Optimization I: Motivation, One-Variable Algorithms

CS 205A:
Mathematical Methods for Robotics, Vision, and Graphics

Doug James (and Justin Solomon)

Optimization Objectives

Problem	**Objective**
Least-squares	$E(\vec{x}) = \|A\vec{x} - \vec{b}\|_2^2$
Project $\vec{b}$ onto $\vec{a}$	$E(c) = \|c\vec{a} - \vec{b}\|_2$
Eigenvectors of symmetric matrix	$E(\vec{x}) = \vec{x}^\top A\vec{x}$
Pseudoinverse	$E(\vec{x}) = \|\vec{x}\|_2^2$
Principal components analysis	$E(C) = \|X - CC^\top X\|_{\text{Fro}}$
Broyden step	$E(J_k) = \|J_k - J_{k-1}\|_{\text{Fro}}^2$

Optimization Constraints

Problem	Constraints
Least-squares	None
Project $\vec{b}$ onto $\vec{a}$	None
Eigenvectors of symmetric matrix	$\|\vec{x}\|_2 = 1$
Pseudoinverse	$A^\top A\vec{x} = A^\top \vec{b}$
Principal components analysis	$C^\top C = I_{d\times d}$
Broyden step	$J_k \cdot \Delta\vec{x} = \Delta f(\vec{x})$

Variational Problem-Solving

Define **objective function** measuring desirable properties and minimize it.

General Motivation

So far:

Optimality conditions solvable in closed-form

General Motivation

So far:

Optimality conditions solvable in closed-form

What if:

We're not so lucky?

Today

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

No constraints on $\vec{x}$.

Nonlinear Least-Squares

E.g. for fitting an exponential:

$$E(a,c) = \sum_i (y_i - ce^{ax_i})^2$$

Maximum Likelihood Estimation

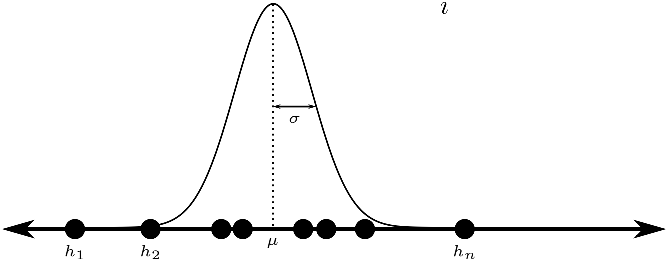
$$g(h;\mu,\sigma) \equiv \frac{1}{\sigma\sqrt{2\pi}} e^{-(h-\mu)^2/2\sigma^2}$$

Maximum Likelihood Estimation

$$g(h;\mu,\sigma) \equiv \frac{1}{\sigma\sqrt{2\pi}} e^{-(h-\mu)^2/2\sigma^2}$$

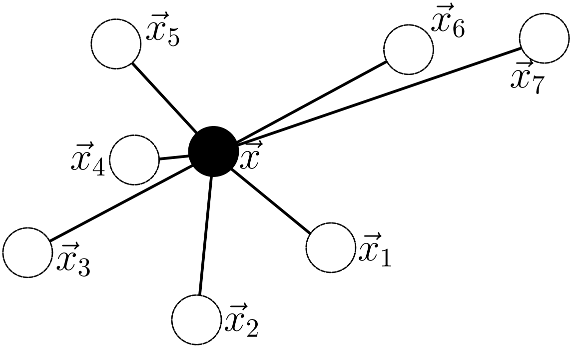
$$\Downarrow \text{ (independent sample)}$$

$$P(\{h_1,\ldots,h_n\};\mu,\sigma) = \prod_i g(h_i;\mu,\sigma)$$

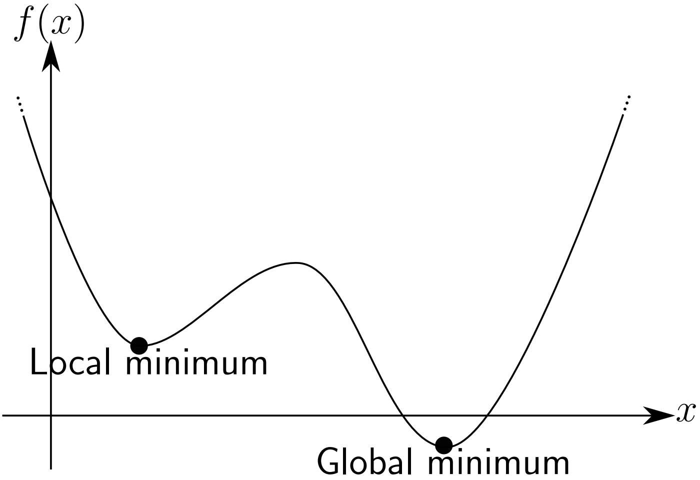


Geometric Median Problem

$$E(\vec{x}) \equiv \sum_i \|\vec{x} - \vec{x}_i\|_2$$



What are we looking for?



