Large-scale Optimization

Georgios Paschos

Director of Science, Amazon

Introduction

- '02–'06 PhD – **University of Patras**
- '07–'08 Postdoc – **VTT, Helsinki**
- '08–'12 Lecturer – **University of Thessaly, Volos**
- '12–'14 Researcher – **MIT, Cambridge**
- '14–'19 Principal Scientist – **Huawei Technologies, Paris**
- '19–now Director, Applied Science – **Amazon, Luxembourg**

Best way to reach out about the course: gpasxos@gmail.com

Mathematical Programming

$$\begin{aligned} \underset{x}{\text{minimize}} \quad & f(x) \\ \text{subject to} \quad & g_i(x) \leq 0, \quad i = 1, \ldots, m \\ & h_j(x) = 0, \quad j = 1, \ldots, p \end{aligned}$$

- $x \in \mathbb{R}^n$ points available to choose
- $f : \mathbb{R}^n \to \mathbb{R}$ objective function to minimize
- $g_i(x) \leq 0$ the inequality constraints
- $h_j(x) = 0$ the equality constraints

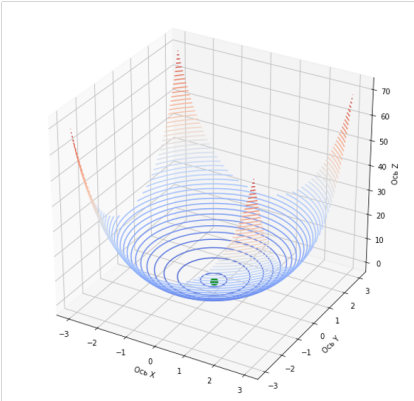

Fig from stackoverflow

Computer Sci, Engineering, Data Sci, Operation Research, Machine Learning, Economics, etc

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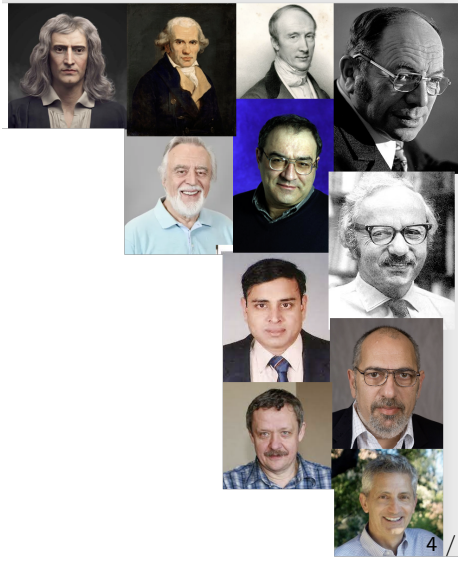
History

- Newton 1669 (Newton's method)
- Monge 1781 (optimal transport)
- Cauchy 1847 (steepest descent)
- Kantorovich 1939 (linear programming)
- Dantzig 1947 (simplex method)
- Karush/Kuhn-Tucker 1951 (KKT)
- Robbins et al 1952 (SGD)
- Glowinski et al 1975 (ADMM)
- Nemirovski 1979 (mirror descent)
- Khatchiyan 1979 (ellipsoid)
- Karmarkar 1984 (interior point)
- Orlin 1994 (network simplex)



More: mathematical-tours.github.io/algorithms/

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Where is it used today?

- Finance: portfolio optimization, utility theory
- Decision making with operation research
- Facility planning and flow optimization: trains, airports, petroleum industry, supply chain, etc
- Communication networks: information theory, congestion control protocols, medium access, etc
- Training ML models: backpropagation algorithm, regression
- Supervised/unsupervised learning: RL, clustering
- Transportation, logistics and engineering
- Robotics: model predictive control
- Image/signal processing
- **ADD YOUR FAVORITE...**

Quiz

- Which of the following is different from the rest?
  - Degree in computer science
  - Degree in engineering
  - Degree in pure mathematics
  - A large pizza

Quiz

- Which of the following is different from the rest?
  - Degree in computer science
  - Degree in engineering
  - Degree in pure mathematics
  - A large pizza

With the rest you can feed a family of 4!

Q: How do we solve optimization problems in real-life?

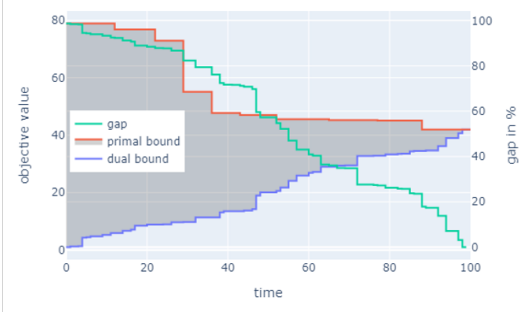
⇒ Cvx-opt - `https://cvxopt.org/`

⇒ SCIP

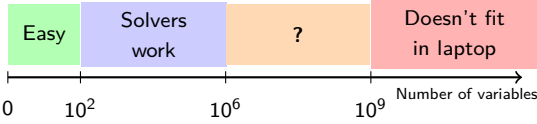
- AIMMS, AMPL, APMonitor, ASTOS, CPLEX
- Couenne – open source for MINLPs
- FICO Xpress, Galahad, GEKKO Python
- Gurobi - free for academic users
- LIONsolver, MIDACO, MINTO
- MOSEK – large scale optimization
- OptimJ, PottersWheel, Pyomo, WORHP

Sometimes solvers fail and you are needed

- LPs: today we solve ∼1M variables/1M constraints (Simplex, IPM, PDLP)

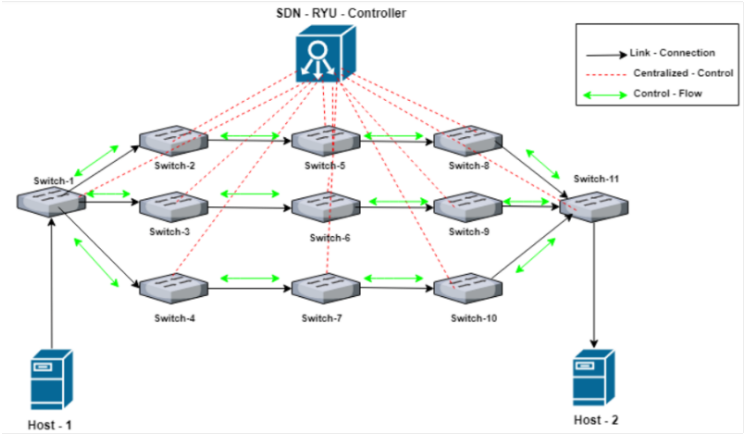


From Gurobi



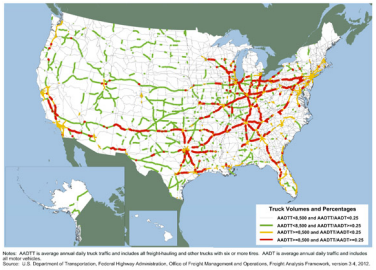
Large-scale example: Internet flow optimization

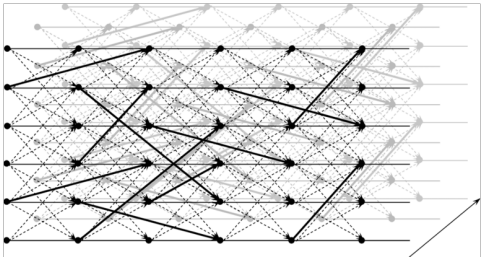
- Huawei SDN controllers: 10k od pairs, 10k links, **100M variables**



Large-scale example: truck scheduling

- Scheduling Amazon's trucks with time-expanded multicommodity flow in Europe
  - 10^3 commodities, 10^2 time slots, 10^2 nodes $\Rightarrow$ **100M var**





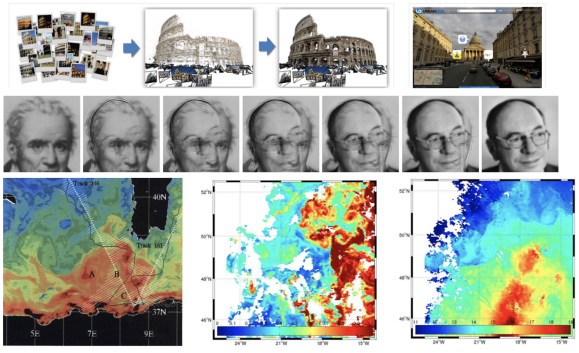
Question

- You have a linear program with 10 million variables representing Amazon's European truck routing.
- **Scenario A**: Gurobi gives you a solution in 2 hours that is provably optimal.
- **Scenario B**: A first-order method gives you a solution in 5 minutes that is 99.5% optimal.
- **Which would you choose and why?**
- **What factors influence this decision in practice?**

Consider: computational cost, business value, time constraints, solution quality needs.

Large-scale example: image processing

- Computer vision
  - 4Mpixels images $\Rightarrow$ $\mathbf{16}\times 10^{12}$ **variables** / pairs of pixels



reconstruction

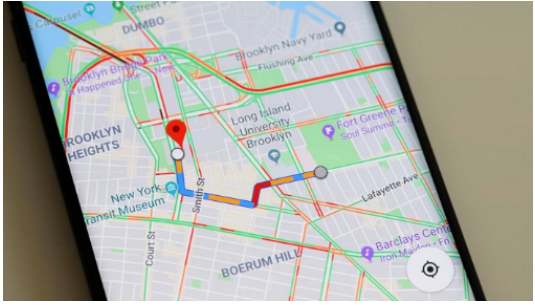
interpolation

weather model calibration

From Papadakis PhD

Large-scale example: Paths in Maps

- Finding a path in Google maps **>100M variables**
  - How does Google maps find the fastest path?



Visualization of a* algorithm https://www.youtube.com/watch?v=CgW0HPHqFE8

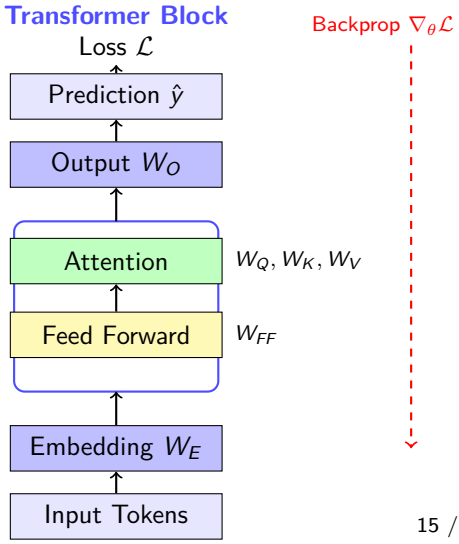
Large-scale example: training ChatGPT

Training = Optimization Problem

Find weights $\theta = \{W_E, W_Q, W_K, W_V, W_{FF}, W_O\}$ that minimize the loss:

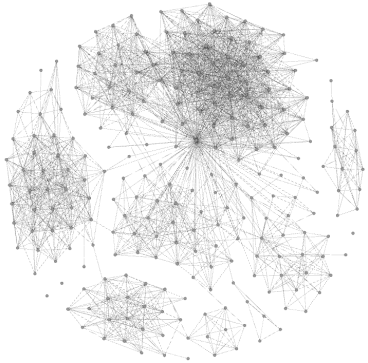
$$\underset{\theta}{\text{minimize}} \quad \mathcal{L}(\theta) = \sum_{i=1}^{N} \ell(y_i, \hat{y}_i(\theta))$$

- GPT-3 davinci: **175 Billion** parameters
- LLaMA-70B: **70 Billion** parameters



Large-scale example: big data clustering

- Finding a community in the Facebook graph $>$**100M variables**



https://snap.stanford.edu/data/

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Large-scale optimization course objectives

- Learn how to...
  - Recognize/classify an optimization problem
  - Solve optimization problems
  - Choose the right method at scale
  - Design new algorithms
- Focus on **convex programming**
- More broadly: how to employ mathematical modeling, algorithms, and python to solve problems.

Complexity map of optimization

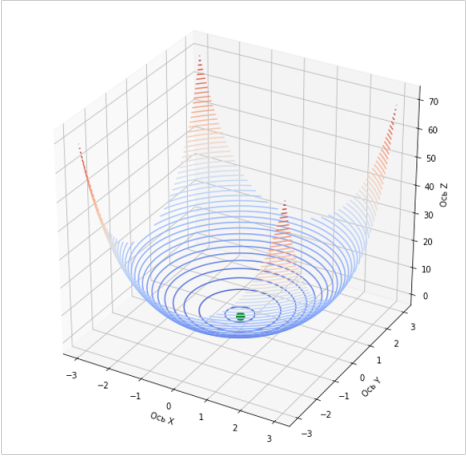
	Continuous	Discrete
Linear	**Linear** programming	**Integer** programming
Non-Linear but convex	**Convex** programming	
Non-Convex		

Question

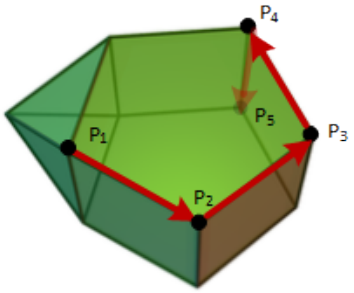
- Consider the problem of training a neural network with 1 billion parameters.
- **Where would you place this problem in our complexity map?**
  - Continuous or discrete?
  - Linear or non-linear?
  - Convex or non-convex?
- **Why is it still solvable in practice despite its classification?**

$$\begin{aligned} \underset{x}{\text{minimize}} \quad & f(x) \\ \text{subject to} \quad & g_i(x) \leq 0, \quad i = 1, \ldots, m \\ & Ax = b \end{aligned}$$

- Introduction to convexity
- First-order methods
- Training neural networks
- Newton methods
- Semi-definite programming ← **Alexios**

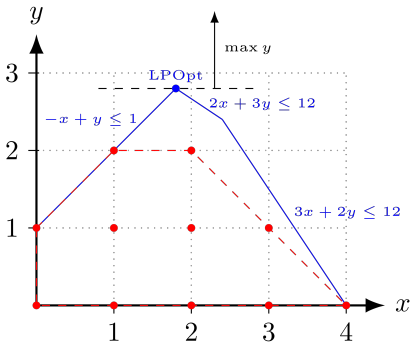


$$\begin{aligned} \underset{x \geq 0}{\text{maximize}} \quad & c^T x \\ \text{subject to} \quad & Ax \leq b \end{aligned}$$



- Simplex method
- LP duality
- Column generation
- **Interior point method** Newton-based
- **Primal-Dual (PDLP)** FOM

$$\begin{aligned} \underset{x}{\text{minimize}} \quad & c^T x \\ \text{subject to} \quad & x \in \mathbb{Z}^n \\ & Ax \leq b \end{aligned}$$



- Complexity – NP-complete problems
- Total unimodularity and shortest paths
- Branch and bound
- Cutting planes and Bender's cut
- Lagrangian relaxation
- Submodularity and greedy (max cover)
- LP Rounding (set cover)
- Heuristics

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Resources

- Presentations
  - **[Paschos]_lsopt_pres.pdf**
- Lecture notes
  - **[Paschos]_lsopt_notes.pdf** ongoing work - feedback welcomed
- Quizes
  - **Train multi-layer perceptron and achieve the best performance on MNIST**
  - **Implement PDHG and Interior Point for LP and compare them**
  - Submit quiz reports by 31/03/2026
- Python notebooks
  - https://github.com/gpasxos/large-scale-optimization
- External references available on Internet (**see next slide**)

References used in this course

[1] S. Boyd and L. Vandenberghe, "Convex Optimization", https://web.stanford.edu/~boyd/cvxbook/bv_cvxbook.pdf

[2] R. Tibshirani, "Convex Optimization", https://www.stat.cmu.edu/~ryantibs/convexopt-F18/

[3] C. Caramanis, "Optimization algorithms", https://www.youtube.com/playlist?list=PLXsmhnDvpjORzPelSDs0LSDrfJcqyLlZc

[4] C. Papadimitriou and K. Steiglitz, "Combinatorial Optimization, Algorithms and Complexity"

[5] G. Peyre, "Numerical tours", https://www.numerical-tours.com/

[6] D. Bertsekas, "Non-linear programming"

[7] Y. Nesterov, "Introductory lectures on convex optimization"

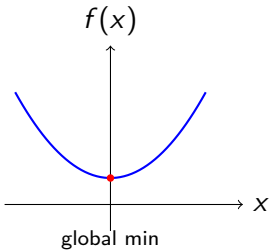
Linear Algebra refresher Prof. Caramanis: https://www.youtube.com/watch?v=FTzZff0uq9U

Part I

Introduction to Convexity

Convex vs Non-Convex

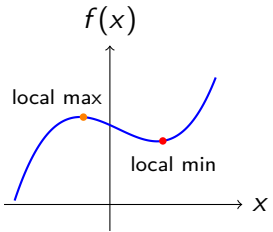
Convex



- Local min $\Rightarrow$ Global min
- Easy to find optimum
- Polynomial-time algorithms

Welcome to Paradise!

Non-Convex



- Can have many local extrema
- Can be very hard
- Worst-case exponential time

Abandon all hope!

