabla f(\mathbf{x}^*) = 0 \qquad \text{(first order NOC)}$$

If in addition $f \in C^2$ within S,

$$\nabla^2 f(\mathbf{x}^*) \text{ positive semidefinite} \qquad \text{(second order NOC)}$$

Sufficient conditions for optimality

- Assume that $\mathbf{x}^*$satisfies the first order NOC

$$\nabla f(\mathbf{x}^*) = 0$$

- and also assume that the second order NOC is strengthened to

$$\nabla^2 f(\mathbf{x}^*) \quad \text{positive } \textit{definite}$$

- Then, for all $\Delta\mathbf{x} \neq 0$, $\Delta\mathbf{x}'\nabla^2 f(\mathbf{x}^*)\Delta\mathbf{x} > 0$. Hence, f tends to increase *strictly* with small excursions from $\mathbf{x}^*$, suggesting SOC…

Sufficient conditions for optimality

Theorem: SOC

Let $f: \mathbb{R}^n \mapsto \mathbb{R}$ be C^2 in an open set S. Suppose that a vector $\mathbf{x}^* \in S$ satisfies the conditions

$$\nabla f(\mathbf{x}^*) = 0 \qquad \text{and} \qquad \nabla^2 f(\mathbf{x}^*) \text{ positive definite}$$

Then $\mathbf{x}^*$ is a strict unconstrained local minimum of f

Special case: convex optimization

A subset C of $\mathbb{R}^n$ is called convex if

$$\alpha \mathbf{x} + (1-\alpha)\mathbf{y} \in C, \quad \forall \mathbf{x}, \mathbf{y} \in C, \forall \alpha \in [0,\ 1]$$

Let C be convex. A function $f: C \rightarrow \mathbb{R}$ is called convex if

$$f(\alpha \mathbf{x} + (1-\alpha)\mathbf{y}) \leq \alpha f(\mathbf{x}) + (1-\alpha) f(\mathbf{y})$$

Special case: convex optimization

Let $f: C \to \mathbb{R}$ be a convex function over a convex set C

- A local minimum of f over C is also a global minimum over C. If in addition f is strictly convex, then there exists at most one global minimum of f
- If f is in C^1 and convex, and the set C is open, $\nabla f(\mathbf{x}^*) = 0$ is a necessary and sufficient condition for a vector $\mathbf{x}^* \in C$ to be a global minimum over C

Discussion

- Optimality conditions are important to filter candidates for global minima
- They often provide the basis for the design and analysis of optimization algorithms
- They can be used for sensitivity analysis

Outline

1. Unconstrained optimization
2. Computational methods for unconstrained optimization
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Computational methods (unconstrained case)

Key idea: iterative descent. We start at some point $\mathbf{x}^0$ (initial guess) and successively generate vectors $\mathbf{x}^1, \mathbf{x}^2, \ldots$ such that f is decreased at each iteration, i.e.,

$$f(\mathbf{x}^{k+1}) \leq f(\mathbf{x}^k), \qquad k = 0, 1, \ldots$$

The hope is to decrease f all the way to the minimum

Gradient methods

Given $\mathbf{x} \in \mathbb{R}^n$ with $\nabla f(\mathbf{x}) \neq 0$, consider the half line of vectors

$$\mathbf{x}_\alpha = \mathbf{x} - \alpha \nabla f(\mathbf{x}), \qquad \forall \alpha \geq 0$$

From first order Taylor expansion (α small)

$$f(\mathbf{x}_\alpha) \approx f(\mathbf{x}) + \nabla f(\mathbf{x})'(\mathbf{x}_\alpha - \mathbf{x}) = f(\mathbf{x}) - \alpha \|\nabla f(\mathbf{x})\|^2$$

So for α small enough $f(\mathbf{x}_{\boldsymbol{\alpha}})$ is smaller than $f(\mathbf{x})$!

Gradient methods

Carrying this idea one step further, consider the half line of vectors

$$\mathbf{x}_\alpha = \mathbf{x} + \alpha\,\mathbf{d}, \qquad \forall\alpha \geq 0$$

where $\nabla f(\mathbf{x})'\mathbf{d} < \mathbf{0}$ (angle $> 90°$)

By Taylor expansion

$$f(\mathbf{x}_\alpha) \approx f(\mathbf{x}) + \alpha \nabla f(\mathbf{x})'\mathbf{d}$$

For small enough α, $f(\mathbf{x} + \alpha\mathbf{d})$ is smaller than $f(\mathbf{x})$!