What are we looking for?

Global minimum

$\vec{x}^* \in \mathbb{R}^n$ is a *global minimum* of $f : \mathbb{R}^n \to \mathbb{R}$ if $f(\vec{x}^*) \leq f(\vec{x})$ for all $\vec{x} \in \mathbb{R}^n$.

What are we looking for?

Global minimum

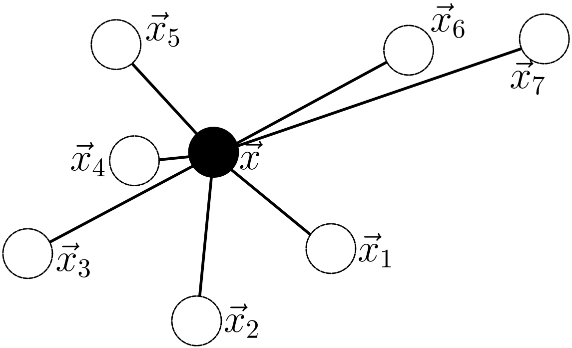
$\vec{x}^* \in \mathbb{R}^n$ is a *global minimum* of $f : \mathbb{R}^n \to \mathbb{R}$ if $f(\vec{x}^*) \leq f(\vec{x})$ for all $\vec{x} \in \mathbb{R}^n$.

Local minimum

$\vec{x}^* \in \mathbb{R}^n$ is a *local minimum* of $f : \mathbb{R}^n \to \mathbb{R}$ if $f(\vec{x}^*) \leq f(\vec{x})$ for all $\vec{x} \in \mathbb{R}^n$ satisfying $\|\vec{x} - \vec{x}^*\|_2 < \varepsilon$ for some $\varepsilon > 0$.

Ex: Equilibrium of Spring System

$$E(\vec{x}) \equiv \frac{1}{2}\sum_i k_i \left(\|\vec{x} - \vec{x}_i\|_2 - L_i\right)^2$$



Differential Optimality

$$f(\vec{x}) \approx f(\vec{x}_0) + \nabla f(\vec{x}_0) \cdot (\vec{x} - \vec{x}_0)$$

Differential Optimality

$$f(\vec{x}) \approx f(\vec{x}_0) + \nabla f(\vec{x}_0) \cdot (\vec{x} - \vec{x}_0)$$

Take: $\vec{x} - \vec{x}_0 = \alpha \nabla f(\vec{x}_0)$:

$$f(\vec{x}_0 + \alpha \nabla f(\vec{x}_0)) \approx f(\vec{x}_0) + \alpha \|\nabla f(\vec{x}_0)\|_2^2$$

Differential Optimality

$$f(\vec{x}) \approx f(\vec{x}_0) + \nabla f(\vec{x}_0) \cdot (\vec{x} - \vec{x}_0)$$

Take: $\vec{x} - \vec{x}_0 = \alpha \nabla f(\vec{x}_0)$:

$$f(\vec{x}_0 + \alpha \nabla f(\vec{x}_0)) \approx f(\vec{x}_0) + \alpha \|\nabla f(\vec{x}_0)\|_2^2$$

When $\|\nabla f(\vec{x}_0)\|_2 \neq 0$, the sign of α determines whether f increases or decreases.

Stationary Point

$$\nabla f(\vec{x}_0) = \vec{0}$$

Doesn't change to first order

Typical Strategy

1. Find critical point
2. Check if it is a local minimum
3. Repeat [optional]

Hessian

$$H_f(\vec{x}) = \begin{pmatrix} \frac{\partial^2 f}{\partial x_1^1} & \frac{\partial^2 f}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_n} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial^2 x_2} & \cdots & \frac{\partial^2 f}{\partial x_2 \partial x_n} \\ \vdots & \vdots & \cdots & \vdots \\ \frac{\partial^2 f}{\partial x_n \partial x_1} & \frac{\partial^2 f}{\partial x_n \partial x_2} & \cdots & \frac{\partial^2 f}{\partial^2 x_n} \end{pmatrix}$$