Applications of Convex Programming

Finance & Economics:

- Portfolio optimization
- Optimal advertising
- Utility maximization

Machine Learning:

- Linear/Ridge/Lasso regression
- Logistic regression
- Support Vector Machines
- Neural network training

Engineering:

- Power allocation (wireless)
- Internet congestion control
- Network slicing
- Signal processing

Operations Research:

- Resource allocation
- Combinatorial relaxations

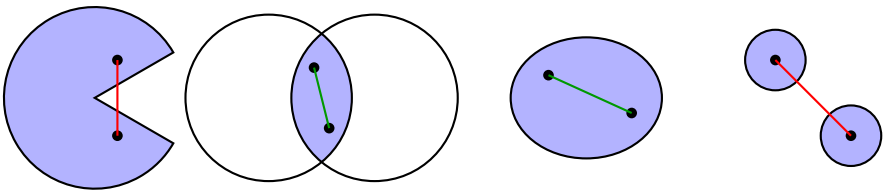
Outline

- **Convex sets** – definitions and examples
- **Convex functions** – definitions and examples
- **Operations preserving convexity**
- **Optimality conditions**
- **Smoothness and strong convexity**

Convex Sets

Definition. A set $\mathcal{X} \subseteq \mathbb{R}^n$ is **convex** if for any $x, y \in \mathcal{X}$:

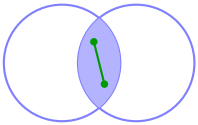
$$\theta x + (1-\theta)y \in \mathcal{X} \quad \text{for all } \theta \in [0,1]$$



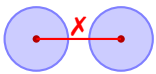
Non-convex Convex Convex Non-convex

Operations Preserving Set Convexity

Intersection: If $\mathcal{X}_1, \mathcal{X}_2$ are convex, then $\mathcal{X}_1 \cap \mathcal{X}_2$ is convex



Intersection is convex

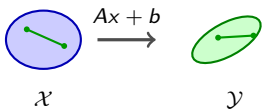


Union is NOT convex

Adding constraints to an optimization problem $\equiv$ intersecting with constraint sets

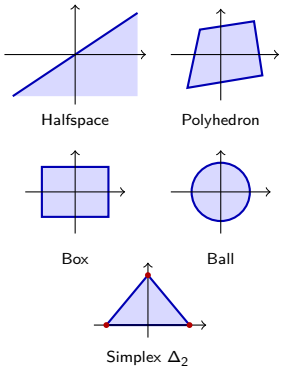
Affine maps: If $\mathcal{X}$ is convex and $y = Ax + b$, then

- $\mathcal{Y} = \{Ax + b : x \in \mathcal{X}\}$ is convex



Examples of Convex Sets

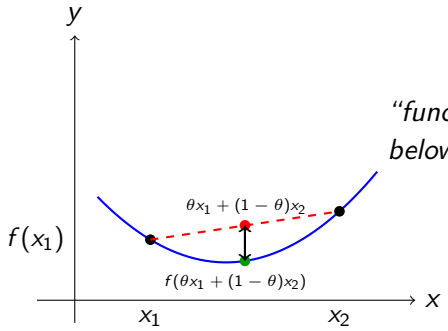
- **Hyperplane:** $\{x : a^\top x = b\}$
  Budget constraints, conservation laws, normalization
- **Halfspace:** $\{x : a^\top x \leq b\}$
  Capacity limits, resource constraints
- **Polyhedron:** $\{x : Ax \leq b,\ Cx = d\}$
  LP feasible regions, network flows, supply chains
- **Box:** $\{x : l \leq x \leq u\}$
  Variable bounds (prices, production levels)
- **Nonnegative orthant:** $\mathbb{R}^n_+ = \{x : x \geq 0\}$
  Physical quantities, costs, probabilities
- **Euclidean ball:** $\{x : \|x - x_0\|_2 \leq r\}$
  Regularization, trust regions, uncertainty sets
- **Simplex:** $\Delta_n = \{x : \sum_i x_i = 1,\ x \geq 0\}$
  Portfolio weights, probability distributions amazon



Convex Functions

Definition. A function $f : \mathcal{X} \to \mathbb{R}$ (where $\mathcal{X}$ is convex) is **convex** if:

$$f(\theta x + (1-\theta)y) \leq \theta f(x) + (1-\theta) f(y) \quad \text{for all } x, y \in \mathcal{X},\ \theta \in [0,1]$$



Q: *What if the gap is zero for all θ?*

Examples of Convex Functions on $\mathbb{R}$

Convex:

- Linear: $ax + b$
- Quadratic: $ax^2 + bx + c \quad (a > 0)$
- Exponential: e^{ax}
- Powers: x^a on $\mathbb{R}_+$ for $a \geq 1$ or $a \leq 0$
- Negative entropy: $x \log x$ on $\mathbb{R}_+$
- Piecewise linear: $\max_i (a_i x + b_i)$

Concave:

- Logarithm: $\log x$ on $\mathbb{R}_{++}$
- Powers: x^a on $\mathbb{R}_+$ for $0 < a < 1$
- Square root: $\sqrt{x}$

Both convex and concave:

- Affine: $ax + b$

Examples of Convex Functions on $\mathbb{R}^n$

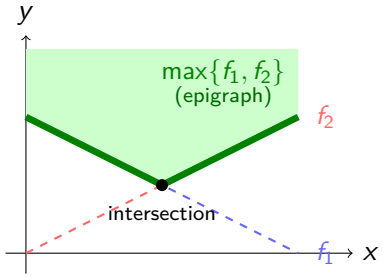
- **Affine:** $a^\top x + b$
- **Quadratic:** $\frac{1}{2}x^\top Qx + b^\top x + c$ where $Q \succeq 0$
- **ℓ_p-norms:** $\|x\|_p = \left(\sum_i |x_i|^p\right)^{1/p}$ for $p \geq 1$
- **Max function:** $\max\{x_1, \ldots, x_n\}$
- **Log-sum-exp:** $\log\left(\sum_{i=1}^n e^{x_i}\right)$ (smooth approximation to max)
- **Negative entropy:** $\sum_i x_i \log x_i$

Concave:

- **Log-determinant:** $\log\det(X)$ on $\mathbb{S}^n_{++}$
- **Geometric mean:** $\left(\prod_i x_i\right)^{1/n}$ on $\mathbb{R}^n_+$

Operations Preserving Function Convexity

- **Nonnegative weighted sum:** $f = w_1 f_1 + \cdots + w_m f_m \quad (w_i \geq 0)$
- **Composition with affine:** $g(x) = f(Ax + b)$
- **Pointwise maximum:** $f(x) = \max\{f_1(x), \ldots, f_m(x)\}$
- **Pointwise supremum:** $f(x) = \sup_{y \in \mathcal{Y}} g(x, y)$



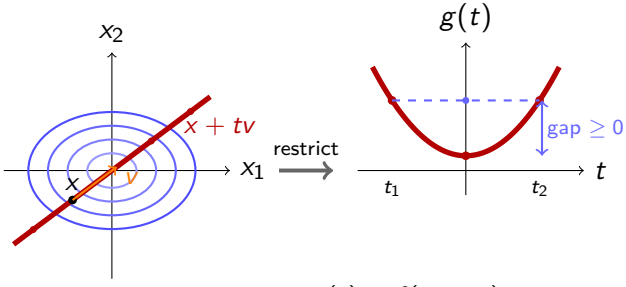
Epigraph of $\max\{f_1, f_2\}$ = intersection of epigraphs (both convex) $\Rightarrow$ convex

Restriction of f to a Line

Key insight: We can check convexity using 1D restrictions

Consider the function $g(t) = f(x + tv)$ where $t \in \mathbb{R}$, $x, v \in \mathbb{R}^n$

$$\boxed{g \text{ is convex in } t \text{ for all } x, v \iff f \text{ is convex}}$$



domain of f with level sets $g(t) = f(x + tv)$ **is convex**

We can disprove convexity in $\mathbb{R}^n$ by finding one violating point in $\mathbb{R}$

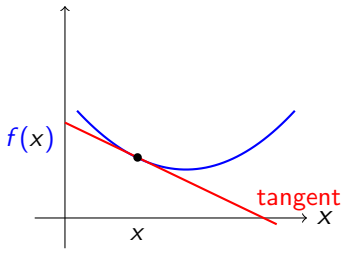
First-Order Condition for Convexity

Theorem. Let f be differentiable on convex $\mathcal{X}$. Then f is convex iff:

$$f(y) \geq f(x) + \nabla f(x)^\top (y - x) \quad \text{for all } x, y \in \mathcal{X}$$

Interpretation:

- Function lies above all its tangent planes



Important consequence:
If $\nabla f(x^*) = 0$, then for all y:

$$f(y) \geq f(x^*) + 0 = f(x^*)$$

Hence $\nabla f(x^*) = 0$ is a sufficient condition for x^* to be **global minimum**!

Q: *Does that mean we can use $\nabla f(x) = 0$ to solve all convex programs?*

amazon

Second-Order Condition for Convexity

Theorem. Let f be twice differentiable. Then f is convex iff:

$$\nabla^2 f(x) \succeq 0 \quad \text{for all } x \in \mathcal{X}$$

where the Hessian is:

$$\nabla^2 f(x) = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} & \cdots \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2^2} & \cdots \\ \vdots & \vdots & \ddots \end{bmatrix}$$

Interpretation:

- Hessian is symmetric: $\nabla^2 f(x) = \sum_i^n \lambda_i e_i e_i^T$
- All eigenvalues of Hessian are ≥ 0
- Curvature in every direction v is non-negative: $v^T \nabla^2 f(x) v = \sum_i^n \lambda_i v_i^2 \geq 0$
- If $\nabla^2 f(x) \succ 0$ (strictly positive definite), then f is **strictly convex**

Example: Log-Sum-Exp is Convex

Log-sum-exp: $f(x_1, x_2) = \log(e^{x_1} + e^{x_2})$ (smooth approximation to max)

Step 1: Gradient

$$\nabla f = \begin{bmatrix} \frac{e^{x_1}}{e^{x_1}+e^{x_2}} \\ \frac{e^{x_2}}{e^{x_1}+e^{x_2}} \end{bmatrix} = \begin{bmatrix} p_1 \\ p_2 \end{bmatrix}$$

where $p_i = \text{softmax}(x)_i, \quad p_1 + p_2 = 1$

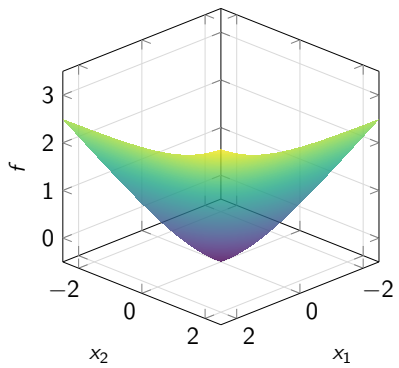
Step 2: Hessian

$$\nabla^2 f = \begin{bmatrix} p_1(1-p_1) & -p_1 p_2 \\ -p_1 p_2 & p_2(1-p_2) \end{bmatrix}$$

Since $p_1 + p_2 = 1$: $\quad \nabla^2 f = p_1 p_2 \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}$

Step 3: Check $\nabla^2 f \succeq 0$ For any $v \in \mathbb{R}^2$:

$$v^\top \nabla^2 f \, v = p_1 p_2 (v_1 - v_2)^2 \geq 0 \ \checkmark$$



Surface curves upward in all directions

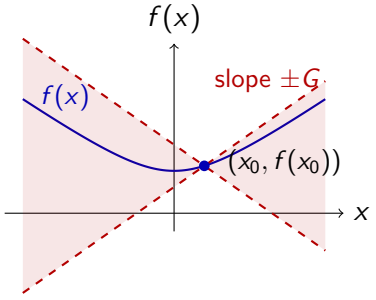
General case: $f(x) = \log \sum_{i=1}^{n} e^{x_i}$ has $\nabla^2 f = \text{diag}(p) - pp^\top \succeq 0$ (used in softmax, attention)

Lipschitz Continuity

Definition. Function f is G-**Lipschitz continuous** if:

$$|f(x) - f(y)| \leq G\|x - y\| \quad \text{for all } x, y \in \mathcal{X}$$

Equivalent condition (for differentiable f): $\|\nabla f(x)\| \leq G$



Bounded gradient norm $\Longrightarrow$ blanket assumption for most proofs

Examples: Lipschitz Continuity

Recall: f is G-Lipschitz if $|f(x) - f(y)| \leq G\|x - y\|$ (equivalently: $\|\nabla f(x)\| \leq G$)

1. **Linear:** $f(x) = a^\top x$

$$\nabla f = a \;\Rightarrow\; G = \|a\|$$

2. **Sigmoid:** $\sigma(z) = \frac{1}{1+e^{-z}}$

$$\sigma'(z) = \sigma(z)(1 - \sigma(z)) \leq \frac{1}{4}$$

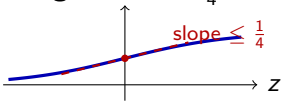
$\Rightarrow G = \frac{1}{4}$

3. **ReLU:** $f(z) = \max(0, z)$

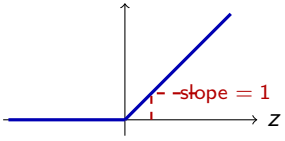
$$f'(z) \in \{0, 1\} \;\Rightarrow\; G = 1$$

4. **Softmax cross-entropy:**

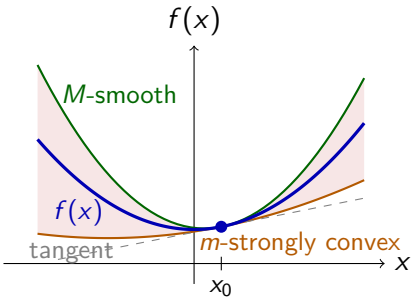
Sigmoid: $G = \frac{1}{4}$



ReLU: $G = 1$



Can we sandwich f within quadratic bounds?



M-**Smoothness:** $f(y) \leq f(x) + \nabla f(x)^\top (y - x) + \frac{M}{2}\|x - y\|^2$

m-**Strong convexity:** $f(y) \geq f(x) + \nabla f(x)^\top (y - x) + \frac{m}{2}\|x - y\|^2$

For $m = 0$: recover first-order convexity condition

Consequence of Strong Convexity

Useful bound: From strong convexity, minimizing the RHS over y:

$$f(y) \geq f(x) + \nabla f(x)^\top (y - x) + \frac{m}{2}\|x - y\|^2$$

Setting $\nabla_y(\text{RHS}) = 0$ gives $y^* = x - \frac{1}{m}\nabla f(x)$

Substituting back:

$$f(y) \geq f(x) - \frac{1}{2m}\|\nabla f(x)\|^2 \quad \text{for all } y$$

Key insight:

$$f(x) - f^* \leq \frac{1}{2m}\|\nabla f(x)\|^2$$

Small gradient $\Rightarrow$ we're close to the minimum — provides stopping criterion!

Strong Convexity: Examples

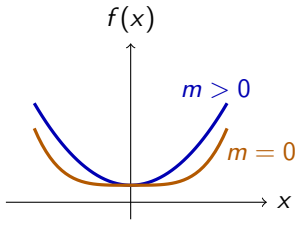
Recall: f is m-strongly convex if $\nabla^2 f(x) \succeq mI$ for all x

Strongly convex:

Function	m
$f(x) = \frac{1}{2}\|x\|^2$	1
$f(x) = \frac{1}{2}x^\top Qx, \quad Q \succ 0$	$\lambda_{\min}(Q)$
$f(x) = \|Ax - b\|^2, \quad A$ full rank	$2\lambda_{\min}(A^\top A)$

Not strongly convex:

$f(x) = \|Ax - b\|^2$	A rank-deficient
$f(x) = \|x\|_1$	not even smooth
$f(x) = \log \sum_i e^{x_i}$	$\lambda_{\min}(\nabla^2 f) = 0$



Blue: strongly convex (quadratic) Orange: convex, not strongly (x^4)

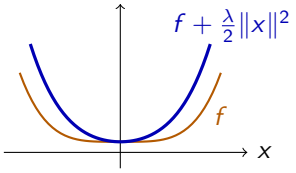
Regularization ⇒ Strong Convexity

Key trick: Adding $\frac{\lambda}{2}\|x\|^2$ to any convex f makes it strongly convex

Claim: If f is convex, then

$$g(x) = f(x) + \frac{\lambda}{2}\|x\|^2$$

is λ-strongly convex.



Proof:

$$\nabla^2 g(x) = \underbrace{\nabla^2 f(x)}_{\succeq 0} + \lambda I \succeq \lambda I \quad \checkmark$$

Ridge regression: $\|Ax - b\|^2 + \lambda\|x\|^2$

Weight decay: $\mathcal{L}(w) + \frac{\lambda}{2}\|w\|^2$

$\Rightarrow$ Unique minimum, faster convergence, better conditioning

Condition Number

Definition: The **condition number** of a smooth, strongly convex function:

$$\kappa = \frac{M}{m} \geq 1$$

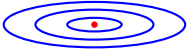
Well-conditioned (κ small):

- Nearly spherical level sets
- Fast convergence
- Algorithms work well

Ill-conditioned (κ large):

- Elongated level sets
- Slow convergence
- Algorithms struggle

$\kappa \approx 1$



$\kappa \gg 1$

Function Properties for Algorithm Analysis

Property	**Hessian**	**What it gives us**
Convex	$\nabla^2 f \succeq 0$	Local min = global min; no need to escape local minima
G-Lipschitz	$\|\nabla f\| \leq G$	Bounded gradients; controls step size in gradient & subgradient methods
M-smooth	$\nabla^2 f \preceq MI$	Bounded curvature; guarantees descent with step size $\eta = 1/M$; no line search needed
m-str. convex	$\nabla^2 f \succeq mI$	Unique minimum; linear convergence rate $O(\rho^k)$; stopping criterion

Condition number $\kappa = M/m$ determines convergence speed; smaller is better

Q: *Which is your favorite function now?*

amazon

Convex Programs

Definition 2.11 (Convex program). An optimization problem:

$$\begin{aligned} \underset{x}{\text{minimize}} \quad & f(x) \\ \text{subject to} \quad & g_i(x) \leq 0, \quad i = 1, \ldots, m \\ & Ax = b \end{aligned}$$

is a convex program if:

- f is convex
- g_i are convex for all i
- Equality constraints are affine

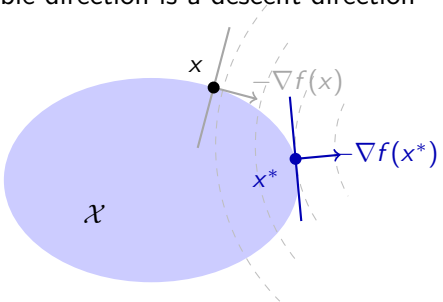
Key property: Every local optimum is a global optimum!

First-Order Optimality Condition for Convex Programs

Theorem. For a convex program with differentiable f, x^* is optimal if and only if:

$$\nabla f(x^*)^\top (y - x^*) \geq 0 \quad \text{for all feasible } y \in \mathcal{X}$$

Interpretation: No feasible direction is a descent direction



Special case – Unconstrained: Plugin $y = x^* - \nabla f(x^*)$ to get $\boxed{\nabla f(x^*) = 0}$

Optimality via $\nabla f = 0$: A System of Equations

Problem: $\min_{x \in \mathbb{R}^n} f(x)$ (unconstrained)

First-order necessary condition: $\nabla f(x^*) = 0$

System of n (generally nonlinear) equations

$$\begin{aligned} \frac{\partial f}{\partial x_1}(x^*) &= 0 \\ &\vdots \\ \frac{\partial f}{\partial x_n}(x^*) &= 0 \end{aligned}$$

Convex f:

- $\nabla f(x^*) = 0$ is **sufficient**
- Every solution is a **global minimum**

Non-convex f:

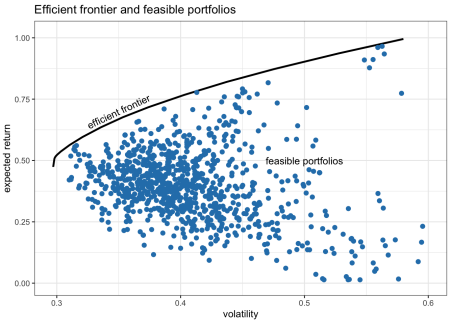
- $\nabla f(x^*) = 0$ is only **necessary**
- Solutions are **local extrema**

Q: *Why can't we just find all solutions to this system and compare?*

Example: Portfolio Optimization

Problem: Minimize risk for target return

$$\begin{aligned} \underset{x}{\text{minimize}} \quad & \frac{1}{2} x^\top \Sigma x \\ \text{subject to} \quad & \mathbf{1}^\top x = 1 \\ & \mu^\top x \geq r_{\min} \\ & x \geq 0 \end{aligned}$$



Efficient frontier: return vs. risk

- $\Sigma \succ 0$: covariance matrix
- μ: expected returns
- x_i: fraction in asset i

✓ Convex QP: $\Sigma \succ 0$

Example: Linear Regression

Least squares:

$$\underset{x}{\text{minimize}} \quad \|Ax - b\|_2^2$$

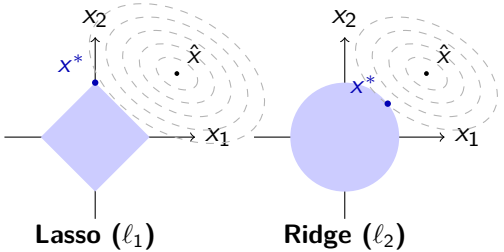
Ridge (L2 regularization):

$$\underset{x}{\text{minimize}} \quad \|Ax - b\|_2^2 + \lambda \|x\|_2^2$$

LASSO (L1, sparse solutions):

$$\underset{x}{\text{minimize}} \quad \|Ax - b\|_2^2 + \lambda \|x\|_1$$

✓ All three are convex!