Gradient methods

Broad and important class of algorithms:
gradient methods

$$\mathbf{x}^{k+1} = \mathbf{x}^k + \alpha^k \mathbf{d}^k, \qquad k = 0, 1, \ldots$$

where if $\nabla f\left(\mathbf{x}^{\mathrm{k}}\right) \neq 0$, $\mathbf{d}^{\mathrm{k}}$ is chosen so that

$$\nabla f(\mathbf{x}^k)'\mathbf{d}^k < 0$$

and the stepsize α is chosen to be positive

Gradient descent

Most often the stepsize is chosen so that

$$f(\mathbf{x}^k + \alpha^k \mathbf{d}^k) < f(\mathbf{x}^k), \qquad k = 0, 1, \ldots$$

and the method is called gradient descent.
"Tuning" parameters:

- selecting the descent direction
- selecting the stepsize

Selecting the descent direction

General class

$$\mathbf{d}^k = -D^k \nabla f(\mathbf{x}^k), \qquad \text{where } D^k > 0$$

(Obviously, $\nabla f\left(\mathbf{x}^k\right)' \mathbf{d}^k < 0$)

Popular choices:

- Steepest descent: $D^k = I$
- Newton's method: $D^k = \left(\nabla^2 f(\mathbf{x}^k)\right)^{-1}$, provided $\nabla^2 f(\mathbf{x}^k) > 0$

Selecting the stepsize

- Minimization rule: α^k is selected such that the cost function is minimized along the direction $\mathbf{d}^k$, i.e.,

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

- Constant stepsize: $\alpha^k = s$
  - the method might diverge
  - convergence rate could be very slow

- Diminishing stepsize: $\alpha^k \to 0$ and $\sum_{k=0}^{+\infty} \alpha^k = \infty$
  - it does not guarantee descent at each iteration

Undiscussed in this class

Mathematical analysis:

- convergence (to stationary points)
- termination criteria
- convergence rate

Derivative-free methods, e.g.,

- coordinate descent
- Nelder-Mead

Constrained optimization

- Constraint set usually specified in terms of equality and inequality constraints
- Sophisticated collection of optimality conditions, involving some auxiliary variables, called Lagrange multipliers

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Viewpoints:

- <u>Penalty viewpoint</u>: we disregard the constraints and we add to the cost a high penalty for violating them
- <u>Feasibility direction viewpoint</u>: it relies on the fact that at a local minimum there can be no cost improvement when traveling a small distance along a direction that leads to feasible points

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Optimization with equality constraints

$$\begin{aligned} \min \quad & f(\mathbf{x}) \\ \text{subject to} \quad & h_i(\mathbf{x}) = 0, \qquad i = 1, \ldots, m \end{aligned}$$

- $f: \mathbb{R}^n \to \mathbb{R}$ and h_i: $\mathbb{R}^n \to \mathbb{R}$ are C^1
- notation: $\mathbf{h} \coloneqq (h_1, \ldots, h_m)$

Lagrange multipliers

- Basic Lagrange multiplier theorem: for a given local minimum $\mathbf{x}^*$ there exist scalars $\lambda_1, \ldots, \lambda_m$ called Lagrange multipliers such that

$$\nabla f(\mathbf{x}^*) + \sum_{i=1}^{m} \lambda_i \nabla h_i(\mathbf{x}^*) = 0$$