Hessian-Based Optimality

$$f(\vec{x}) \approx f(\vec{x}_0) + \nabla f(\vec{x}_0) \cdot (\vec{x} - \vec{x}_0) + \frac{1}{2}(\vec{x} - \vec{x}_0)^\top H_f(\vec{x} - \vec{x}_0)$$

Hessian-Based Optimality

$$f(\vec{x}) \approx f(\vec{x}_0) + \nabla f(\vec{x}_0) \cdot (\vec{x} - \vec{x}_0) + \frac{1}{2}(\vec{x} - \vec{x}_0)^\top H_f (\vec{x} - \vec{x}_0)$$

- H_f is *positive definite* $\implies$ local minimum
- H_f is *negative definite* $\implies$ local maximum
- H_f is *indefinite* $\implies$ saddle point
- H_f is *not invertible* $\implies$

Hessian-Based Optimality

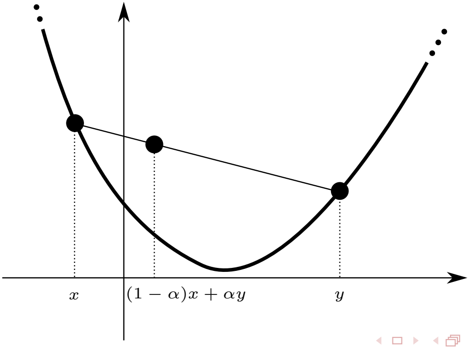
$$f(\vec{x}) \approx f(\vec{x}_0) + \nabla f(\vec{x}_0) \cdot (\vec{x} - \vec{x}_0) + \frac{1}{2}(\vec{x} - \vec{x}_0)^\top H_f(\vec{x} - \vec{x}_0)$$

- H_f is *positive definite* $\implies$ local minimum
- H_f is *negative definite* $\implies$ local maximum
- H_f is *indefinite* $\implies$ saddle point
- H_f is *not invertible* $\implies$ **nothing**

Alternative Optimality

Convex

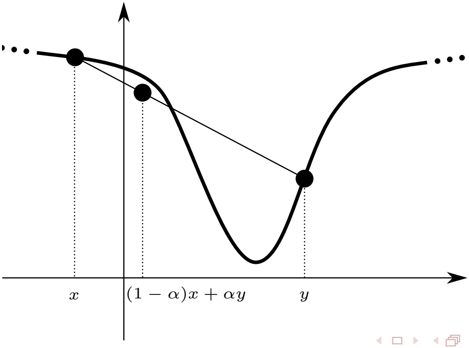
$f : \mathbb{R}^m \to \mathbb{R}$ is *convex* when for all $\vec{x}, \vec{y} \in \mathbb{R}^m$ and $\alpha \in (0,1)$, $f((1-\alpha)\vec{x} + \alpha\vec{y}) \leq (1-\alpha)f(\vec{x}) + \alpha f(\vec{y})$.



Alternative Optimality

Quasi-Convex

$f:\mathbb{R}^m\to\mathbb{R}$ is *convex* when for all $\vec{x},\vec{y}\in\mathbb{R}^m$ and $\alpha\in(0,1)$, $f((1-\alpha)\vec{x}+\alpha\vec{y})\leq\max(f(\vec{x}),f(\vec{y}))$.



Newton's Method

Minimize $f \leftrightarrow$ find roots of f'

Newton's Method

Minimize $f \leftrightarrow$ find roots of f'

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

Newton's Method

Minimize $f \leftrightarrow$ find roots of f'

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

Question:

What do you need for secant?

Newton's Method

Minimize $f \leftrightarrow$ find roots of f'

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

Question:

What do you need for secant?

Alternative: Successive parabolic interpolation

Imitate Bisection?

Question:

Analog of Intermediate Value Theorem?

Imitate Bisection?

Question:

Analog of Intermediate Value Theorem?

Unimodular

$f : [a, b] \to \mathbb{R}$ is *unimodular* if there exists $x^* \in [a, b]$ such that f is decreasing for $x \in [a, x^*]$ and increasing for $x \in [x^*, b]$.