LASSO vs Ridge constraint geometry

Geometry: Equivalent to $\min_x \|Ax - b\|^2$ s.t. $\|x\|_p \leq r$. Solution is where smallest ellipse touches the boundary. ℓ_1 ball has corners $\Rightarrow$ solution lands on axis $\Rightarrow$ **sparse!**

Example: Logistic Regression

Binary classification: $y_i \in \{0, 1\}$

Model:

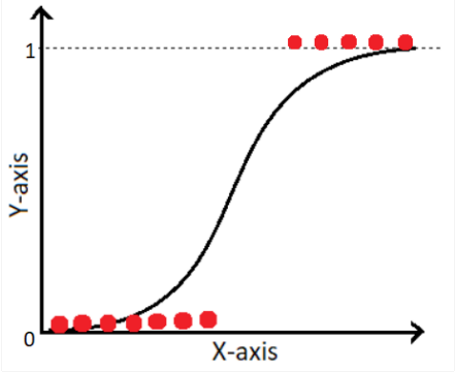
$$P(Y = 1 \mid x) = \frac{e^{a^\top x + b}}{1 + e^{a^\top x + b}}$$

Minimize negative log-likelihood:

$$\underset{a,b}{\text{minimize}} \sum_{i=1}^{m} [-y_i z_i + \log(1 + e^{z_i})]$$

where $z_i = a^\top x_i + b$

✓ Convex: $\log(1 + e^z)$ is convex



Sigmoid function & decision boundary

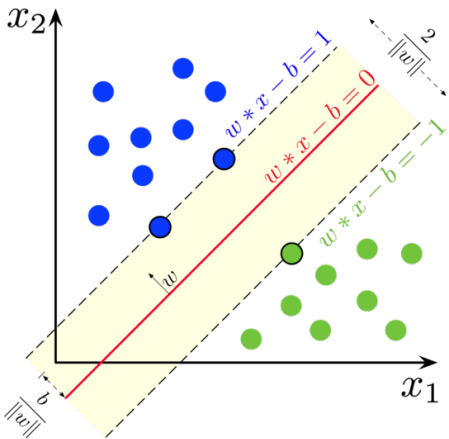
Example: Support Vector Machines

Maximum margin classifier:

$$\begin{aligned} \underset{w,b,\xi}{\text{minimize}} \quad & \frac{1}{2}\|w\|^2 + C\sum_{i=1}^{m}\xi_i \\ \text{subject to} \quad & y_i(w^\top x_i + b) \geq 1 - \xi_i \\ & \xi_i \geq 0 \end{aligned}$$

Equivalent (hinge loss):

$$\underset{w,b}{\text{minimize}} \quad \frac{1}{2}\|w\|^2 + C\sum_{i}[1 - y_i(w^\top x_i + b)]_+$$



Maximum margin & support vectors

✓ Convex QP

From Professor Winston: https://www.youtube.com/watch?v=_PwhiWxHK8o

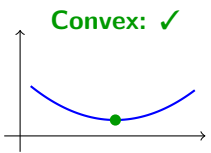
Why Convexity Matters

Convex programs are tractable:

- ✓ Local optima are global
- ✓ Polynomial-time algorithms
- ✓ Scalable to millions of variables
- ✓ Duality gives optimality certificates
- ✓ Rich theory for analysis

Recipe for success:

1. Recognize/formulate as convex program
2. Apply standard solver
3. Get guaranteed global optimum



Many local minima ⇒ hard to find global

Next: Gradient descent, Newton's method, Interior point methods

References for Convexity

[1] S. Boyd and L. Vandenberghe, "Convex Optimization", https://web.stanford.edu/~boyd/cvxbook/

[2] R. Tibshirani, "Convex Optimization", https://www.stat.cmu.edu/~ryantibs/convexopt-F18/

[3] Y. Nesterov, "Introductory Lectures on Convex Optimization"

[4] D. Bertsekas, "Convex Optimization Theory"

Part II

First-Order Methods for Unconstrained Optimization

Outline

Goal: Solve unconstrained convex optimization

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

using only function values $f(x)$ and gradients $\nabla f(x)$

- **Gradient descent** – the fundamental algorithm
- **Convergence analysis** – rates under different assumptions
- **Subgradient methods** – handling non-smooth functions
- **Lower bounds** – fundamental limits
- **Accelerated methods** – momentum and Nesterov's method

Iterative Algorithms

All methods generate a sequence $x^{(0)}, x^{(1)}, x^{(2)}, \ldots$ converging to x^*

General update:

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

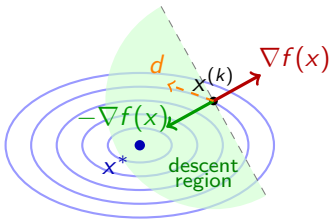
Key design choices:

- Direction $d^{(k)}$
- Step size $\eta^{(k)} > 0$

Key questions:

- Does it converge?
- How many iterations for $f(x^{(k)}) - f^* \leq \epsilon$?

Descent direction: $d^T \nabla f(x) < 0$



Any d with $d^T \nabla f(x) < 0$ decreases f; steepest descent uses $d = -\nabla f(x)$

Gradient Descent

$$x^{(k+1)} = x^{(k)} - \underbrace{\eta^{(k)}}_{\text{step size}} \underbrace{\nabla f(x^{(k)})}_{\text{direction } d}$$

Why negative gradient?

- $-\nabla f(x)$ points to locally steepest *decrease*
- The *direction* of $-\nabla f(x)$ minimizes $d^T \nabla f(x)$ over unit d

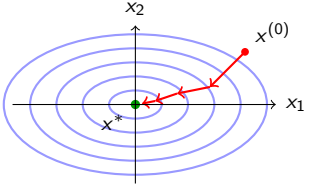
Motivation via quadratic model:

Minimize
$\hat{f}(y) = f(x) + \nabla f(x)^T (y - x) + \frac{1}{2\eta} \|y - x\|^2$

Setting $\nabla_y \hat{f} = 0$: $\quad y = x - \eta \nabla f(x)$

$\Rightarrow$ Each step minimizes a local quadratic model

Augustin-Louis Cauchy (1847)



Example 1d: Gradient Descent on $f(x) = 2x^2 + 1$

Setup:

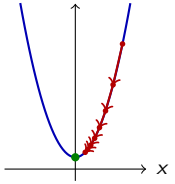
- Optimum: $x^* = 0$
- Gradient: $\nabla f(x) = 4x$
- Update: $x^{(k+1)} = (1 - 4\eta)x^{(k)}$

Convergence:

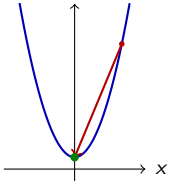
- $0 < \eta < \frac{1}{4}$: monotone
- $\eta = \frac{1}{4}$: one step!
- $\frac{1}{4} < \eta < \frac{1}{2}$: oscillates
- $\eta \geq \frac{1}{2}$: diverges

Key insight:

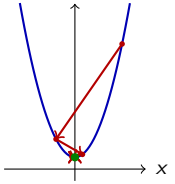
Step size must be small enough to converge, but larger $\Rightarrow$ faster



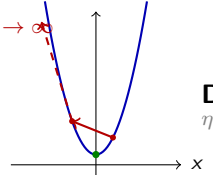
Too small
$\eta = 0.05$



Optimal
$\eta = 0.25$



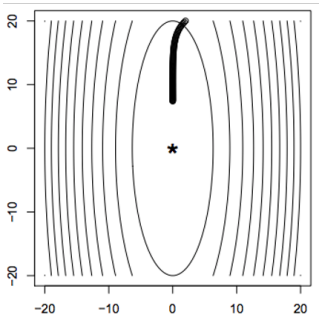
Oscillating
$\eta = 0.35$



Diverging
$\eta = 0.6$

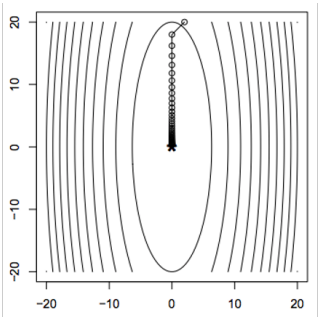
amazon

Effect of Step Size



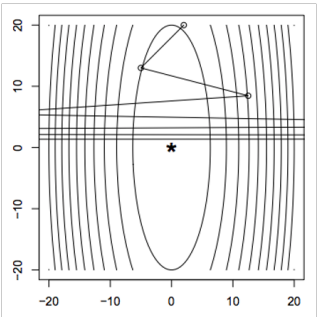
Too small

slow convergence



Just right

fast & stable



Too big

oscillates/diverges

Step Size Selection

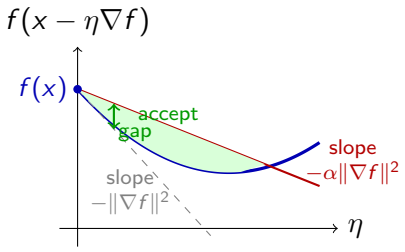
Four common strategies:

1. **Constant:** $\eta^{(k)} = \eta$ for all k
   - Simple, but requires knowing smoothness constant M
2. **Diminishing:** $\eta^{(k)} = c/\sqrt{k+1}$ or $\eta^{(k)} = c/(k+1)$
   - Conditions: $\sum_k \eta^{(k)} = \infty$ and $\sum_k (\eta^{(k)})^2 < \infty$
   - Essential for stochastic gradient descent
3. **Exact line search:** $\eta^{(k)} = \arg\min_{\eta \geq 0} f(x^{(k)} - \eta \nabla f(x^{(k)}))$
   - Optimal along gradient direction, but expensive
4. **Backtracking (Armijo's rule):** adaptive, practical
   - Start large, shrink until sufficient decrease

Armijo Rule (Backtracking Line Search)

Idea: Accept step η if it gives sufficient decrease:

$$f(x - \eta \nabla f(x)) \leq f(x) - \alpha \eta \|\nabla f(x)\|^2, \quad \alpha \in (0, 0.5)$$



Why terminates: Function slope $>$ Armijo slope at $\eta = 0$

$\Rightarrow$ gap always exists for small η

Backtracking:

1. Start with $\eta = 1$
2. While condition fails: $\eta \leftarrow \beta \eta$
3. Return η

Typical: $\alpha = 0.3$, $\beta = 0.5$

α	Effect
small	large steps
large	small steps
> 0.5	may reject $\frac{1}{M}$

Convergence Analysis: Setup

Recall function properties:

Property	Condition	Meaning
G-Lipschitz	$\|\nabla f(x)\| \leq G$	bounded gradients
M-smooth	$\nabla^2 f(x) \preceq MI$	bounded curvature
m-strongly convex	$\nabla^2 f(x) \succeq mI$	curved away from flat

Notation:

- $R = \|x^{(0)} - x^*\|$ (initial distance to optimum)
- $f_k^{\text{best}} = \min_{i \leq k} f(x^{(i)})$ (best value found so far)
- $\kappa = M/m$ (condition number)

More assumptions $\Rightarrow$ faster convergence rates

Convergence of Gradient Descent

Theorem (Convergence rates)

Let f be convex with bounded gradients $\|\nabla f(x)\| \leq G$.

1. **Lipschitz case:** With $\eta^{(k)} = R/(G\sqrt{k})$:

$$f_k^{\text{best}} - f^* \leq \frac{RG}{\sqrt{k}} \qquad \text{(convergence in } O(1/\epsilon^2) \text{ steps)}$$

2. **Smooth case:** If additionally M-smooth, with $\eta = 1/M$:

$$f_k^{\text{best}} - f^* \leq \frac{MR^2}{2k} \qquad \text{(convergence in } O(1/\epsilon) \text{ steps)}$$

3. **Strongly convex case:** If additionally m-strongly convex, with $\eta = 1/M$:

$$f(x^{(k)}) - f^* \leq \left(1 - \frac{1}{\kappa}\right)^k (f(x^{(0)}) - f^*) \quad (O(\kappa \log(1/\epsilon)) \text{ steps})$$

amazon

Proof Sketch: Lipschitz Case

Step 1: Track distance to optimum

$$\|x^{(k+1)} - x^*\|^2 = \|x^{(k)} - \eta^{(k)}\nabla f(x^{(k)}) - x^*\|^2 \qquad \text{expand norm} \|a-b\|^2 = \|a\|^2 - 2a^T b + \|b\|^2$$

$$= \|x^{(k)} - x^*\|^2 - 2\eta^{(k)}\nabla f(x^{(k)})^T(x^{(k)} - x^*) + (\eta^{(k)})^2\|\nabla f(x^{(k)})\|^2$$

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Step 2: Plug-in convexity $\nabla f(x^{(k)})^T(x^{(k)} - x^*) \geq f(x^{(k)}) - f^*$

$$\|x^{(k+1)} - x^*\|^2 \leq \|x^{(k)} - x^*\|^2 - 2\eta^{(k)}(f(x^{(k)}) - f^*) + (\eta^{(k)})^2\|\nabla f(x^{(k)})\|^2$$

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Step 3: Telescope and rearrange (using $\|\nabla f\| \leq G$, $\|x^{(0)} - x^*\| = R$)

$$f_k^{\text{best}} - f^* \leq \frac{R^2 + G^2\sum_{i=0}^{k-1}(\eta^{(i)})^2}{2\sum_{i=0}^{k-1}\eta^{(i)}}$$

Proof Sketch: Lipschitz Case

Step 1: Track distance to optimum

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Step 4: Optimize step size — for constant η:

$$f_k^{\text{best}} - f^* \leq \underbrace{\frac{R^2}{2k\eta}}_{\downarrow \text{ as } \eta\uparrow} + \underbrace{\frac{\eta G^2}{2}}_{\downarrow \text{ as } \eta\downarrow}$$

Proof Sketch: Lipschitz Case

Step 1: Track distance to optimum

$$\|x^{(k+1)} - x^*\|^2 = \|x^{(k)} - \eta^{(k)}\nabla f(x^{(k)}) - x^*\|^2 \qquad \text{expand norm} \|a-b\|^2 = \|a\|^2 - 2a^T b + \|b\|^2$$

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Setting $\frac{d}{d\eta}(\cdot) = 0$: $\quad \eta^* = \frac{R}{G\sqrt{k}} \quad \Rightarrow \quad \boxed{f_k^{\text{best}} - f^* \leq \frac{RG}{\sqrt{k}}}$

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Summary: Gradient Descent Convergence Rates

Assumptions	**Error after k**	**Iters for ϵ**	**Step size**
Convex, G-Lipschitz	$O(1/\sqrt{k})$	$O(1/\epsilon^2)$	$\eta = R/(G\sqrt{k})$
Convex, M-smooth	$O(1/k)$	$O(1/\epsilon)$	$\eta = 1/M$
m-SC, M-smooth	$O((1-1/\kappa)^k)$	$O(\kappa \log(1/\epsilon))$	$\eta = 1/M$

Example derivation If $\epsilon = \frac{C}{\sqrt{k}}$, then the number of iterations we need are: $k = \frac{C^2}{\epsilon^2}$

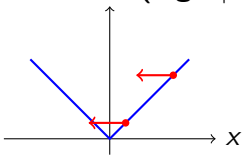
Interpreting the rates:

- $O(1/\sqrt{k})$: Slow – halving error requires $4\times$ iterations
- $O(1/k)$: Sublinear – halving error requires $2\times$ iterations
- $O(\rho^k)$: Linear – constant factor reduction per iteration

Why Smoothness Helps

Key insight: For smooth functions, the gradient "self-tunes"

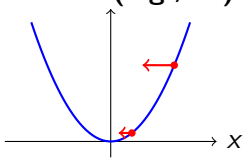
Non-smooth (e.g., $|x|$)



Gradient $= \pm 1$ always

Must use diminishing step size

Smooth (e.g., x^2)



Gradient $\to 0$ near x^*

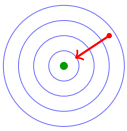
Fixed step size $\eta = 1/M$ works

From smoothness: $f(x^{(k+1)}) \leq f(x^{(k)}) - \frac{1}{2M}\|\nabla f(x^{(k)})\|^2$

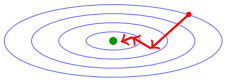
The gradient magnitude shrinks automatically as we approach the minimum!

Dependence on Condition Number

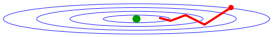
Condition number: $\kappa = M/m \geq 1$



$\kappa = 1$
circular, fast



$\kappa = 10$
elliptical, slower



$\kappa = 100$
narrow valley, zigzag

Convergence rate: $(1 - 1/\kappa)^k$

- $\kappa = 2$: error halves every ≈ 1.4 iterations
- $\kappa = 100$: error halves every ≈ 69 iterations
- $\kappa = 10000$: error halves every ≈ 6931 iterations

Ill-conditioned problems are hard for gradient descent!

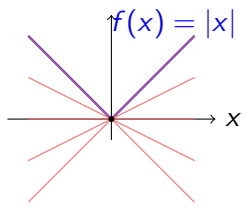
Subgradients for Non-Smooth Functions

Problem: f is convex but not differentiable everywhere

Definition: g is a **subgradient** of f at x if for all y:

$$f(y) \geq f(x) + g^T(y - x)$$

The **subdifferential** $\partial f(x)$ is the set of all subgradients at x



$\partial f(0) = [-1, 1]$

Examples:

- $f(x) = |x|$: $\partial f(0) = [-1, 1]$
- $f(x) = \|x\|_1$:
$$(\partial f(x))_i = \begin{cases} \text{sign}(x_i) & x_i \neq 0 \\ [-1, 1] & x_i = 0 \end{cases}$$
- $f(x) = \max_i(a_i^T x + b_i)$:

$$\partial f(x) = \text{conv}\{a_i : i \in I(x)\}$$

Optimality condition: $0 \in \partial f(x^*)$

where $I(x) = \{i : a_i^T x + b_i = f(x)\}$ (active set)

Subgradient Method

Algorithm:

$$x^{(k+1)} = x^{(k)} - \eta^{(k)} g^{(k)}, \quad \text{where } g^{(k)} \in \partial f(x^{(k)})$$

Warning

Subgradient direction is **not** necessarily a descent direction!
Function value may increase: $f(x^{(k+1)}) > f(x^{(k)})$
$\Rightarrow$ Track best iterate: $f_k^{\text{best}} = \min_{i \le k} f(x^{(i)})$

Theorem (Convergence)

With $\|g\| \le G$ for all $g \in \partial f(x)$ and step size $\eta^{(k)} = R/(G\sqrt{k})$:

$$f_k^{\text{best}} - f^* \le \frac{RG}{\sqrt{k}} \qquad \text{(convergence in } O(1/\epsilon^2) \text{ steps)}$$

Same rate as Lipschitz gradient descent – but cannot do better for non-smooth!

Lower Bounds: Fundamental Limits

Question: How fast can *any* first-order method converge?

Theorem (Nesterov's lower bounds)

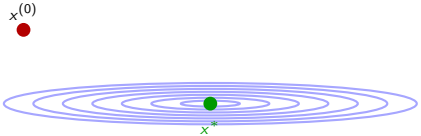
Using only $f(x)$ and $\nabla f(x)$ queries, to achieve $f(x^{(k)}) - f^* \leq \epsilon$:

Setting	**Lower bound**	**GD achieves**
G-Lipschitz convex	$\Omega(1/\epsilon^2)$	$O(1/\epsilon^2)$ ✓
M-smooth convex	$\Omega(1/\sqrt{\epsilon})$	$O(1/\epsilon)$ ✗
m-SC, M-smooth	$\Omega(\sqrt{\kappa}\log(1/\epsilon))$	$O(\kappa\log(1/\epsilon))$ ✗

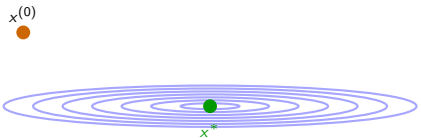
Key insight: GD is optimal for non-smooth, but suboptimal for smooth!