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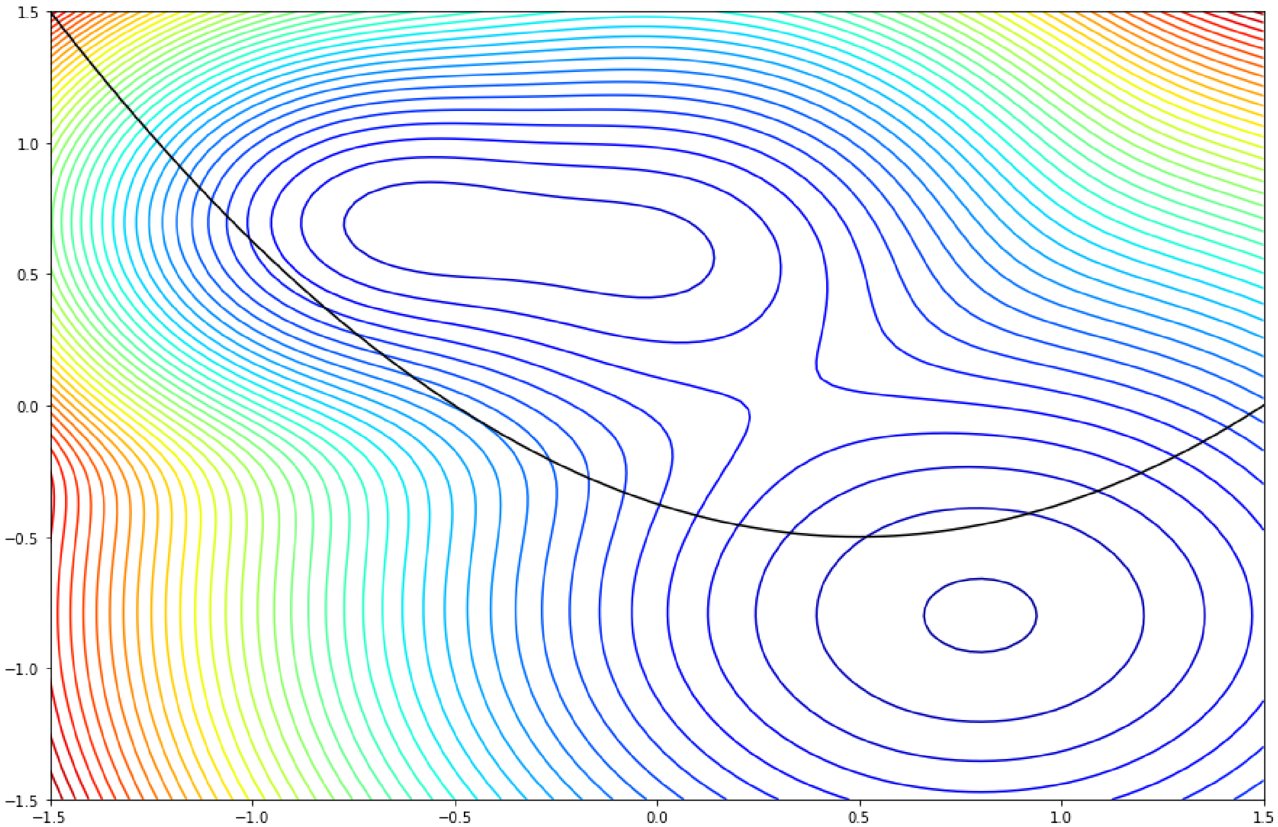