Observations about Unimodular Functions

Consider $a < x_0 < x_1 < b$:

- $f(x_0) \geq f(x_1) \implies f(x) \geq f(x_1)$ for all $x \in [a, x_0] \implies [a, x_0]$ can be discarded
- $f(x_1) \geq f(x_0) \implies f(x) \geq f(x_0)$ for all $x \in [x_1, b] \implies [x_1, b]$ can be discarded

Unimodular Optimization v1.0

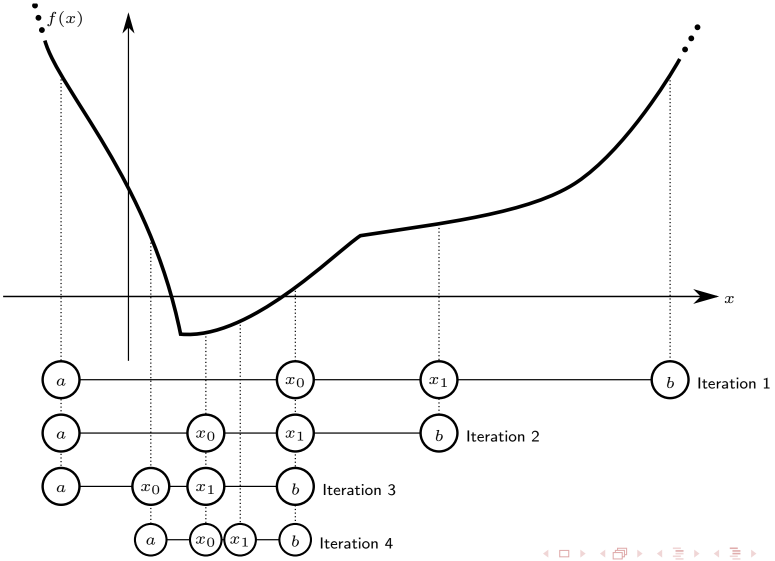
Iteratively remove $1/3$ of interval in each iteration.

Unimodular Optimization v1.0

Iteratively remove $^1/_3$ of interval in each iteration.

Requires two evaluations per iteration.

New Idea


f(x)
x
a
x0
x1
b
Iteration 1
a
x0
x1
b
Iteration 2
a
x0
x1
b
Iteration 3
a
x0
x1
b
Iteration 4

Reuse Evaluations?

$$x_0 = \alpha \quad x_1 = 1 - \alpha$$

$$\alpha \in (0, 1/2)$$

Reuse Evaluations?

$$x_0 = \alpha \quad x_1 = 1 - \alpha$$

$$\alpha \in (0, 1/2)$$

Remove right interval $[x_1, b]$
$\longrightarrow$new interval is $[0, 1 - \alpha]$.

Reuse Evaluations?

$$x_0 = \alpha \quad x_1 = 1 - \alpha$$

$$\alpha \in (0, 1/2)$$

Remove right interval $[x_1, b]$
$\longrightarrow$new interval is $[0, 1 - \alpha]$.

New bounds:

$$\tilde{x}_0 = \alpha(1 - \alpha)$$

$$\tilde{x}_1 = (1 - \alpha)^2$$

Reuse Evaluations?

To reuse: $(1-\alpha)^2 = \alpha$

$$\implies \quad \alpha = \frac{1}{2}(3-\sqrt{5})$$

$$1-\alpha = \frac{1}{2}(\sqrt{5}-1) \equiv \tau$$

Reuse Evaluations?

To reuse: $(1-\alpha)^2 = \alpha$

$$\implies \quad \alpha = \frac{1}{2}(3-\sqrt{5})$$

$$1-\alpha = \frac{1}{2}(\sqrt{5}-1) \equiv \tau$$

Golden ratio...

Golden Section Search

1. Initialize a and b so that f is unimodular on $[a, b]$.
2. Take $x_0 = a + (1 - \tau)(b - a), x_1 = a + \tau(b - a)$; initialize $f_0 = f(x_0), f_1 = f(x_1)$.
3. Iterate until $b - a$ is sufficiently small:
   - **3.1** If $f_0 \geq f_1$, then remove the interval $[a, x_0]$:
     - Move left side: $a \leftarrow x_0$
     - Reuse previous iteration: $x_0 \leftarrow x_1$, $f_0 \leftarrow f_1$
     - Generate new sample: $x_1 \leftarrow a + \tau(b - a)$, $f_1 \leftarrow f(x_1)$
   - **3.2** If $f_1 > f_0$, then remove the interval $[x_1, b]$:
     - Move right side: $b \leftarrow x_1$
     - Reuse previous iteration: $x_1 \leftarrow x_0$, $f_1 \leftarrow f_0$
     - Generate new sample: $x_0 \leftarrow a + (1 - \tau)(b - a)$, $f_0 \leftarrow f(x_0)$

Next