Can we close these gaps? **Yes!** $\rightarrow$ Accelerated methods

The Problem with Gradient Descent

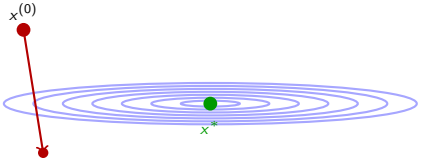


Gradient Descent

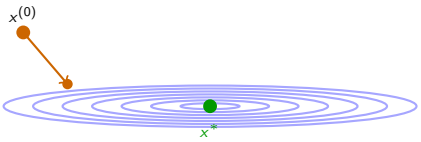


Momentum Method

The Problem with Gradient Descent



Gradient Descent



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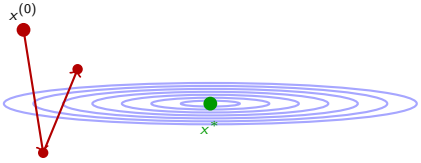
The Problem with Gradient Descent



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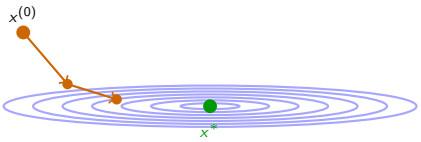

Momentum Method

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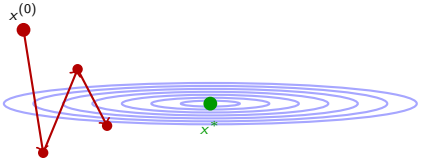

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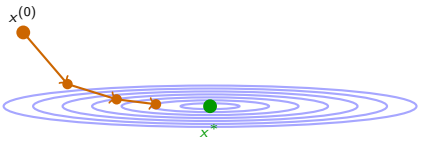
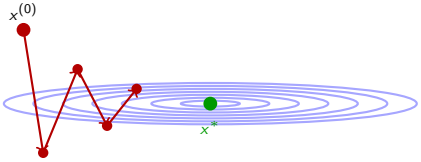


Momentum Method

The Problem with Gradient Descent



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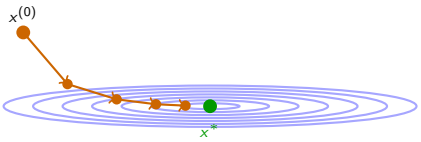
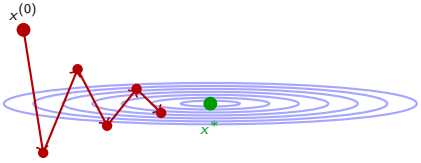
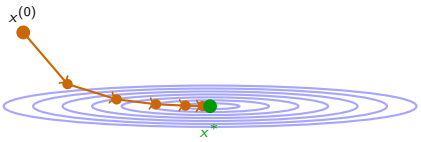


Momentum Method

The Problem with Gradient Descent



Gradient Descent



Momentum Method

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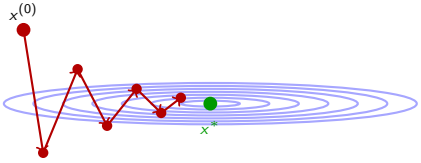

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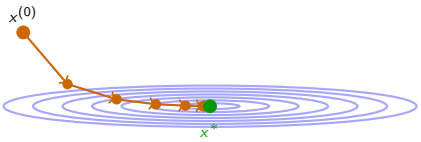

Momentum Method

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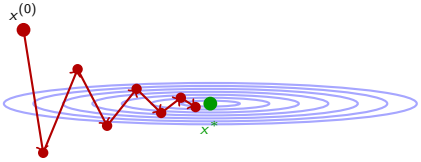

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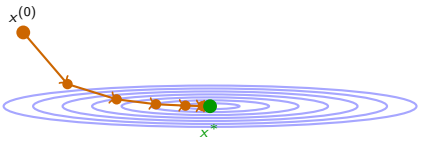

Momentum Method

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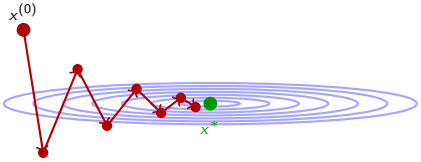
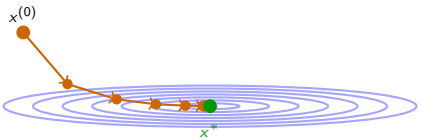


Gradient Descent

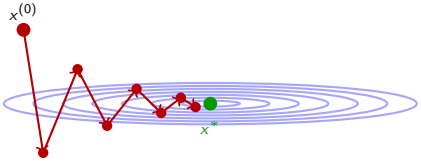
Gradient points to nearest contour, not toward optimum $\Rightarrow$ **zigzag**



Momentum Method

Momentum averages directions, cancels oscillations $\Rightarrow$ **smooth**

The Problem with Gradient Descent



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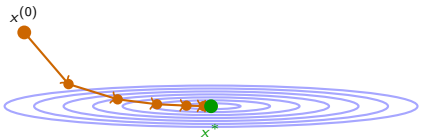

Momentum Method

Momentum averages directions, cancels oscillations $\Rightarrow$ **smooth**

Key insight: Momentum builds speed along consistent directions, dampens oscillations

Heavy Ball Method (Polyak, 1964)

$$\boxed{x^{(k+1)} = x^{(k)} - \eta \nabla f(x^{(k)}) + \beta(x^{(k)} - x^{(k-1)})}$$

new gradient step momentum term (previous)

Intuition: A heavy ball rolling downhill

- Without momentum ($\beta = 0$): gets bounced in valleys
- With momentum ($\beta > 0$): accumulates speed along consistent directions, cancels oscillations across inconsistent ones

Optimal parameters (for quadratics with eigenvalues in $[m, M]$):

$$\eta^* = \frac{4}{(\sqrt{M} + \sqrt{m})^2}, \quad \beta^* = \left(\frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1}\right)^2$$

Nesterov's Accelerated Gradient (1983)

Key innovation: Evaluate gradient at *lookahead* point

$$\begin{aligned} x^{(k+1)} &= y^{(k)} - \eta \nabla f(y^{(k)}) && \text{(gradient step from lookahead)} \\ y^{(k+1)} &= x^{(k+1)} + \frac{k}{k+3}(x^{(k+1)} - x^{(k)}) && \text{(momentum/extrapolation)} \end{aligned}$$

Momentum coefficient: $\frac{k}{k+3}$ grows from 0 toward 1

- Early: rely on gradient information
- Later: trust momentum built from history

Theorem (Optimal rate for smooth convex)

With $\eta = 1/M$:

$$f(x^{(k)}) - f^* \leq \frac{2M\|x^{(0)} - x^*\|^2}{(k+1)^2} \qquad \text{(convergence in } O(1/\sqrt{\epsilon}) \text{ steps)}$$

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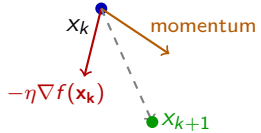
From Heavy Ball to Nesterov's Accelerated Gradient

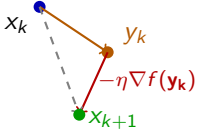
Key idea: Evaluate gradient at lookahead point instead of current point

Heavy Ball



$$x_{k+1} = x_k - \eta\nabla f(\mathbf{x_k}) + \beta(x_k - x_{k-1})$$

Nesterov



$$x_{k+1} = x_k - \eta\nabla f(\mathbf{y_k}) + \beta_k(x_k - x_{k-1})$$
where $y_k = x_k + \beta_k(x_k - x_{k-1})$

	Heavy Ball	**Nesterov**
Gradient at	current x_k	lookahead y_k
Momentum β	fixed (needs tuning)	$\frac{k-1}{k+2} \to 1$
Smooth + strongly cvx	$O\left(\left(1 - \sqrt{m/M}\right)^k\right)$	$O\left(\left(1 - \sqrt{m/M}\right)^k\right)$
Smooth only	may diverge	$O\left(\frac{1}{k^2}\right)$

Acceleration for Strongly Convex Functions

For m-strongly convex, M-smooth functions:

Nesterov variant: Use constant momentum $\beta = \frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}$

$$f(x^{(k)}) - f^* \leq \left(1 - \frac{1}{\sqrt{\kappa}}\right)^k (f(x^{(0)}) - f^*)$$

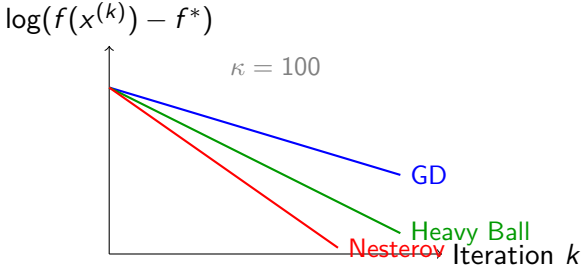
Comparison of rates:

Method	**Rate per iteration**	**Iters for ϵ**
Gradient Descent	$1 - \frac{1}{\kappa}$	$O(\kappa \log(1/\epsilon))$
Nesterov	$1 - \frac{1}{\sqrt{\kappa}}$	$O(\sqrt{\kappa} \log(1/\epsilon))$

Example: $\kappa = 10000$

- GD: $\approx 10000 \times \log(1/\epsilon)$ iterations
- Nesterov: $\approx 100 \times \log(1/\epsilon)$ iterations – 100× speedup!

Comparing Momentum Methods



Method	Step size	Momentum	Rate
Gradient Descent	$1/M$	–	$(1 - 1/\kappa)^k$
Heavy Ball	$4/(\sqrt{M} + \sqrt{m})^2$	$(\frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1})^2$	$(1 - 1/\sqrt{\kappa})^k$
Nesterov	$1/M$	$\frac{k}{k+3}$ or fixed	$(1 - 1/\sqrt{\kappa})^k$

Source: Nice illustrations of momentum methods for machine learning

Summary: First-Order Methods

Method	Assumptions	Rate	Optimal?
Subgradient	G-Lipschitz	$O(1/\sqrt{k})$	✓
GD	G-Lipschitz	$O(1/\sqrt{k})$	✓
GD	M-smooth	$O(1/k)$	✗
GD	m-SC, M-smooth	$O((1-1/\kappa)^k)$	✗
Heavy Ball	m-SC, M-smooth	$O((1-1/\sqrt{\kappa})^k)$	✓
Nesterov	M-smooth	$O(1/k^2)$	✓
Nesterov	m-SC, M-smooth	$O((1-1/\sqrt{\kappa})^k)$	✓

Practical guidance:

- Non-smooth $\rightarrow$ Subgradient with diminishing step sizes
- Smooth $\rightarrow$ Nesterov (if you know M) or GD with backtracking
- Strongly convex + smooth $\rightarrow$ Heavy Ball or Nesterov variant

Practical Tips

Choosing a method:

1. Know your function properties (G, M, m if possible)
2. Start with GD + backtracking (robust baseline)
3. Try momentum if convergence is slow
4. Use Nesterov for smooth problems when M is known

Debugging convergence issues:

- Diverging? $\rightarrow$ Reduce step size
- Oscillating? $\rightarrow$ Reduce step size or add momentum
- Converging too slowly? $\rightarrow$ Increase step size or use acceleration
- Stuck at suboptimal point? $\rightarrow$ Check convexity!

Step size heuristics:

- Start with $\eta = 1$ and backtrack
- For quadratics: $\eta = 1/\lambda_{\max}(Q)$
- For neural networks: typical range 10^{-4} to 10^{-1}

References

[1] S. Boyd and L. Vandenberghe, "Convex Optimization", https://web.stanford.edu/~boyd/cvxbook/

[2] Y. Nesterov, "Introductory Lectures on Convex Optimization: A Basic Course", Springer, 2004

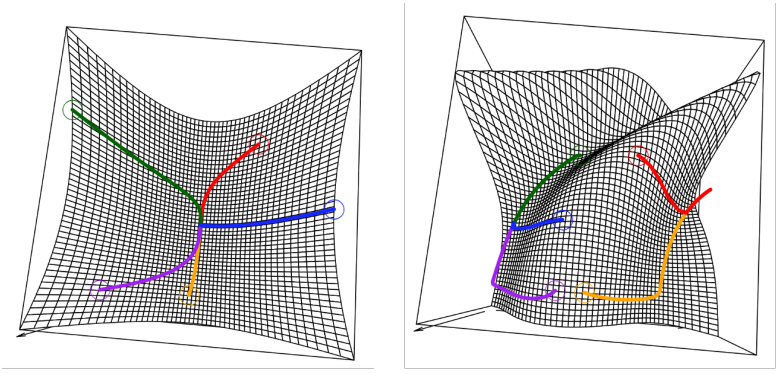
[3] B. Polyak, "Some methods of speeding up the convergence of iteration methods", USSR Computational Mathematics and Mathematical Physics, 1964

[4] Y. Nesterov, "A method of solving a convex programming problem with convergence rate $O(1/k^2)$", Soviet Mathematics Doklady, 1983

[5] A. Beck and M. Teboulle, "A Fast Iterative Shrinkage-Thresholding Algorithm for Linear Inverse Problems", SIAM J. Imaging Sciences, 2009

Convex vs Non-Convex Optimization

Convex | **Non-Convex**



GD on non-convex: converges to **stationary point** ($\nabla f = 0$), but no guarantee it's global optimum. Active research area in deep learning!

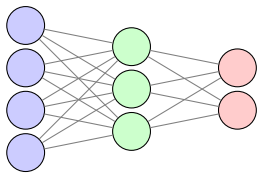
Part III

Training Neural Networks

Why This Matters

The Deep Learning Revolution:

- Image recognition
- Natural language processing
- Game playing (AlphaGo)
- Protein folding
- Large Language Models



At its core:

Training a neural network =
Solving an optimization problem

Find weights that minimize prediction error

Empirical Risk Minimization

Given n data points (a_i, b_i):

$$f(x) = \frac{1}{n} \sum_{i=1}^{n} \ell(h_x(a_i), b_i)$$

- h_x = model with parameters x
- ℓ = loss function (e.g., squared error, cross-entropy)
- n = number of training samples

The Scalability Problem

Full gradient descent:

$$x^{(k+1)} = x^{(k)} - \eta \nabla f(x^{(k)}) = x^{(k)} - \eta \cdot \frac{1}{n} \sum_{i=1}^{n} \nabla f_i(x^{(k)})$$

Cost per iteration: $O(n)$ gradient evaluations

Dataset	**Size** n
MNIST	60,000
ImageNet	1,200,000
Common Crawl	100,000,000,000+

Computing the full gradient once can take hours or days!

The Key Idea: Stochastic Gradients

Instead of computing the full gradient:

$$\nabla f(x) = \frac{1}{n}\sum_{i=1}^{n} \nabla f_i(x) \quad \text{(expensive: } O(n)\text{)}$$

Use a random sample as an estimate:

$$\nabla f_{i_k}(x) \quad \text{where } i_k \sim \text{Uniform}\{1, \ldots, n\} \quad \text{(cheap: } O(1)\text{)}$$

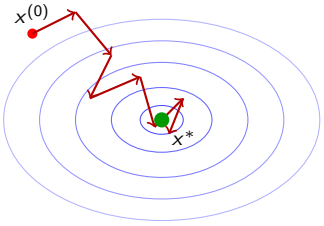
Why does this work?

$$\mathbb{E}_{i_k}[\nabla f_{i_k}(x)] = \frac{1}{n}\sum_{i=1}^{n} \nabla f_i(x) = \nabla f(x)$$

Unbiased estimate! On average, we point in the right direction.

Stochastic Gradient Descent

1. **Input:** Initial $x^{(0)}$, step sizes $\{\eta^{(k)}\}$, iterations K
2. **For** $k = 0, 1, \ldots, K-1$:
   - Sample i_k uniformly from $\{1, \ldots, n\}$
   - $x^{(k+1)} \leftarrow x^{(k)} - \eta^{(k)} \nabla f_{i_k}(x^{(k)})$
3. **Return** average $\bar{x}^{(K)} = \frac{1}{K} \sum_{k=0}^{K-1} x^{(k)}$



Key properties:

- Cost per iteration: $O(1)$ instead of $O(n)$
- Noisy updates, but correct *on average*

Why return the average?

- In theory: full average; in practice: last few iterates

Mini-Batch SGD

Idea: Use a small batch of b samples instead of just one:

$$x^{(k+1)} = x^{(k)} - \eta^{(k)} \cdot \frac{1}{b} \sum_{j \in B_k} \nabla f_j(x^{(k)})$$

where $B_k \subset \{1, \ldots, n\}$ is a random subset of size b.

Why mini-batches?

Variance Reduction	**Parallelism**	**Hardware**
Averaging b samples reduces variance by factor b	b gradients computed in parallel on GPU	Modern GPUs optimized for batch operations

Typical batch sizes: 32, 64, 128, 256, 512

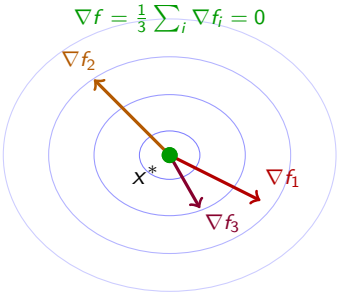
Convergence Analysis: The Variance Challenge

Key insight: At x^*, the full gradient vanishes but individual gradients do not!

Full gradient is the average:

$$\nabla f(x^*) = \frac{1}{n}\sum_{i=1}^{n} \nabla f_i(x^*) = 0$$

But each $\nabla f_i(x^*) \neq 0$ in general!



Individual gradients cancel on average, but SGD sees only one at a time

With constant step η: oscillates in neighborhood of size $\sim \eta\sigma$. To converge $\Rightarrow$ **diminishing step sizes**

Convergence of SGD

Theorem. Let $f(x) = \frac{1}{n}\sum_{i=1}^{n} f_i(x)$ with each f_i convex and M-smooth, and $\sigma^2 < \infty$.

***M*-smooth case:** With constant step size η:

$$\mathbb{E}[f(\bar{x}^{(K)})] - f^* \leq \underbrace{\frac{R^2}{\eta K}}_{\text{optimization}} + \underbrace{\eta\sigma^2}_{\text{noise}}$$

- If $\sigma^2 = 0$: set $\eta = \frac{1}{M} \Rightarrow O\left(\frac{MR^2}{K}\right)$ (recovers GD rate $O(1/K)$)
- If $\sigma^2 > 0$: set $\eta = \frac{R}{\sigma\sqrt{K}} \Rightarrow O\left(\frac{R\sigma}{\sqrt{K}}\right)$ (noise dominates)

***m*-strongly convex case:** With step size $\eta^{(k)} = \frac{2}{m(k+1)}$:

$$\mathbb{E}[f(\bar{x}^{(K)})] - f^* = O\left(\frac{\sigma^2}{mK}\right) \qquad \text{GD had rate: } O\left(\left(1 - \frac{m}{M}\right)^K\right)$$

Key insight: Noise σ^2 forces smaller step sizes, which slows convergence from $O(1/K)$ to $O(1/\sqrt{K})$.

SGD vs Full Gradient Descent (Convex + Smooth)

	Full GD	**SGD**	**Winner**
Cost per iteration	$O(n)$	$O(1)$	SGD
Iterations for ϵ accuracy	$O(1/\epsilon)$	$O(1/\epsilon^2)$	GD
Total cost for ϵ accuracy	$O(n/\epsilon)$	$O(1/\epsilon^2)$	**Depends!**

When does SGD win?

SGD is faster when: $\frac{1}{\epsilon^2} < \frac{n}{\epsilon}$, i.e., when $\boxed{n > \frac{1}{\epsilon}}$

Translation: SGD wins when we have many samples and don't need extreme precision.

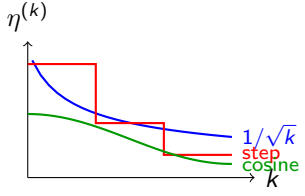
This is exactly the regime of modern machine learning!

Practical Considerations: Step Size Schedules

The step size $\eta^{(k)}$ is critical for SGD performance.

Common schedules:

- $1/\sqrt{k}$ **decay:** $\eta^{(k)} = \frac{\eta_0}{\sqrt{k+1}}$ (theoretically motivated)
- $1/k$ **decay:** $\eta^{(k)} = \frac{\eta_0}{k+1}$ (for strongly convex)
- **Step decay:** Reduce by factor 10 at fixed epochs (common in deep learning)
- **Cosine annealing:** $\eta^{(k)} = \eta_{\min} + \frac{1}{2}(\eta_0 - \eta_{\min})(1 + \cos(\pi k/K))$

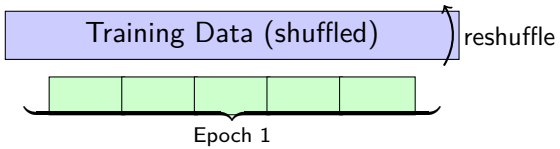


Epochs and Shuffling

Epoch: One complete pass through all n training samples

In practice:

1. Shuffle the data at the start of each epoch
2. Process mini-batches sequentially (not random sampling with replacement)
3. Repeat for multiple epochs



Why shuffle?