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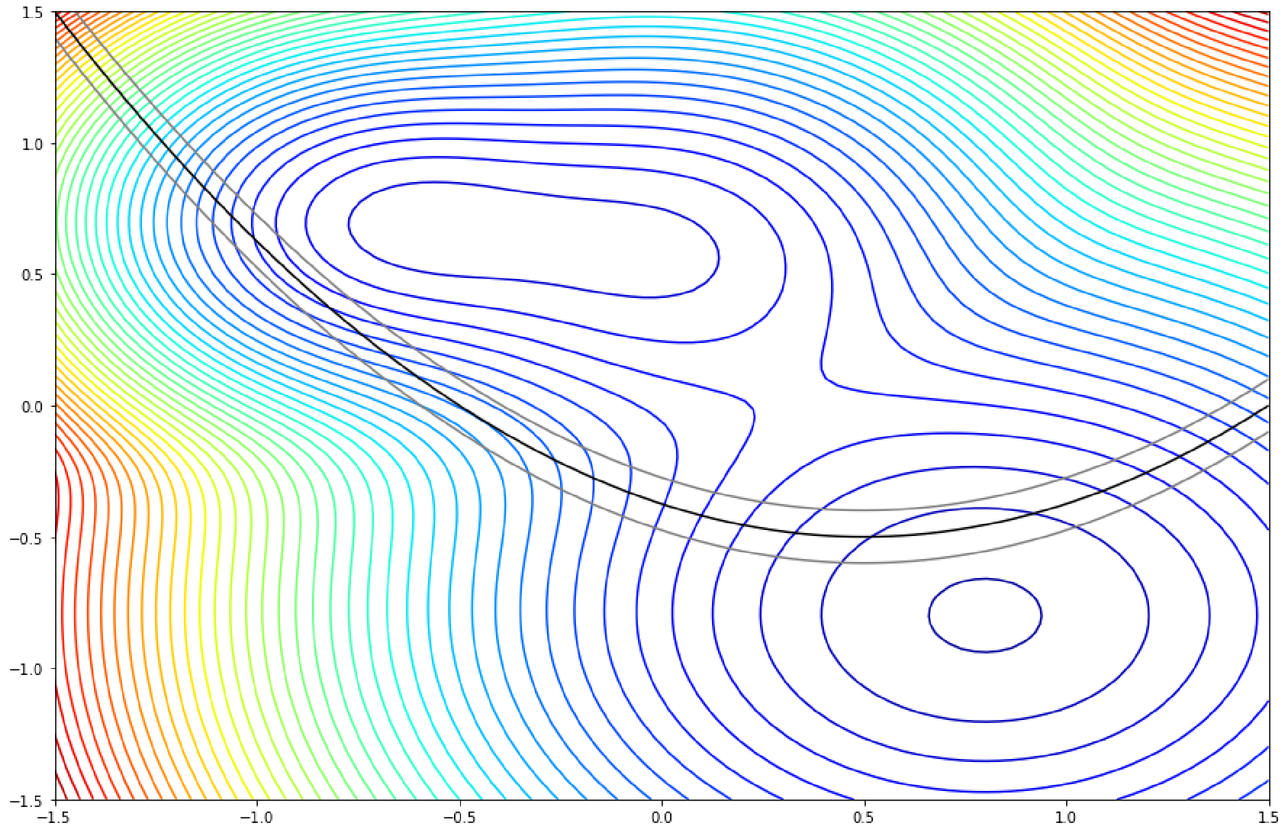

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- Example

$$\begin{aligned} \text{min} \quad & x_1 + x_2 \\ \text{subject to} \quad & x_1^2 + x_2^2 = 2 \end{aligned}$$

Lagrange multipliers

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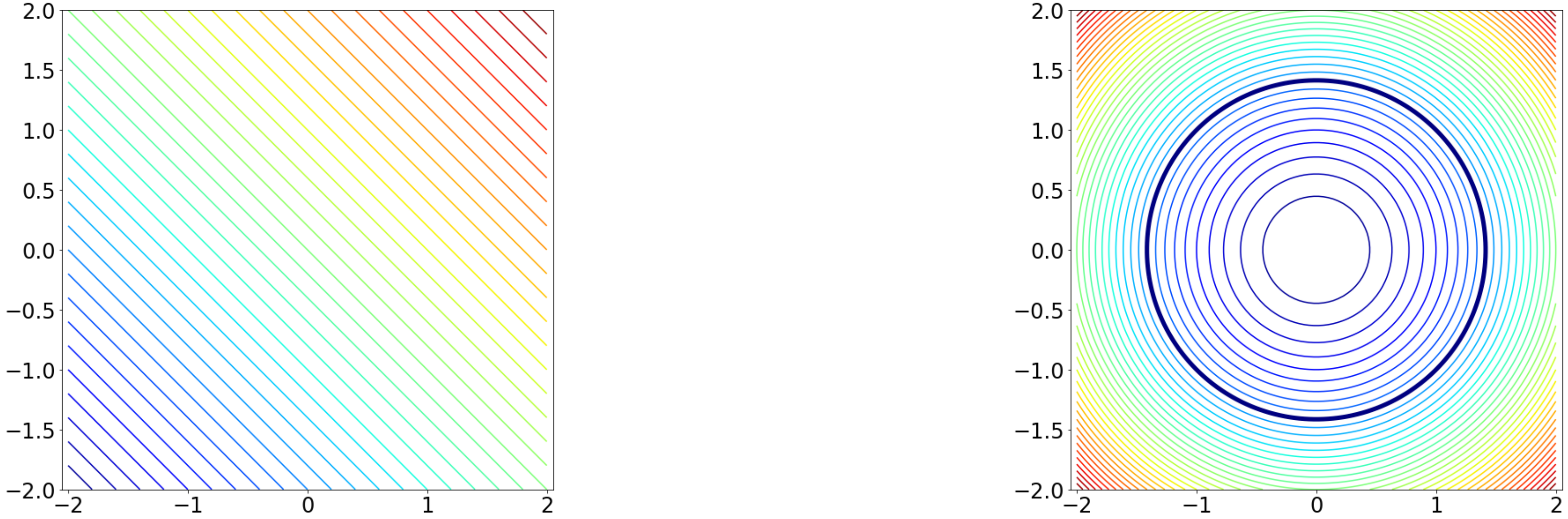
$f(\mathbf{x}) = x_1 + x_2$ $\qquad$ $h(\mathbf{x}) = x_1^2 + x_2^2 - 2$