- Ensures batches are approximately independent
- Reduces variance compared to fixed ordering
- Required for theoretical guarantees

SGD with Momentum

Problem: SGD gradients are noisy $\Rightarrow$ oscillates, slow convergence
Solution: Use a smoothed gradient via **exponential moving average (EMA)**

$$m^{(k+1)} = \beta\, m^{(k)} + (1-\beta)\nabla f_{i_k}(x^{(k)}), \qquad x^{(k+1)} = x^{(k)} - \eta\, m^{(k+1)}$$

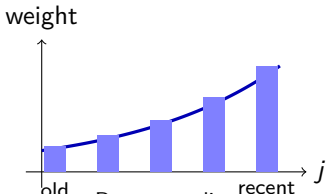
What does EMA compute? Unrolling the recursion:

$$m^{(k+1)} = (1-\beta)\sum_{j=0}^{k} \beta^{k-j}\nabla f_{i_j}(x^{(j)})$$

Weighted average of past gradients:

- Recent gradients: high weight
- Old gradients: exponentially forgotten
- Window $\approx \frac{1}{1-\beta}$ steps

$\beta = 0.9 \Rightarrow$ averages over ≈ 10 steps
$\beta = 0.99 \Rightarrow$ averages over ≈ 100 steps



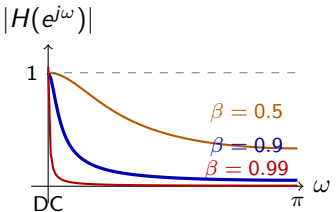
EMA is a Low-Pass Filter

Recall: $m^{(k+1)} = \beta\, m^{(k)} + (1-\beta)\, \nabla f_{i_j}(x^{(j)})$

This is a **first-order IIR filter** with transfer function:

$$H(z) = \frac{1-\beta}{1-\beta z^{-1}}$$

Frequency response:



Interpretation for SGD:

Signal	SGD meaning
Input	noisy gradient $g^{(k)}$
Output	momentum $m^{(k)}$
Low freq	true gradient
High freq	noise

Trade-off: large $\beta \Rightarrow$ filters out noise but adapts slowly. small $\beta \Rightarrow$ fast but noisy.

Typical $\beta = 0.9$: good balance for SGD momentum

Adam: Adaptive Moment Estimation

Idea: Momentum + **per-parameter adaptive learning rate**

$$m^{(k+1)} = \beta_1 m^{(k)} + (1-\beta_1)\, g \qquad \text{(EMA of gradient)}$$

$$v^{(k+1)} = \beta_2 v^{(k)} + (1-\beta_2)\, g \odot g \qquad \text{(EMA of squared gradient)}$$

$$x^{(k+1)} = x^{(k)} - \eta \cdot \hat{m}^{(k+1)} / (\sqrt{\hat{v}^{(k+1)}} + \epsilon) \qquad \text{(adaptive update)}$$

where $g \odot g = \left[\left(\frac{\partial f}{\partial x_1}\right)^2, \ldots, \left(\frac{\partial f}{\partial x_n}\right)^2 \right]^\top$ tracks one magnitude per parameter

Bias correction: Since $m^{(0)} = v^{(0)} = 0$, early estimates are biased toward zero:

$$\hat{m}^{(k)} = \frac{m^{(k)}}{1-\beta_1^k}, \qquad \hat{v}^{(k)} = \frac{v^{(k)}}{1-\beta_2^k}$$

Per-parameter adaptation: Each x_j has effective learning rate $\frac{\eta}{\sqrt{\hat{v}_j}+\epsilon}$

Large gradients $\Rightarrow$ large $\hat{v}_j \Rightarrow$ smaller step. Defaults: $\beta_1 = 0.9$, $\beta_2 = 0.999$, $\eta = 0.001$

Kingma and Ba, "Adam: A Method for Stochastic Optimization", ICLR 2015. https://arxiv.org/abs/1412.6980

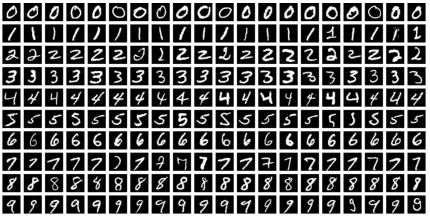
Problem Setup: MNIST Classification

The Dataset:

- 70,000 grayscale images
- Handwritten digits (0–9)
- Each image: 28×28 pixels
- Task: predict which digit
- https://en.wikipedia.org/wiki/MNIST_database

Why MNIST?

- Small enough to train on laptop
- Rich enough to illustrate key ideas
- The "Hello World" of ML



Sample digits from MNIST

$28 \times 28 = 784$ pixels per image

Mathematical Formulation

Input and Output:

- Input: $a \in \mathbb{R}^{784}$ (flattened image)
- Label: $y \in \{0, 1, \ldots, 9\}$ (true digit)
- Prediction: $\hat{p} \in \mathbb{R}^{10}$ (probability distribution over classes)

Goal: Learn a function $h_\theta : \mathbb{R}^{784} \to \mathbb{R}^{10}$ such that:

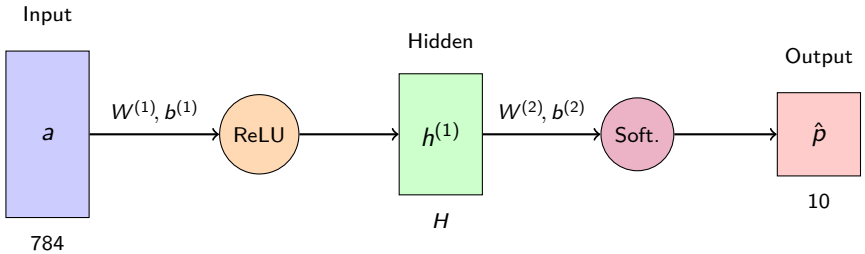
$$h_\theta(a) \approx \text{probability distribution peaking at true class } y$$

Key Questions:

1. What form should h_θ take? $\longrightarrow$ **Network Architecture**
2. How do we measure "good"? $\longrightarrow$ **Loss Function**
3. How do we find θ? $\longrightarrow$ **Optimization (SGD)**

The Multilayer Perceptron (MLP)

Core idea: Stack simple building blocks to create complex functions



Forward computation:

$$z^{(1)} = W^{(1)}a + b^{(1)} \quad \text{(linear transformation)}$$

$$h^{(1)} = \text{ReLU}(z^{(1)}) \quad \text{(nonlinear activation)}$$

$$z^{(2)} = W^{(2)}h^{(1)} + b^{(2)} \quad \text{(linear transformation)}$$

$$\hat{p} = \text{softmax}(z^{(2)}) \quad \text{(probabilities)}$$

amazon

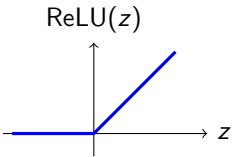
Network Components

Parameters to learn: $\theta = (W^{(1)}, b^{(1)}, W^{(2)}, b^{(2)})$

- $W^{(1)} \in \mathbb{R}^{H \times 784}$, $b^{(1)} \in \mathbb{R}^{H}$ first layer
- $W^{(2)} \in \mathbb{R}^{10 \times H}$, $b^{(2)} \in \mathbb{R}^{10}$ second layer

ReLU Activation:

$$\text{ReLU}(z) = \max(0, z)$$



Softmax:

$$\text{softmax}(z)_j = \frac{e^{z_j}}{\sum_{k=1}^{10} e^{z_k}}$$

Converts scores to probabilities:

- All outputs in $(0, 1)$
- Sum to exactly 1

Example: $H = 128$ hidden units $\Rightarrow 784 \times 128 + 128 + 128 \times 10 + 10 = \mathbf{101{,}770}$ parameters

Loss Function for Multi-class Classification: Cross-Entropy

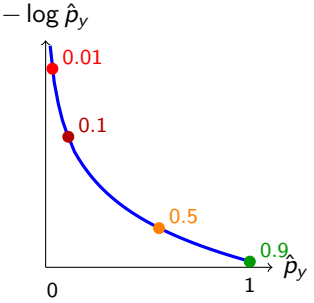
For true label y and predicted probabilities $\hat{p}$:

$$\ell(\hat{p}, y) = -\log \hat{p}_y = -\log \frac{e^{z_y^{(2)}}}{\sum_{k=0}^{9} e^{z_k^{(2)}}}$$

Example: Image shows a "3", so true label $y = 3$

Prediction	$\hat{p}_3$	**Loss**
Confident & correct	0.9	$-\log(0.9) = 0.1$
Uncertain	0.5	$-\log(0.5) = 0.7$
Unsure	0.1	$-\log(0.1) = 2.3$
Confident & wrong	0.01	$-\log(0.01) = 4.6$

Key property:
Confident mistakes are **severely** penalized!



The Optimization Problem

Given n training examples $\{(a_i, y_i)\}_{i=1}^n$, find weights that minimize:

$$\boxed{\underset{\theta}{\text{minimize}} \quad f(\theta) = \frac{1}{n}\sum_{i=1}^{n} \ell(h_\theta(a_i), y_i)}$$

where $\theta = (W^{(1)}, b^{(1)}, W^{(2)}, b^{(2)})$ collects all network parameters.

Two key observations:

1. This is **Empirical Risk Minimization** $\Longrightarrow$ **SGD** is the natural algorithm
2. The problem is **non-convex** due to nonlinear activations
   $\Longrightarrow$ No guarantee of global minimum, but SGD works well in practice

Backpropagation

Challenge: To apply SGD, we need to compute $\nabla_\theta \ell$ for each sample

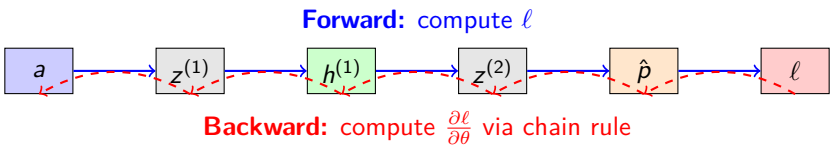
Chain rule: For composed functions $\ell = \ell(g(h(x)))$:

$$\frac{d\ell}{dx} = \frac{d\ell}{dg} \cdot \frac{dg}{dh} \cdot \frac{dh}{dx}$$

Our network is exactly this: a composition of simple functions

$$\ell = \ell\Big(\text{softmax}(W^{(2)} \cdot \text{ReLU}(W^{(1)} a + b^{(1)}) + b^{(2)}),\ y\Big)$$

Backpropagation: Systematically apply chain rule layer by layer starting from the end



Forward Pass: Compute and Store

Starting from input, compute all intermediate values:

1. **Input layer:** a (given)
2. **Hidden pre-activation:** $z^{(1)} = W^{(1)}a + b^{(1)}$
3. **Hidden activation:** $h^{(1)} = \text{ReLU}(z^{(1)})$
4. **Output pre-activation:** $z^{(2)} = W^{(2)}h^{(1)} + b^{(2)}$
5. **Output probabilities:** $\hat{p} = \text{softmax}(z^{(2)})$
6. **Loss:** $\ell = -\log \hat{p}_y$

Important: Store all intermediate values!
We need them for the backward pass.

Backward Pass

Goal: Compute all partial derivatives $\frac{\partial \ell}{\partial W^{(1)}}$, $\frac{\partial \ell}{\partial b^{(1)}}$, $\frac{\partial \ell}{\partial W^{(2)}}$, $\frac{\partial \ell}{\partial b^{(2)}}$ using chain rule

Step 1: Gradient w.r.t. output scores $z^{(2)}$
For cross-entropy + softmax, there's a clean formula:

$$\frac{\partial \ell}{\partial z^{(2)}} = \hat{p} - e_y$$

where e_y is one-hot encoding of true label y

Step 2: Gradients for $W^{(2)}$ and $b^{(2)}$ (chain rule)

$$\frac{\partial \ell}{\partial W^{(2)}} = \frac{\partial \ell}{\partial z^{(2)}} (h^{(1)})^\top, \qquad \frac{\partial \ell}{\partial b^{(2)}} = \frac{\partial \ell}{\partial z^{(2)}}$$

Backward Pass: Hidden Layer

Step 3: Gradient w.r.t. hidden activations $h^{(1)}$

$$\frac{\partial \ell}{\partial h^{(1)}} = (W^{(2)})^\top \frac{\partial \ell}{\partial z^{(2)}}$$

Step 4: Gradient w.r.t. hidden pre-activations $z^{(1)}$

Apply chain rule through ReLU:

$$\frac{\partial \ell}{\partial z^{(1)}} = \frac{\partial \ell}{\partial h^{(1)}} \odot \underbrace{\mathbf{1}[z^{(1)} > 0]}_{\text{ReLU derivative}}$$

($\odot$ = elementwise multiplication; ReLU derivative is 1 where $z^{(1)} > 0$, else 0)

Step 5: Gradients for $W^{(1)}$ and $b^{(1)}$

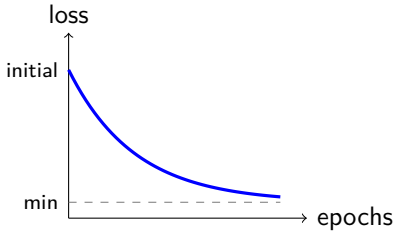
$$\frac{\partial \ell}{\partial W^{(1)}} = \frac{\partial \ell}{\partial z^{(1)}} a^\top, \qquad \frac{\partial \ell}{\partial b^{(1)}} = \frac{\partial \ell}{\partial z^{(1)}}$$

Done! We have all four gradients needed for SGD update.

The Complete Training Algorithm

Mini-Batch SGD + Backprop:

1. Initialize weights randomly
2. **For each epoch:**
   - 2.1 Shuffle training data
   - 2.2 **For each mini-batch $\mathcal{B}$:**
     - Forward pass (compute ℓ)
     - Backward pass (compute $\nabla \ell$)
     - Average gradients over batch
     - Update: $\theta \leftarrow \theta - \eta \cdot \nabla$
3. Evaluate accuracy



Hyperparameters:

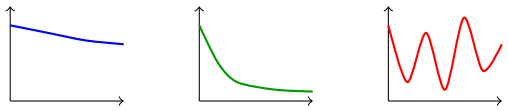
- Learning rate η
- Batch size B
- Number of epochs
- Hidden size H

Practical Considerations

Initialization matters:

- Too large $\Rightarrow$ exploding gradients
- Too small $\Rightarrow$ vanishing gradients
- Common: $W_{ij} \sim \mathcal{N}(0, 1/\sqrt{\text{fan-in}})$

Learning rate is critical:

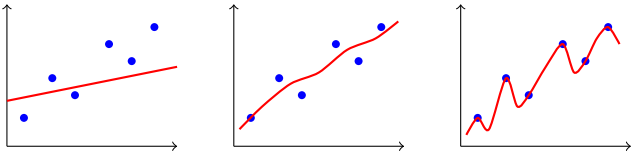


Shuffling: Ensures mini-batches are independent (required for SGD theory)

Regularization: Often add $\frac{\lambda}{2}\|\theta\|^2$ to prevent overfitting

Regularization: Preventing Overfitting

Problem: Network can memorize training data instead of learning patterns



Solution: Add a penalty for large weights

$$\underset{\theta}{\text{minimize}} \quad \underbrace{\frac{1}{n}\sum_{i=1}^{n} \ell(h_\theta(a_i), y_i)}_{\text{fit the data}} + \underbrace{\frac{\lambda}{2}\|\theta\|^2}_{\text{keep weights small}}$$

Why it works:

- Large weights $\Rightarrow$ sharp, complex decision boundaries $\Rightarrow$ memorization
- Small weights $\Rightarrow$ smooth, simple functions $\Rightarrow$ generalization

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Quiz 1: MNIST Classification Challenge / Submit by 31/03/2026

Task: Build an ML model to classify handwritten digits (0–9)

Model Interface:

- `model.fit(X, y)` – train on images $X \in \mathbb{R}^{n \times 784}$, labels $y \in \{0, ..., 9\}^n$
- `model.predict(X)` – return predicted labels

Rules:

1. Only `numpy` allowed
2. No pre-computed weights – training must happen in `fit()`
3. Time budget: 120s (hard stop: 180s)
4. Minimum accuracy: 97%

Evaluation:

- You develop with `seed=42`
- Grading uses an *unknown* seed $\Rightarrow$ your model must generalize

https://github.com/gpasxos/large-scale-optimization/blob/main/Quiz_2026.ipynb

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Part IV

Duality

Outline

Goal: Solve (or bound) constrained convex optimization

$$\underset{x \in \mathbb{R}^n}{\text{minimize}} \quad f(x) \quad \text{subject to} \quad g_i(x) \leq 0, \quad h_j(x) = 0$$

- **The Lagrangian** – combining objective and constraints
- **Weak and strong duality** – provide bounds
- **KKT conditions** – necessary and sufficient for optimality
- **Complementary slackness** – active constraints and multipliers
- **Fenchel duality** – conjugates and saddle points

Duality: every constrained problem has a "mirror" problem

Motivating Example: Constrained Minimum

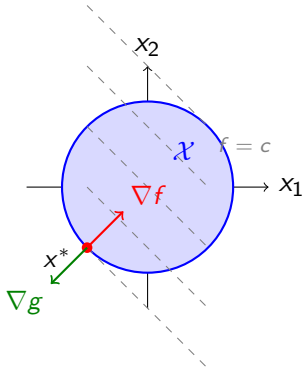
$$\begin{aligned} \underset{x \in \mathbb{R}^2}{\text{minimize}} \quad & x_1 + x_2 \\ \text{subject to} \quad & x_1^2 + x_2^2 \leq 2 \end{aligned}$$

Observations:

- Linear objective $\Rightarrow$ optimum on boundary
- At optimum: gradients are *parallel*
- $\nabla f(x^*) = \lambda \nabla g(x^*)$

Solution:

- $x^* = (-1, -1)$, $\lambda^* = 1/2$
- $f^* = -2$



At optimum: $\nabla f(x^*)$ and $\nabla g(x^*)$ are parallel (true for active constraints)

Why Must Gradients Be Parallel?

Suppose they weren't parallel at x^*...

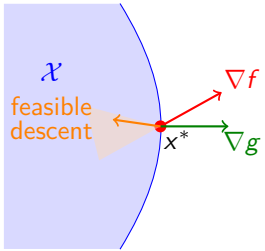
Then $-\nabla f(x^*)$ and $-\nabla g(x^*)$ span a cone of directions that:

- Decrease the objective ($d^T \nabla f < 0$)
- Stay feasible ($d^T \nabla g < 0$)

$\Rightarrow$ We could improve! Contradiction.

At a true minimum:

- Only way to decrease f is to leave feasible region: $\nabla f = \lambda \nabla g$ for some $\lambda \geq 0$



If gradients not parallel:

there exists feasible descent direction

The Lagrangian Function

Definition (Lagrangian)

For problem $\min_x f(x)$ s.t. $g_i(x) \leq 0$, $h_j(x) = 0$:

$$L(x, \lambda, \mu) = f(x) + \sum_{i=1}^{m} \lambda_i g_i(x) + \sum_{j=1}^{p} \mu_j h_j(x)$$

Dual variables:

- $\lambda_i \geq 0$: multiplier for $g_i(x) \leq 0$
- $\mu_j \in \mathbb{R}$: multiplier for $h_j(x) = 0$

Also called **Lagrange multipliers**

Interpretation:

- λ_i = "price" of violating constraint i
- Large $\lambda_i \Rightarrow$ violation is expensive
- At right λ: minimizing L gives constrained optimum

Stationarity: $\nabla_x L(x^*, \lambda^*, \mu^*) = 0 \Leftrightarrow \nabla f(x^*) + \sum_i \lambda_i^* \nabla g_i(x^*) + \sum_j \mu_j^* \nabla h_j(x^*) = 0$

The Lagrange Dual Function

Definition (Dual function)

$$D(\lambda, \mu) = \inf_x L(x, \lambda, \mu) = \inf_x \left[f(x) + \sum_{i=1}^{m} \lambda_i g_i(x) + \sum_{j=1}^{p} \mu_j h_j(x) \right]$$

Key property:

Concavity

$D(\lambda, \mu)$ is **always concave**
(even if primal is nonconvex!)

Why? Pointwise infimum of affine functions in (λ, μ)

Implication:

- Dual problem is concave maximization
- Always "easy" (in principle)
- Can solve even when primal is hard

Computing D**:** Minimize L over x (often has closed form for structured problems)

Weak Duality: A Universal Lower Bound

Theorem (Weak Duality)

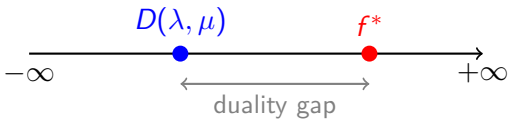
For any $\lambda \geq 0$ and any μ:

$$D(\lambda, \mu) \leq f^*$$

Proof: Let x^* be primal optimal. Then:

$$D(\lambda, \mu) = \inf_x L(x, \lambda, \mu) \leq L(x^*, \lambda, \mu)$$

$$= f(x^*) + \underbrace{\sum_i \lambda_i g_i(x^*)}_{\leq 0 \text{ (since } \lambda_i \geq 0, g_i(x^*) \leq 0)} + \underbrace{\sum_j \mu_j h_j(x^*)}_{=0} \leq f(x^*) = f^*$$



The Dual Problem

Question: What's the *tightest* lower bound?

Definition (Dual Problem)

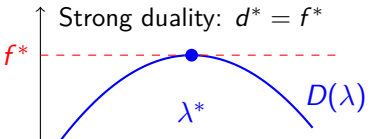
$$d^* = \underset{\lambda,\mu}{\text{maximize}} \; D(\lambda, \mu) \quad \text{subject to} \quad \lambda \geq 0$$

Properties:

- Concave maximization (tractable!)
- $d^* \leq f^*$ always (weak duality)
- $f^* - d^*$ = **duality gap**

Strong duality: $d^* = f^*$

- Gap is zero
- Dual finds the optimal primal value!
- When does this hold?



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When Does Strong Duality Hold?

Definition (Slater's Condition)

A problem satisfies **Slater's condition** if there exists a **strictly feasible** point $\tilde{x}$:

$$g_i(\tilde{x}) < 0 \quad \forall i, \qquad h_j(\tilde{x}) = 0 \quad \forall j$$

Theorem (Strong Duality)

If the primal is convex and Slater's condition holds, then:

$$d^* = f^* \qquad \text{(strong duality)}$$

and the dual optimum is attained.

Slater satisfied:

- $\min\{x_1 + x_2 : x_1^2 + x_2^2 \leq 1\}$
- Take $\tilde{x} = (0, 0)$: $0 < 1$ ✓

Slater fails:

- $\min\{x : x^2 \leq 0\}$
- Only feasible point: $x = 0$

Complementary Slackness

Theorem

If strong duality holds with optimal (x^*, λ^*, μ^*), then:

$$\lambda_i^* g_i(x^*) = 0 \qquad \forall i = 1, \ldots, m$$

Equivalently:

$$\lambda_i^* > 0 \;\Rightarrow\; g_i(x^*) = 0 \qquad \text{and} \qquad g_i(x^*) < 0 \;\Rightarrow\; \lambda_i^* = 0$$

Economic interpretation:

- λ_i^* = "shadow price" of constraint i
- Slack constraint ($g_i < 0$): not binding, price $= 0$
- Tight constraint ($g_i = 0$): may have positive price
- Positive price $\Rightarrow$ constraint must be tight

Example: Plant Crops

Problem: x_1 acres of wheat (\$5k/acre profit) and x_2 acres of corn (\$4k/acre profit)

$$\begin{aligned} \underset{x_1, x_2 \geq 0}{\text{maximize}} \quad & 5x_1 + 4x_2 \\ \text{subject to} \quad & x_1 + x_2 \leq 6 \quad \text{(land: 6 acres)} \\ & x_1 \leq 4 \quad \text{(wheat irrigation capacity)} \\ & x_2 \leq 5 \quad \text{(corn irrigation capacity)} \end{aligned}$$

Solution: $x^* = (4, 2)$, profit $= \$28$k

	Land	**Wheat irr.**	**Corn irr.**
Used	6	4	2
Limit	6	4	5
Tight?	Yes	Yes	No
λ_i^*	4	1	0

$\lambda_1^*(6-6) = 0$ ✓ $\lambda_2^*(4-4) = 0$ ✓
$\lambda_3^*\underbrace{(2-5)}_{\neq 0} = 0$ ✓

Shadow prices:

- $\lambda_1^* = 4$: extra acre of land $\Rightarrow$ profit +\$4k
- $\lambda_2^* = 1$: extra wheat irrigation $\Rightarrow$ profit +\$1k
- $\lambda_3^* = 0$: extra corn irrigation $\Rightarrow$ **worthless** (3 acres already unused!)

Advice: Invest in land first (\$4k return per acre), then wheat irrigation (\$1k return).

The KKT Conditions

Definition (Karush-Kuhn-Tucker Conditions)

(x^*, λ^*, μ^*) satisfies the **KKT conditions** if:

1. **Stationarity:** $\nabla f(x^*) + \sum_i \lambda_i^* \nabla g_i(x^*) + \sum_j \mu_j^* \nabla h_j(x^*) = 0$
2. **Complementary slackness:** $\lambda_i^* g_i(x^*) = 0$ for all i
3. **Primal feasibility:** $g_i(x^*) \leq 0, \quad h_j(x^*) = 0$ for all i, j
4. **Dual feasibility:** $\lambda_i^* \geq 0$ for all i

Theorem (KKT for Convex Problems)

For convex problems with strong duality:
x^* is primal optimal, (λ^*, μ^*) is dual optimal $\Leftrightarrow$ KKT conditions hold

Key insight: KKT reduces constrained optimization to solving a system of equations!

Example: Equality constrained QP

Problem: $\min \frac{1}{2}\|x\|^2$ subject to $Ax = b$

Lagrangian: $L(x, \mu) = \frac{1}{2}x^T x + \mu^T(Ax - b)$

KKT conditions:

Stationarity: $x^* + A^T\mu^* = 0 \;\Rightarrow\; x^* = -A^T\mu^*$

Primal feas.: $Ax^* = b$

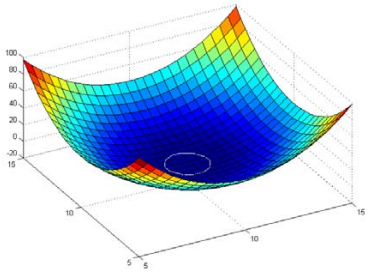
Solve: Substitute into feasibility:

$$A(-A^T\mu^*) = b \;\;\Rightarrow\;\; \mu^* = -(AA^T)^{-1}b$$

Solution:

$$\boxed{x^* = A^T(AA^T)^{-1}b}$$

Optimum is closest point to origin on the affine subspace $Ax = b$



Plot of $\frac{1}{2}\|x\|^2$ for $d = 2$.

Application: Power Allocation over Fading Channels

Problem: Allocate power p_i to n channels with noise levels $N_i > 0$

$$\underset{p \geq 0}{\text{maximize}} \quad \sum_{i=1}^{n} \log(1 + p_i/N_i) \quad \text{s.t.} \quad \sum_{i=1}^{n} p_i = P$$

Lagrangian (with $\lambda_i \geq 0$ for $-p_i \leq 0$, and μ for equality):

$$L(p, \lambda, \mu) = -\sum_{i=1}^{n} \log(1 + p_i/N_i) - \sum_{i=1}^{n} \lambda_i p_i + \mu\Big(\sum_{i=1}^{n} p_i - P\Big)$$

Stationarity: $\dfrac{\partial L}{\partial p_i} = -\dfrac{1}{N_i + p_i} - \lambda_i + \mu = 0 \;\Rightarrow\; \lambda_i = \mu - \dfrac{1}{N_i + p_i}$

Comp. slackness: $\lambda_i \, p_i = 0 \;\; \forall \, i$

Primal feasibility: $p_i \geq 0, \quad \sum_i p_i = P$

Dual feasibility: $\lambda_i \geq 0 \;\; \forall \, i$

Substituting stationarity into complementary slackness: $p_i \left(\mu - \frac{1}{N_i + p_i}\right) = 0, \quad i = 1, \ldots, n$

For each channel: either $p_i = 0$ or $p_i = \frac{1}{\mu} - N_i$. **Q:** *Which one?*

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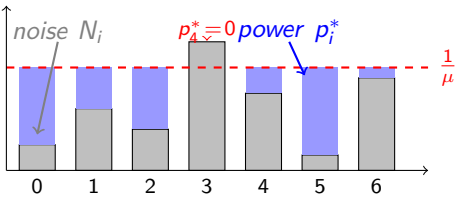
Solution: Water-Filling

Decide $p_i = 0$ or $p_i = \frac{1}{\mu} - N_i$ using KKT conditions:

Case 1: $1/\mu > N_i$ (good channel)
If we tried $p_i = 0$: stationarity gives $\lambda_i = \mu - 1/N_i < 0$ ✗ violates $\lambda_i \geq 0$
$\Rightarrow$ Must have $p_i = \frac{1}{\mu} - N_i > 0$

Case 2: $1/\mu \leq N_i$ (bad channel)
If we tried $p_i > 0$: need $\mu = \frac{1}{N_i + p_i} < \frac{1}{N_i}$
✗ contradicts $1/\mu \leq N_i$
$\Rightarrow$ Must have $p_i = 0$ (channel shut off)

Solution: $\boxed{p_i^* = \left(\frac{1}{\mu} - N_i\right)^+}$ where μ satisfies $\sum_{i=1}^n \left(\frac{1}{\mu} - N_i\right)^+ = P$



Intuition: Pour P water on top of N_i "rocks"

- Water level $1/\mu$ rises uniformly
- Good channels (low N_i) get more power
- Bad channels (high N_i) get **nothing** — better to reallocate!
- μ is the shadow price of power budget

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From Constraints to Min-Max

Goal: Reformulate constrained problem as unconstrained

$$\min_x f(x) \quad \text{s.t.} \quad g(x) \leq 0$$

Key observation: What happens when we maximize L over $\lambda \geq 0$?

$$\sup_{\lambda \geq 0} L(x, \lambda) = \sup_{\lambda \geq 0} [f(x) + \lambda g(x)] = \begin{cases} f(x) & \text{if } g(x) \leq 0 \\ +\infty & \text{if } g(x) > 0 \end{cases}$$

Why?

- If $g(x) \leq 0$: maximizing $\lambda g(x)$ over $\lambda \geq 0$ gives $\lambda^* = 0$, so $\sup = f(x)$
- If $g(x) > 0$: take $\lambda \to +\infty$, so $\sup = +\infty$

The sup over λ acts as an **infinite penalty** for constraint violation!

Constrained Optimization = Min-Max Game

Combining the insights:

$$\min_x \{f(x) : g(x) \leq 0\} \quad = \quad \min_x \sup_{\lambda \geq 0} L(x, \lambda)$$

Interpretation as a two-player game:

Player 1 (minimizer):

- Chooses x
- Wants to minimize cost
- Must respect constraints (or pay ∞)

Player 2 (maximizer):

- Chooses $\lambda \geq 0$
- "Adversary" or "referee"
- Penalizes constraint violations

The game:

1. Player 1 announces x
2. Player 2 responds with worst-case λ (infinite penalty if cheating)
3. Player 1's best strategy: choose feasible x that minimizes f

What If We Swap the Order?

Primal: Player 1 moves first, Player 2 responds

$$f^* = \min_x \sup_{\lambda \geq 0} L(x, \lambda)$$

Dual: Player 2 moves first, Player 1 responds

$$d^* = \sup_{\lambda \geq 0} \min_x L(x, \lambda) = \sup_{\lambda \geq 0} D(\lambda)$$

Who has the advantage?

- Moving **second** is always better (you see opponent's move)
- In primal: Player 2 moves second $\Rightarrow$ can punish violations
- In dual: Player 1 moves second $\Rightarrow$ can optimize against fixed λ

Max-Min Inequality or ... Weak Duality (always holds)

$$\underbrace{\sup_{\lambda} \min_x L(x, \lambda)}_{d^* \text{ (dual)}} \leq \underbrace{\min_x \sup_{\lambda} L(x, \lambda)}_{f^* \text{ (primal)}}$$

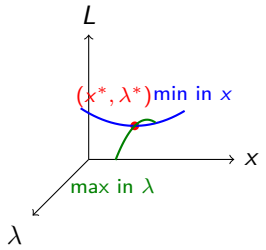
Saddle Points: When Order Doesn't Matter

Question: When does $\min \sup = \sup \min$? **Answer:** When there exists a **saddle point**

Definition (Saddle Point)

(x^*, λ^*) is a saddle point of L if:

$$L(x^*, \lambda) \leq L(x^*, \lambda^*) \leq L(x, \lambda^*) \quad \text{for all } x, \lambda \geq 0$$



At a saddle point:

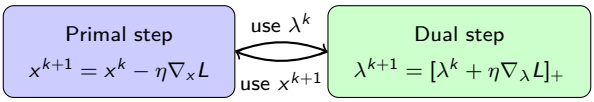
- x^* minimizes $L(\cdot, \lambda^*)$
- λ^* maximizes $L(x^*, \cdot)$
- Neither player wants to deviate
- **Nash equilibrium!**

Saddle point exists $\Leftrightarrow$ strong duality holds $\Leftrightarrow$ $d^* = f^*$

Why Saddle Points Matter for Algorithms

Saddle point formulation: $\min_x \max_{\lambda \geq 0} L(x, \lambda)$

Enables primal-dual algorithms:



Key benefits:

- **Decoupling:** Primal and dual updates can be simple (even closed-form)
- **Certificates:** Gap $f(x^k) - D(\lambda^k)$ measures distance to optimality
- **Parallelization:** Dual often decomposes across constraints

Examples: Uzawa's method, ADMM, Chambolle-Pock, Arrow-Hurwicz...

A Universal Template for Convex Optimization

Observation: Almost any convex problem can be written as:

$$\min_x \quad f(x) + g(Ax)$$

How? Use **indicator functions** $\delta_C(z) = \begin{cases} 0 & z \in C \\ +\infty & z \notin C \end{cases}$

Problem	**As** $\min_x f(x) + g(Ax)$
$\min f(x)$ s.t. $Ax = b$	$f(x) + \delta_{\{b\}}(Ax)$
$\min f(x)$ s.t. $Ax \leq b$	$f(x) + \delta_{\{z : z \leq b\}}(Ax)$
$\min f(x)$ s.t. $x \in C$	$f(x) + \delta_C(x)$ (take $A = I$)
LASSO	$\lambda\|x\|_1 + \frac{1}{2}\|Ax - b\|^2$

Constraints become functions, everything is $f + g \circ A$

Fenchel Duality for $f + g \circ A$

Since $\min_x f(x) + g(Ax)$ covers (almost) everything, let's derive its dual.

Fenchel dual: For any convex g: $g(z) = \max_y \{\langle z, y\rangle - g^*(y)\}$
Our template as a saddle-point:

$$\min_x \{f(x) + g(Ax)\} = \min_x \left\{ f(x) + \max_y [\langle Ax, y\rangle - g^*(y)] \right\}$$
$$= \min_x \max_y \{f(x) + \langle Ax, y\rangle - g^*(y)\}$$

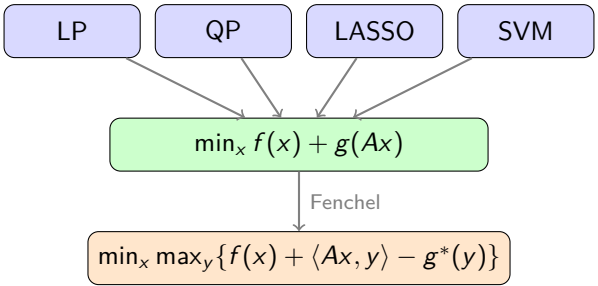
Swapping min and max gives the Fenchel dual:

$$\max_y \left\{ \underbrace{-f^*(-A^T y)}_{-\max_x[\langle -A^T y, x\rangle - f(x)]} \quad -g^*(y) \right\}$$

To use this, we need to know f^* and g^* — the **convex conjugates**

Why This Perspective is Powerful

One framework, many problems:



Benefits:

- **Unified theory:** One duality framework for all these problems
- **Unified algorithms:** Primal-dual methods work on the saddle point form
- **Modular:** Swap f, g, or A — same algorithm structure

Convex Conjugates: A Deeper Duality

To apply Fenchel duality, we need conjugates f^* and g^*

Definition (Convex Conjugate / Fenchel Conjugate)

$$f^*(y) = \sup_x \{\langle y, x\rangle - f(x)\}$$

Geometric interpretation:

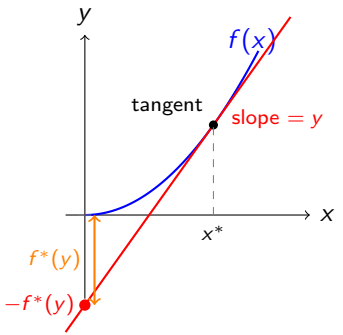
- Find $\ell(x)$, the tangent of f with slope y:

$$\ell(x) = yx - f^*(y)$$

- $f^*(y) =$ negative of y-intercept

Key properties:

- f^* is always convex
- $f^{**} = f$ (for convex, closed f)
- $f(x) + f^*(y) \geq \langle y, x\rangle$



For $f(x) = \frac{1}{2}x^2$: slope y tangent touches at $x^* = y$, giving $f^*(y) = \frac{1}{2}y^2$

Common Conjugates

Function $f(x)$	**Conjugate** $f^*(y)$
$\frac{1}{2}x^T Qx \quad (Q \succ 0)$	$\frac{1}{2}y^T Q^{-1} y$
$\frac{1}{2}\|x\|_2^2$	$\frac{1}{2}\|y\|_2^2$
$\|x\|$ (any norm)	$\delta_{\{\|y\|_* \leq 1\}}(y)$ (indicator of dual ball)
$\|x\|_1$	$\delta_{\{\|y\|_\infty \leq 1\}}(y)$
$\delta_{\mathcal{C}}(x)$ (indicator)	$\sigma_{\mathcal{C}}(y) = \sup_{x \in \mathcal{C}} \langle y, x \rangle$ (support fn)
e^x	$y \log y - y \quad (y > 0)$

Key pattern: Conjugate "inverts" the (derivative of the) function

- Quadratic with $Q \leftrightarrow$ Quadratic with Q^{-1}
- ℓ_1 norm $\leftrightarrow$ ℓ_∞ ball indicator
- $y = \nabla f(x) \Leftrightarrow x = \nabla f^*(y)$

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From Saddle Point to Algorithm

Saddle point: $\min_x \max_y \{f(x) + \langle Ax, y\rangle - g^*(y)\}$

Algorithm: Alternate proximal gradient descent (in x) and ascent (in y)

$$\boxed{\begin{aligned} x^{k+1} &= \text{prox}_{\tau f}\left(x^k - \tau A^T y^k\right) \quad \text{(primal update)} \\ y^{k+1} &= \text{prox}_{\sigma g^*}\left(y^k + \sigma A x^{k+1}\right) \quad \text{(dual update)} \end{aligned}}$$

Ingredients you need:

1. $\text{prox}_{\tau f}$ — proximal operator of f (look up in table)
2. $\text{prox}_{\sigma g^*}$ — use identity: $\text{prox}_{\sigma g^*}(y) = y - \sigma \text{prox}_{g/\sigma}(y/\sigma)$
3. Step sizes: $\tau, \sigma > 0$ with $\tau\sigma\|A\|^2 < 1$

This is the **Primal-Dual Hybrid Gradient (PDHG)** or **Chambolle-Pock** algorithm.