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- Example

$$\begin{aligned} \min \quad & x_1 + x_2 \\ \text{subject to} \quad & x_1^2 + x_2^2 = 2 \end{aligned}$$

Solution: $\mathbf{x}^*$= (-1, -1)

Lagrange multipliers

$$\nabla f(\mathbf{x}^*) + \sum_{i=1}^{m} \lambda_i \nabla h_i(\mathbf{x}^*) = 0$$

Interpretations:

1. The cost gradient $\nabla f(\mathbf{x}^*)$ belongs to the subspace spanned by the constraint gradients at $\mathbf{x}^*$. That is, the constrained solution will be at a point of tangency of the constrained cost curves and the constraint function

Lagrange multipliers

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Interpretations:

1. The cost gradient $\nabla f(\mathbf{x}^*)$ belongs to the subspace spanned by the constraint gradients at $\mathbf{x}^*$. That is, the constrained solution will be at a point of tangency of the constrained cost curves and the constraint function
2. The cost gradient $\nabla f(\mathbf{x}^*)$ is orthogonal to the subspace of first order feasible variations

$$V(\mathbf{x}^*) = \{\Delta\mathbf{x} | \nabla h_i(\mathbf{x}^*)' \Delta\mathbf{x} = 0, \ i = 1, \ldots, m\}$$

This is the subspace of variations $\Delta\mathbf{x}$ for which the vector $\mathbf{x} = \mathbf{x}^* + \Delta\mathbf{x}$ satisfies the constraint $\mathbf{h}(\mathbf{x}) = 0$ up to first order. Hence, at a local minimum, the first order cost variation $\nabla f(\mathbf{x}^*)' \Delta \boldsymbol{x}$ is zero for all variations $\Delta\mathbf{x}$ in this subspace

NOC

Theorem: NOC

Let $\mathbf{x}^*$ be a local minimum of f subject to $\mathbf{h}(\mathbf{x}) = 0$ and assume that the constraint gradients $\nabla h_1(\mathbf{x}^*), \dots, \nabla h_m(\mathbf{x}^*)$ are linearly independent. Then there exists a unique vector $(\lambda_1, \dots, \lambda_m)$, called a Lagrange multiplier vector, such that

$$\nabla f(\mathbf{x}^*) + \sum_{i=1}^{m} \lambda_i \nabla h_i(\mathbf{x}^*) = 0$$

(2^{nd} order NOC and SOC are provided in AA203-Notes)

Discussion

- A feasible vector $\mathbf{x}$ for which $\{\nabla h_i(\mathbf{x})\}_i$ are linearly independent is called *regular**
- Proof relies on transforming the constrained problem into an unconstrained one
    1. penalty approach: we disregard the constraints while adding to the cost a high penalty for violating them → extends to inequality constraints
    2. elimination approach: we view the constraints as a system of m equations with n unknowns, and we express m of the variables in terms of the remaining $n - m$, thereby reducing the problem to an unconstrained problem

* There may not exist Lagrange multipliers for a local minimum that is not regular