When to Use Which Duality

Fenchel duality: Best when f, g have "simple" structure

Simple g	**Conjugate** g^*
$\|z\|_1$	$\delta_{\|y\|_\infty \leq 1}$
$\|z\|_2$	$\delta_{\|y\|_2 \leq 1}$
$\frac{1}{2}\|z\|^2$	$\frac{1}{2}\|y\|^2$
$\delta_{\{b\}}(z)$	$\langle b, y \rangle$
$\delta_{\{z \leq b\}}$	Easy (separable)

Lagrangian duality: Best for general nonlinear constraints $g(x) \leq 0$

- Dual variables λ handle constraints directly
- No need to compute conjugates of complicated sets

Rule of thumb: Linear constraints + structured objectives $\rightarrow$ Fenchel
Nonlinear constraints $\rightarrow$ Lagrangian

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Part V

First-Order Methods for Constrained Optimization

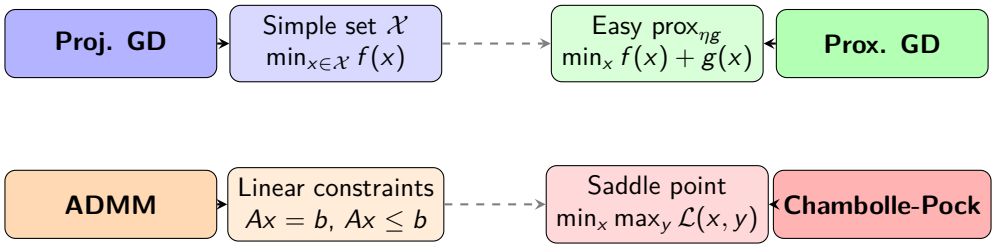
Goal: Solve constrained convex optimization

$$\underset{x}{\text{minimize}} \quad f(x) + g(x)$$

where f is smooth, g may be non-smooth (encodes constraints/regularization)

- **Projected gradient descent**
  $g(x) = \delta_{\mathcal{X}}(x)$ (indicator of set with cheap projection: box, ball, polyhedron)
- **Proximal gradient methods**
  $g(x) = \lambda\|x\|_1$ or other non-smooth regularizer with cheap prox
- **ADMM**
  $g(x) = h(Ax)$ or separable $g(x) = \sum_i g_i(x_i)$ (splitting structure)
- **Mirror descent**
  $g(x) = \delta_{\Delta_n}(x)$ (indicator of simplex constraints)
- **Primal-dual methods**
  $g(x) = h(Kx)$ with linear operator K (e.g., $K = \nabla$ for TV)

The Constrained Optimization Landscape



Key insight: Match algorithm to problem structure!

Projected Gradient Descent

Problem: $\min_{x \in \mathcal{X}} f(x), \quad \mathcal{X}$ closed convex

Algorithm:

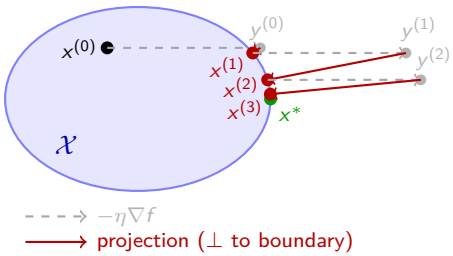
$$\boxed{x^{(k+1)} = \Pi_{\mathcal{X}}\left(x^{(k)} - \eta \nabla f(x^{(k)})\right)}$$

Two steps:

1. Gradient step (may leave $\mathcal{X}$)
2. Project back onto $\mathcal{X}$

Projection:

$$\Pi_{\mathcal{X}}(y) = \text{argmin}_{x \in \mathcal{X}} \|x - y\|^2$$



Projection finds the **nearest point** on boundary

Key property: Projection is **non-expansive**: $\|\Pi_{\mathcal{X}}(y_1) - \Pi_{\mathcal{X}}(y_2)\| \leq \|y_1 - y_2\|$

Common Projections

Set $\mathcal{X}$	Projection $\Pi_{\mathcal{X}}(y)$	Cost	
Box $[l, u]$	$\text{clip}(y, l, u)$	$O(n)$	✓
ℓ_2-ball $\|x\| \leq r$	$\begin{cases} y & \|y\| \leq r \\ r \cdot y/\|y\| & \text{else} \end{cases}$	$O(n)$	✓
Halfspace $a^T x \leq b$	$y - \frac{(a^T y - b)^+}{\|a\|^2} a$	$O(n)$	✓
Simplex Δ_n	Sort + threshold	$O(n \log n)$	✓
Affine $Ax = b$	$y - A^T(AA^T)^{-1}(Ay - b)$	$O(mn)^*$	✗
Polyhedron $Ax \leq b$	Solve QP	expensive	✗

Box projection:

$$[\Pi(y)]_i = \min(\max(y_i, l_i), u_i)$$

Ball projection:

$$\Pi(y) = \frac{r}{\max(r, \|y\|)} \cdot y$$

Projected GD: Convergence

Theorem (Convergence of Projected GD)

Let f be convex and M-smooth, $\mathcal{X}$ closed convex. With $\eta = 1/M$:

M-smooth:

$$f(x^{(k)}) - f^* \leq \frac{M\|x^{(0)} - x^*\|^2}{2k} \qquad (O(1/\epsilon) \text{ iterations})$$

m-strongly convex:

$$\|x^{(k)} - x^*\|^2 \leq \left(1 - \frac{m}{M}\right)^k \|x^{(0)} - x^*\|^2 \qquad (O(\kappa \log(1/\epsilon)) \text{ iterations})$$

Key insight: Same rates as unconstrained GD!

Why? Non-expansiveness of projection: constraint doesn't slow us down (if projection is cheap)

Projected Gradient Descent: Example Problems

1. Box-constrained regression

$$\min_{l \le x \le u} \frac{1}{2}\|Ax - b\|^2$$

Physical bounds on parameters (e.g., concentrations ≥ 0, probabilities ≤ 1). Projection: $O(n)$ clipping.

2. Portfolio optimization

$$\min_{x \in \Delta_n} x^T \Sigma x - \mu^T x$$

Weights on simplex $\Delta_n = \{x \geq 0, \mathbf{1}^T x = 1\}$. Projection: $O(n \log n)$ sort.

3. Low-rank matrix completion

$$\min_{\|X\|_F \le r} \sum_{(i,j) \in \Omega} (X_{ij} - M_{ij})^2$$

Frobenius ball: projection is $O(mn)$ scaling.

4. Signal recovery with energy budget

$$\min_{\|x\|_2 \le P} \|Ax - b\|^2$$

Power constraint in communications. ℓ_2-ball projection: $O(n)$ scaling.

5. SVM dual

$$\min_{0 \le \alpha \le C} \frac{1}{2}\alpha^T Q \alpha - \mathbf{1}^T \alpha$$

Box constraints on dual variables. Projection: $O(n)$ clipping.

6. Constrained least squares

$$\min_{\{x:\, a^T x \le b\}} \|Ax - c\|^2$$

Halfspace: projection is $O(n)$ closed-form.

Proximal Operators: Beyond Projection

Problem: $\min_x f(x) + g(x)$ where f smooth, g **non-smooth**

Definition (Proximal Operator)

$$\text{prox}_{\eta g}(y) = \text{argmin}_x \left\{ g(x) + \frac{1}{2\eta}\|x - y\|^2 \right\}$$

Interpretation:

- Balance minimizing $g(x)$...
- ...with staying close to y
- η controls the trade-off

Special case:
For $g = \delta_{\mathcal{X}}$ (indicator):

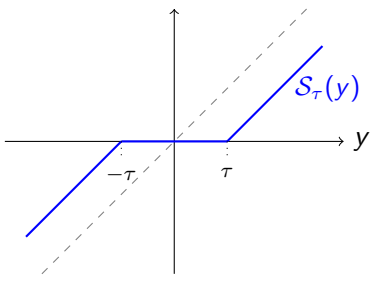
$$\text{prox}_{\eta \delta_{\mathcal{X}}}(y) = \Pi_{\mathcal{X}}(y)$$

Projection is a proximal operator!

Soft-Thresholding: Prox of ℓ_1 Norm

For $g(x) = \lambda\|x\|_1$:

$$\boxed{[\text{prox}_{\eta g}(y)]_i = \text{sign}(y_i) \cdot \max(|y_i| - \eta\lambda, 0) = \mathcal{S}_{\eta\lambda}(y_i)}$$



Effect:

- $\|x\|_1$ wants $x = 0$ ($\uparrow$ with λ)
- $\|x - y\|^2$ wants $x = y$ ($\downarrow$ with η)

Why it works:

- Values in $[-\tau, \tau] \to$ **zero**
- Other values shrunk by τ
- **Induces sparsity!**

Common Proximal Operators

Function $g(x)$	**Prox**$_{\eta g}(y)$	**Name**
$\delta_{\mathcal{X}}(x)$	$\Pi_{\mathcal{X}}(y)$	Projection
$\lambda\|x\|_1$	$\text{sign}(y) \odot (\|y\| - \eta\lambda)^+$	Soft-threshold
$\frac{\lambda}{2}\|x\|_2^2$	$\frac{y}{1+\eta\lambda}$	Shrinkage
$\lambda\|x\|_2$	$\left(1 - \frac{\eta\lambda}{\|y\|_2}\right)^+ y$	Group soft-thresh
$\delta_{\{\|x\|_2 \le r\}}(x)$	$\frac{r}{\max(r, \|y\|_2)} y$	Ball projection

Separability: If $g(x) = \sum_i g_i(x_i)$, then prox decomposes:

$$\left[\text{prox}_{\eta g}(y)\right]_i = \text{prox}_{\eta g_i}(y_i) \qquad \text{(solve } n \text{ independent 1D problems)}$$

Proximal Gradient Method (ISTA)

Problem: $\min_x f(x) + g(x)$ (f smooth, g non-smooth)

ISTA (Iterative Shrinkage-Thresholding Algorithm)

1: **for** $k = 0, 1, \ldots$ **do**
2: $\quad y^{(k)} \leftarrow x^{(k)} - \eta \nabla f(x^{(k)})$ // cheap forward step on f
3: $\quad x^{(k+1)} \leftarrow \text{prox}_{\eta g}(y^{(k)})$ // backward step on g (works for some functions)
4: **end for**

Interpretation: Minimize local quadratic model of f, plus exact g:

$$x^{(k+1)} = \text{argmin}_x \left\{ \underbrace{f(x^{(k)}) + \nabla f(x^{(k)})^T (x - x^{(k)}) + \frac{1}{2\eta} \|x - x^{(k)}\|^2}_{\text{quadratic approx of } f} + g(x) \right\}$$

Convergence

With $\eta = 1/M$: $\quad F(x^{(k)}) - F^* \leq \dfrac{M \|x^{(0)} - x^*\|^2}{2k}$

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Why "Forward-Backward Splitting"?

Forward step (explicit, on f): Evaluate gradient at **current** point

$$y^{(k)} = x^{(k)} - \eta \nabla f(x^{(k)})$$

Backward step (implicit, on g): Optimality of $\text{prox}_{\eta g}$ gives

$$0 \in \partial g(x^{(k+1)}) + \tfrac{1}{\eta}(x^{(k+1)} - y^{(k)})$$

which rearranges to

$$x^{(k+1)} = y^{(k)} - \eta\, \partial g(x^{(k+1)})$$

Subgradient evaluated at the **next** (unknown) point!

ISTA = forward on f + backward on g:

$$x^{(k+1)} = \underbrace{\text{prox}_{\eta g}}_{\text{backward}}\Big(\underbrace{x^{(k)} - \eta \nabla f(x^{(k)})}_{\text{forward}}\Big)$$

FISTA: Accelerated Proximal Gradient (ISTA + Nesterov)

Algorithm 1 *

FISTA (Fast ISTA)

1: $y^{(0)} \leftarrow x^{(0)}$, $t_0 \leftarrow 1$
2: **for** $k = 0, 1, \ldots$ **do**
3: $\quad x^{(k+1)} \leftarrow \text{prox}_{\eta g}(y^{(k)} - \eta \nabla f(y^{(k)}))$
4: $\quad t_{k+1} \leftarrow (1 + \sqrt{1 + 4t_k^2})/2$
5: $\quad y^{(k+1)} \leftarrow x^{(k+1)} + \frac{t_k - 1}{t_{k+1}}(x^{(k+1)} - x^{(k)})$
6: **end for**

Optimal Convergence ($F = f + g$)

$$F(x^{(k)}) - F^* \leq \frac{2M\|x^{(0)} - x^*\|^2}{(k+1)^2}$$

	ISTA	**FISTA**
Rate	$O(1/k)$	$O(1/k^2)$
Iters for ϵ	$O(1/\epsilon)$	$O(1/\sqrt{\epsilon})$

Key insight: Momentum term $\frac{t_k - 1}{t_{k+1}} \approx \frac{k-1}{k+2}$ uses past iterates to "look ahead"; achieves optimal first-order rate for smooth + non-smooth composite problems.

Application: LASSO for Sparse Recovery

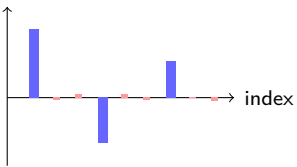
$$\min_x \frac{1}{2}\|Ax - b\|^2 + \lambda\|x\|_1$$

ISTA for LASSO:

1. $y = x - \eta A^T(Ax - b)$
2. $x^+ = \mathcal{S}_{\eta\lambda}(y)$

Step size: $\eta = 1/\lambda_{\max}(A^TA)$

Each iteration: $O(mn)$ for matrix-vector products



Sparse signal + noise

Effect of λ:

- Small λ: fits noise
- Large λ: too sparse
- Just right: recovers signal

Dual Ascent

Problem: $\min_x f(x)$ s.t. $Ax = b$ f is strictly convex

Lagrangian: $L(x, \lambda) = f(x) + \lambda^T(Ax - b)$

Dual function: $D(\lambda) = \inf_x L(x, \lambda)$ (concave in λ)

Algorithm:

$$x^{(k+1)} = \text{argmin}_x L(x, \lambda^{(k)})$$

$$\lambda^{(k+1)} = \lambda^{(k)} + \eta(Ax^{(k+1)} - b)$$

Interpretation:

- Step 1: Find best x for current prices λ
- Step 2: Gradient ascent on dual $D(\lambda)$

Subgradient of dual

If $x^* \in \text{argmin}_x L(x, \lambda)$, then

$$g = Ax^* - b$$

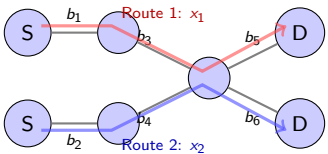
is a subgradient of D at λ.

The **constraint residual** tells us which direction to move λ!

Raise λ_i when constraint i is violated ($[Ax - b]_i > 0$); lower when slack

Application: Internet Congestion Control

Network: Links $\ell = 1, \ldots, L$ with capacities b_ℓ; Routes $r = 1, \ldots, R$ with rates $x_r \geq 0$



Optimization problem:

$$\max_{x \geq 0} \sum_r U_r(x_r) \quad \text{s.t.} \quad \sum_{r:\ell \in r} x_r \leq b_\ell \quad \forall \ell$$

- $U_r(x_r)$: utility of route r (concave, e.g. $\log x_r$)
- Capacity constraints couple all routes sharing a link

Challenge: Routes are controlled by **different users** who don't know each other's utilities!

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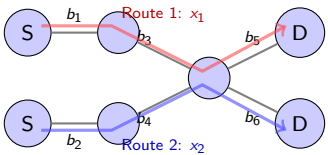

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Lagrangian:

$$L(x, \lambda) = \sum_r U_r(x_r) - \sum_\ell \lambda_\ell \left(\sum_{r:\ell \in r} x_r - b_\ell \right) = \sum_r \Big[U_r(x_r) - x_r \underbrace{\sum_{\ell \in r} \lambda_\ell}_{q_r \text{ (path price)}} \Big] + \sum_\ell \lambda_\ell b_\ell$$

Lagrangian **decomposes by route** for fixed λ! Each user solves independently.

Congestion Control via Dual Ascent

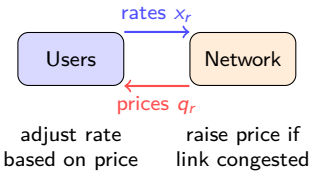
For fixed prices λ, each route independently solves:

$$x_r^*(\lambda) = \text{argmax}_{x_r \geq 0} \left\{ U_r(x_r) - x_r \cdot q_r \right\}, \qquad q_r = \sum_{\ell \in r} \lambda_\ell$$

For $U_r(x) = \log(x)$: $\quad x_r^* = 1/q_r \quad$ ("proportional fairness")

Distributed protocol:

1. **Network signals path delay:**
   Send price $q_r = \sum_{\ell \in r} \lambda_\ell$ to route r
2. **Users regulate rate:**
   Set rate $x_r = (U_r')^{-1}(q_r)$
3. **Rates generate link delays:**
   Update link prices:
   $\lambda_\ell^+ = \left[\lambda_\ell + \eta(\text{load}_\ell - b_\ell)\right]^+$



Q: *Why must we project λ_ℓ onto $\mathbb{R}_+$?*

This is how TCP works!

Dual Ascent: Dual Converges, But What About Primal?

Good news: $D(\lambda)$ is always concave, so dual ascent (= gradient ascent on D) converges to λ^* under standard conditions

Bad news: Having λ^* doesn't mean we can recover x^*!

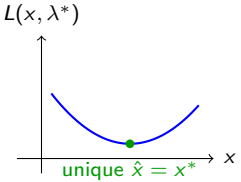
Primal recovery: Given λ^*, solve $\hat{x} \in \operatorname{argmin}_x L(x, \lambda^*)$ and hope $\hat{x} = x^*$

f strictly convex:

$\operatorname{argmin}_x L(x, \lambda^*)$ is a **unique point**

Since x^* must be in this set $\Rightarrow \hat{x} = x^*$

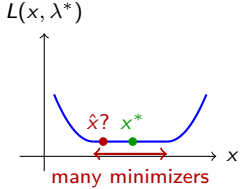
Moreover $x(\lambda)$ continuous, so $\lambda^{(k)} \to \lambda^*$ implies $x^{(k)} \to x^*$



f convex, not strictly:

$\operatorname{argmin}_x L(x, \lambda^*)$ has a **set** of minimizers which includes x^* and **infeasible** points!

Algorithm can pick: $\Rightarrow Ax^{(k)} \neq b$



What Goes Wrong Without Strict Convexity

Example: $\min_{x \in \mathbb{R}^3} \frac{1}{2}(x_1^2 + x_2^2)$ s.t. $x_1 + x_2 + x_3 = 1$

f is convex but **not** strictly convex (doesn't depend on x_3; Hessian $= \text{diag}(1, 1, 0)$)

What dual ascent does:

$L(x, \lambda) = \frac{1}{2}(x_1^2 + x_2^2) + \lambda(x_1 + x_2 + x_3 - 1)$

$\frac{\partial L}{\partial x_1} = x_1 + \lambda = 0 \Rightarrow x_1 = -\lambda$

$\frac{\partial L}{\partial x_2} = x_2 + \lambda = 0 \Rightarrow x_2 = -\lambda$

$\frac{\partial L}{\partial x_3} = \lambda$

If $\lambda \neq 0$: $\inf_{x_3} L = -\infty$ (unbounded!)