The Lagrangian function

- It is often convenient to write the necessary conditions in terms of the Lagrangian function $L: \mathbb{R}^{n+m} \to \mathbb{R}$

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

- Then, if $\mathbf{x}^*$ is a local minimum which is regular, the NOC conditions are compactly written

$$\nabla_{\mathbf{x}} L(\mathbf{x}^*, \lambda^*) = 0$$
$$\nabla_{\lambda} L(\mathbf{x}^*, \lambda^*) = 0$$

System of $n + m$ equations with $n + m$ unknowns

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$$\begin{aligned} \min \quad & f(\mathbf{x}) \\ \text{subject to} \quad & h_i(\mathbf{x}) = 0, \qquad i = 1, \ldots, m \\ & g_j(\mathbf{x}) \leq 0, \qquad j = 1, \ldots, r \end{aligned}$$

- f, h_i, g_j are C^1
- Inequality Constrained Problem (ICP) in compact form

$$\begin{aligned} \min \quad & f(\mathbf{x}) \\ \text{subject to} \quad & \mathbf{h}(\mathbf{x}) = 0 \\ & \mathbf{g}(\mathbf{x}) \leq 0 \end{aligned}$$

Active constraints

For any feasible point, the set of active inequality constraints is denoted

$$A(\mathbf{x}) := \{j \mid g_j(\mathbf{x}) = 0\}$$

If $j \notin A(\mathbf{x})$, then the constraint is *inactive* at $\mathbf{x}$.

Active constraints

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Key points

- if $\mathbf{x}^*$ is a local minimum of the ICP, then $\mathbf{x}^*$ is also a local minimum for the identical ICP without the inactive constraints
- at a local minimum, active inequality constraints can be treated to a large extent as equalities

Active constraints

- Hence, if $\mathbf{x}^*$ is a local minimum of ICP, then $\mathbf{x}^*$ is also a local minimum for the equality constrained problem

$$\begin{aligned} \min \quad & f(\mathbf{x}) \\ \text{subject to} \quad & \mathbf{h}(\mathbf{x}) = 0 \\ & g_j(\mathbf{x}) = 0, \qquad \forall j \in A(\mathbf{x}^*) \end{aligned}$$

Active constraints

- Thus if $\mathbf{x}^*$ is regular, there exist Lagrange multipliers $(\lambda_1, \dots, \lambda_m)$ and $\mu_j^*, j \in A(\mathbf{x}^*)$, such that

$$\nabla f(\mathbf{x}^*) + \sum_{i=1}^{m} \lambda_i^* \nabla h_i(\mathbf{x}^*) + \sum_{j \in A(\mathbf{x}^*)} \mu_j^* \nabla g_j(\mathbf{x}^*) = 0$$

- or equivalently

$$\nabla f(\mathbf{x}^*) + \sum_{i=1}^{m} \lambda_i^* \nabla h_i(\mathbf{x}^*) + \sum_{j=1}^{r} \mu_j^* \nabla g_j(\mathbf{x}^*) = 0$$

$$\mu_j^* = 0 \quad \forall j \notin A(\mathbf{x}^*) \qquad (\text{indeed } \mu_j^* \geq 0)$$

Karush-Kuhn-Tucker NOC

Define the Lagrangian function

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

Theorem: KKT NOC

Let $\mathbf{x}^*$ be a local minimum for ICP where f, h_i, g_j are C^1 and assume $\mathbf{x}^*$ is regular (equality + active inequality constraints gradients are linearly independent). Then, there exist unique Lagrange multiplier vectors $(\lambda_1^*, \dots, \lambda_m^*)$, $(\mu_1^*, \dots, \mu_r^*)$ such that

$$\nabla_{\mathbf{x}} L(\mathbf{x}^*, \lambda^*, \mu^*) = 0$$

$$\mu_j^* \geq 0, \quad j = 1, \dots, r$$

$$\mu_j^* = 0 \qquad \forall j \notin A(\mathbf{x}^*)$$

Example

$$\begin{aligned} \min \quad & x^2 + y^2 \\ \text{s.t.} \quad & 2x + y \leq 2 \end{aligned}$$

Solution: $(0,0)$

Next time

Calculus of variations

(infinite-dimensional optimization!)