If $\lambda = 0$: minimizers $= \{(0, 0, x_3) : x_3 \in \mathbb{R}\}$

$\lambda^* = 0$, but minimizer set is a **line**

True solution: $x^* = (0, 0, 1)$ — but algorithm could pick $(0, 0, 47)$

Observations:

✗ $x(\lambda)$ **not unique**

x_3 is free $\Rightarrow$ infinitely many minimizers

✗ **Primal infeasible**

Algorithm picks arbitrary x_3

$\Rightarrow x_1 + x_2 + x_3 \neq 1$

✗ $D(\lambda)$ **non-smooth**

$$D(\lambda) = \begin{cases} -\lambda & \lambda = 0 \\ -\infty & \lambda \neq 0 \end{cases}$$

Gradient ascent can't even start!

$\Downarrow$

Need a fix!

Augmented Lagrangian: Fixing Dual Ascent

Idea: Add a quadratic penalty for constraint violation

Augmented Lagrangian:

$$\boxed{L_\rho(x, \lambda) = f(x) + \lambda^T(Ax - b) + \frac{\rho}{2}\|Ax - b\|^2}$$

Method of Multipliers:

$$x^{(k+1)} = \text{argmin}_x L_\rho(x, \lambda^{(k)})$$
$$\lambda^{(k+1)} = \lambda^{(k)} + \rho(Ax^{(k+1)} - b)$$

Note: Dual step size $= \rho$ (not a free parameter!)

This is gradient ascent on $D_\rho(\lambda) = \inf_x L_\rho(x, \lambda)$, which is **smooth** with Lipschitz constant $1/\rho$.

Why it fixes dual ascent:

- ✓ $D_\rho(\lambda)$ is **differentiable** (even if f not strictly cvx)
- ✓ Penalty **pushes** $x^{(k)}$ toward feasibility during iterations

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Augmented Lagrangian: The Catch

Comparison:

	Dual Ascent	Aug. Lagrangian
Requires strict cvx	Yes	No
Dual smoothness	Not always	Yes
Primal feasibility	Not guaranteed	Encouraged
Convergence	Fragile	Robust
Decomposable?	**Yes!**	**No!**

The problem:

The penalty $\frac{\rho}{2}\|Ax - b\|^2$ **couples all variables** through A!

Can't distribute the x-update!

Q: *Can we get the best of both Aug. Lagrangian + Dual Ascent?*

$\Downarrow$

ADMM

ADMM: Splitting for Decomposition

Problem structure:

$$\min_{x,z} f(x) + g(z) \quad \text{subject to} \quad Ax + Bz = c$$

Key idea: Split problem into easier subproblems

Augmented Lagrangian:

$$L_\rho(x, z, \lambda) = f(x) + g(z) + \lambda^T(Ax + Bz - c) + \frac{\rho}{2}\|Ax + Bz - c\|^2$$

ADMM alternates:

$$x^+ \leftarrow \text{argmin}_x L_\rho(x, z, \lambda)$$
$$z^+ \leftarrow \text{argmin}_z L_\rho(x^+, z, \lambda)$$
$$\lambda^+ \leftarrow \lambda + \rho(Ax^+ + Bz^+ - c)$$

Why it works:

- x-update: only involves f
- z-update: only involves g
- Each may be easy!
- Penalty ρ couples them

Convergence: $O(1/k)$
Under strong cvx: linear rate

ADMM for LASSO

Reformulate: $\min_{x,z} \frac{1}{2}\|Ax - b\|^2 + \lambda\|z\|_1$ s.t. $x = z$

x-update: Ridge regression

$$x^+ = (A^TA + \rho I)^{-1}(A^Tb + \rho(z - u))$$

z-update: Soft-thresholding

$$z^+ = \mathcal{S}_{\lambda/\rho}(x^+ + u)$$

u-update: (scaled dual)

$$u^+ = u + x^+ - z^+$$

Advantages over ISTA:

- Can precompute $(A^TA + \rho I)^{-1}$
- Often faster for medium-sized problems
- Natural for distributed settings

Choosing ρ:

- Too small: slow convergence
- Too large: ill-conditioning
- Adaptive: balance residuals

ADMM for Distributed Consensus

Problem: $\min_x \sum_{i=1}^{B} f_i(x)$ (agent i knows only f_i)

Reformulation: Give each agent a local copy, enforce consensus

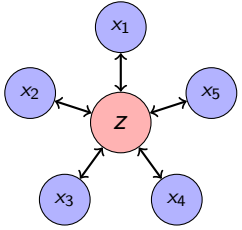
$\min_{x_1,\ldots,x_B,z} \sum_{i=1}^{B} f_i(x_i)$ s.t. $x_i = z \ \forall i$

ADMM updates:

$$x_i^+ = \text{argmin}_{x_i} \left\{ f_i(x_i) + \frac{\rho}{2}\|x_i - z + u_i\|^2 \right\}$$

$$z^+ = \frac{1}{B}\sum_{i=1}^{B}(x_i^+ + u_i)$$

$$u_i^+ = u_i + x_i^+ - z^+$$



Agents solve local problems
Coordinator averages

Communication: Each round, agents send x_i to coordinator, receive z

What About Nonlinear Constraints?

All dual/ADMM methods assumed **affine constraints** $Ax + Bz = c$. Why?

Augmented Lagrangian for $\min_x f(x)$ s.t. $g(x) \leq 0$, g convex:

$$L_\rho(x, \lambda) = f(x) + \lambda^T g(x) + \tfrac{\rho}{2}\|g(x)\|^2$$

Affine: $g(x) = Ax - b$

$\|Ax - b\|^2$ is convex quadratic in x ✓

$\Rightarrow$ x-subproblem is convex ✓

$\Rightarrow$ easy to solve ✓

Nonlinear convex: e.g., $g(x) = x^2 - 1$

$\|g(x)\|^2 = (x^2 - 1)^2 = x^4 - 2x^2 + 1$

$\frac{d^2}{dx^2} = 12x^2 - 4 < 0$ for $|x| < \frac{1}{\sqrt{3}}$ ✗

$\Rightarrow$ penalty is **nonconvex** ✗

What to do for nonlinear convex constraints:

Approach	Idea
Projection	If $\Pi_{\{g \leq 0\}}$ is cheap $\rightarrow$ use projected GD or proximal GD
Linearization	$g(x) \approx g(x^k) + \nabla g(x^k)^T(x - x^k) \leq 0 \rightarrow$ halfspace, then ADMM
Interior point	Barrier $-\sum_i \log(-g_i(x))$ keeps iterates strictly feasible (next Ch.)
Dual ascent	$\lambda^+ = [\lambda + \eta\, g(x^+)]^+$ still valid (dual always concave), but with above limitations

Mirror Descent: Convergence Depends on the Norm

Problem: $\min_{x \in \Delta_n} f(x)$ where $\Delta_n = \{x \geq 0, \sum_i x_i = 1\}$ (probability simplex)

Arises in: bandwidth allocation, portfolio weights, probability distributions, attention mechanisms

Key idea: Replace $\|x - y\|_2^2$ with a **Bregman divergence** $D_\phi(x, y)$:

$$x^{(k+1)} = \text{argmin}_{x \in \Delta_n} \left\{ \nabla f(x^{(k)})^T x + \tfrac{1}{\eta} D_\phi(x, x^{(k)}) \right\}$$

where ϕ is σ-strongly convex w.r.t. $\|\cdot\|_p$ on Δ_n.

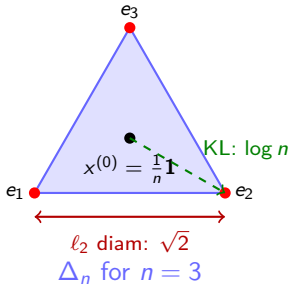
General convergence bound

$$f(\bar{x}^{(k)}) - f^* \;\leq\; L\sqrt{\frac{2\, n^{2-2/p} \cdot Z}{\sigma \cdot k}}$$

$n^{2-2/p}$ — **norm factor** — how gradient scales with dimension n

$Z = D_\phi(x^*, x^{(0)})$ — **initial distance** — Bregman diameter

σ — **strong convexity** of ϕ w.r.t. $\|\cdot\|_p$



Goal: Choose ϕ (and hence p, σ, Z) to minimize $n^{2-2/p} \cdot Z/\sigma$

amazon

Euclidean vs. Entropy: From n to $\log n$

Which norm p minimizes $n^{2-2/p} \cdot Z/\sigma$ over $\Delta_n = \{x \geq 0, \mathbf{1}^T x = 1\}$?

Euclidean ($p = 2$): $\phi = \frac{1}{2}\|x\|_2^2$

Norm factor: $n^{2-2/2} = \mathbf{n}$
Strong cvx: $\sigma = 1$
Diameter: $Z \leq 1$

Product: $\mathbf{n}$

$f(\bar{x}^{(k)}) - f^* \leq L\sqrt{2n/k}$

Iterations for ε: $O(n/\varepsilon^2)$

Entropy ($p = 1$): $\phi = \sum_i x_i \log x_i$

Norm factor: $n^{2-2/1} = n^0 = \mathbf{1}$
Strong cvx: $\sigma = 1$ (w.r.t. $\|\cdot\|_1$)
Diameter: $Z \leq \log n$

Product: $\log \mathbf{n}$

$f(\bar{x}^{(k)}) - f^* \leq L\sqrt{2\log n/k}$

Iterations for ε: $O(\log n/\varepsilon^2)$

	$n = 10^3$	$n = 10^5$	$n = 10^7$
Euclidean iters	$\propto 1000$	$\propto 100{,}000$	$\propto 10{,}000{,}000$
Entropy iters	$\propto 7$	$\propto 12$	$\propto 16$
Speedup	$140\times$	$8{,}300\times$	$620{,}000\times$

Exponentiated Gradient: The Update Rule

Mirror descent with entropy $\phi(x) = \sum_i x_i \log x_i$ on $\Delta_n = \{x \geq 0, \mathbf{1}^T x = 1\}$:

$$x_i^{(k+1)} = \frac{x_i^{(k)} \exp\big(-\eta \left[\nabla f(x^{(k)})\right]_i\big)}{\sum_j x_j^{(k)} \exp\big(-\eta \left[\nabla f(x^{(k)})\right]_j\big)}$$

Why it works:

- Multiply weight by $e^{-\eta \nabla_i f}$
  - Large gradient $\Rightarrow$ aggressive scaling
  - Small gradient $\Rightarrow$ gentle update
- Renormalize so $\sum_i x_i = 1$
- $x_i^{(k)} > 0$ always if $x_i^{(0)} > 0$
- **No projection needed!**

Per-iteration comparison:

	Proj. GD	**Exp. Grad.**
Compute ∇f	$O(n)$	$O(n)$
Project/update	sort $O(n \log n)$	exp $O(n)$
Total/iter	$O(n \log n)$	$O(n)$
Iters for ε	$O(n/\varepsilon^2)$	$O(\log n/\varepsilon^2)$

Also called: Multiplicative Weights Update, Hedge algorithm (online learning)

Init: $x^{(0)} = \mathbf{1}/n$ (minimizes max KL to any vertex)

Savings from **two sources**: fewer iterations ($n \to \log n$) **and** cheaper per-iteration ($n \log n \to n$)

Primal-Dual Methods: Saddle Point View

Problem: $\min_x f(x) + g(Kx)$ (f smooth, g convex, K linear operator)

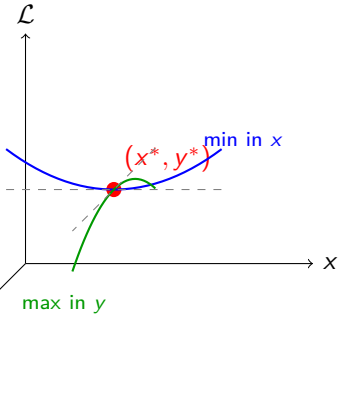
Saddle point reformulation: Using $g(z) = \max_y \{y^T z - g^*(y)\}$:

$$\min_x \max_y \underbrace{f(x) + \langle Kx, y\rangle - g^*(y)}_{\mathcal{L}(x,y)}$$

Examples:

LASSO	: $K = I$, $g = \lambda\|\cdot\|_1$
Equality constr.	: $g = \delta_{\{b\}}$, $g^* = b^T y$
TV denoising	: $K = \nabla$, $g = \lambda\|\cdot\|_1$
Inequality constr.	: $g = \delta_{\leq 0}$, $y \geq 0$

Key insight: Dual variable y acts as Lagrange multiplier for constraint $Kx \in \mathrm{dom}(g)$



From Saddle Point to Algorithms

Goal: $\min_x \max_y \mathcal{L}(x,y) = f(x) + \langle Kx, y\rangle - g^*(y)$

1. Simultaneous GD-Ascent ✗

$$x^{k+1} = x^k - \tau(\nabla f(x^k) + K^T y^k)$$

$$y^{k+1} = y^k + \sigma(Kx^k - \nabla g^*(y^k))$$

Both use **stale** info from step $k \Rightarrow$ oscillates/diverges

2. Simultaneous Proximal ✗

$$x^{k+1} = \text{prox}_{\tau f}(x^k - \tau K^T y^k)$$

$$y^{k+1} = \text{prox}_{\sigma g^*}(y^k + \sigma K x^k)$$

Prox handles f, g^*, but still simultaneous $\Rightarrow$ can diverge

3. Chambolle-Pock ✓

$$y^{k+1} = \text{prox}_{\sigma g^*}(y^k + \sigma K \bar{x}^k)$$

$$x^{k+1} = \text{prox}_{\tau f}(x^k - \tau K^T y^{k+1})$$

$$\bar{x}^{k+1} = x^{k+1} + \theta(x^{k+1} - x^k)$$

Fresh y^{k+1} + **extrapolated** $\bar{x} \Rightarrow$ converges!

4. ADMM ✓

$$x^{k+1} = \text{argmin}_x f(x) + \tfrac{\rho}{2}\|Kx - z^k + u^k\|^2$$

$$z^{k+1} = \text{prox}_{g/\rho}(Kx^{k+1} + u^k)$$

$$u^{k+1} = u^k + Kx^{k+1} - z^{k+1}$$

Quadratic penalty couples K and $x \Rightarrow$ converges!

Two fixes: Chambolle-Pock = alternate + momentum ADMM = augmentation (ρ-penalty)

Chambolle-Pock (PDHG)

Problem: $\min_x \max_y \; f(x) + \langle Kx, y \rangle - g^*(y)$

Algorithm 2 *

Chambolle-Pock (Primal-Dual Hybrid Gradient)

1: Initialize $x^{(0)}$, $y^{(0)}$, $\bar{x}^{(0)} = x^{(0)}$
2: **for** $k = 0, 1, \ldots$ **do**
3: $\quad y^{(k+1)} \leftarrow \text{prox}_{\sigma g^*}(y^{(k)} + \sigma K \bar{x}^{(k)})$
4: $\quad x^{(k+1)} \leftarrow \text{prox}_{\tau f}(x^{(k)} - \tau K^T y^{(k+1)})$
5: $\quad \bar{x}^{(k+1)} \leftarrow x^{(k+1)} + \theta(x^{(k+1)} - x^{(k)})$
6: **end for**

Step sizes: $\tau\sigma\|K\|^2 < 1$, $\theta = 1$

Key ingredients:

- Prox of f (primal)
- Prox of g^* (dual)
- Matrix-vector with K, K^T

Moreau identity:

$$\text{prox}_{\sigma g^*}(y) = y - \sigma \text{prox}_{g/\sigma}(y/\sigma)$$

Compute prox of g^* from prox of g!

Convergence: $O(1/k)$ for convex; linear under strong convexity.

Convergence Rates Summary

Solve: $\text{minimize}_x \quad f(x) + g(x)$

Method	f **Lip. Cvx**[1]	f **Sm. Cvx**	f **Sm.+Str.Cvx**	**Requires**
Subgradient	$O(1/\sqrt{k})$	$O(1/k)$	$O((1-m/M)^k)$	easy proj on $g(x) \leq 0$
ISTA	—	$O(1/k)$	$O((1-m/M)^k)$	∇f, easy prox_g
FISTA	—	$O(1/k^2)$	$O((1-\sqrt{m/M})^k)$	∇f, easy prox_g
Mirror Desc.	$O\left(\sqrt{\frac{\log n}{k}}\right)$[2]	—	—	suitable D_ϕ
ADMM	—	$O(1/k)$	linear	linear split, easy subprob
Chamb.-Pock	—	$O(1/k)$	linear	linear K, easy prox

[1] Non-smooth, bounded subgradient norm.
[2] On simplex Δ_n with entropy.

Key insight: Non-smooth $\Rightarrow O(1/\sqrt{k})$; smooth $\Rightarrow O(1/k)$; acceleration $\Rightarrow O(1/k^2)$.

Method Selection Guide

Problem Structure	**Best Method**	**Alternative**
Simple set (box, ball)	Projected GD	—
Simplex (high-dim)	Mirror descent	Projected GD
ℓ_1 regularization	Proximal GD / FISTA	ADMM
TV regularization	Chambolle-Pock	ADMM
Linear constraints $Ax = b$	ADMM	Chambolle-Pock
Distributed / consensus	ADMM	Dual ascent

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[1] A. Beck and M. Teboulle, "A Fast Iterative Shrinkage-Thresholding Algorithm for Linear Inverse Problems", SIAM J. Imaging Sciences, 2009

[2] S. Boyd, N. Parikh, E. Chu, B. Peleato, J. Eckstein, "Distributed Optimization and Statistical Learning via ADMM", Found. & Trends in ML, 2011

[3] A. Chambolle and T. Pock, "A First-Order Primal-Dual Algorithm for Convex Problems with Applications to Imaging", J. Math. Imaging Vision, 2011

[4] A. Beck, "First-Order Methods in Optimization", SIAM, 2017

[5] S. Bubeck, "Convex Optimization: Algorithms and Complexity", Found. & Trends in ML, 2015

Part VI

Newton's Method and Interior Point Methods

Outline

Goal: Solve convex optimization with high accuracy

$$\underset{x}{\text{minimize}} \quad f(x) \quad \text{subject to} \quad g_i(x) \leq 0, \quad Ax = b$$

- **Newton's method** – second-order information for fast convergence
- **Equality constraints** – Newton via KKT system
- **Interior point methods** – barrier functions for inequalities

Second-order methods: fewer iterations, but $O(n^3)$ per iteration

Newton's Method

Iterative algorithm:

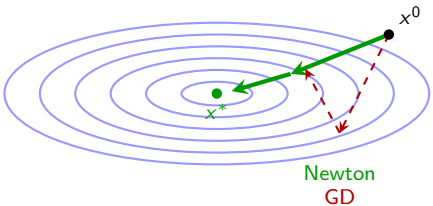
$$x^{k+1} = x^k - \underbrace{\eta^k}_{\text{step size}} \underbrace{[\nabla^2 f(x^k)]^{-1}}_{\text{Hessian inv.}} \underbrace{\nabla f(x^k)}_{\text{gradient}}$$

Newton step:

$$\Delta x_{\text{nt}} = -[\nabla^2 f(x^k)]^{-1} \nabla f(x^k)$$

Step size choices:

- **Pure Newton:** $\eta = 1$
- **Line search:** $\eta^* = \arg\min_\eta f(x^k + \eta \Delta x_{\text{nt}})$
- **Backtracking:** Armijo's rule



Newton takes direct path; GD zigzags on ill-conditioned problems

Newton's Method

Problem: $\text{minimize}_x\, f(x)$

Iterative algorithm:

$$x^{k+1} = x^k - \underbrace{\eta^k}_{\text{step size}} \underbrace{[\nabla^2 f(x^k)]^{-1}}_{\text{Hessian inv.}} \underbrace{\nabla f(x^k)}_{\text{gradient}}$$

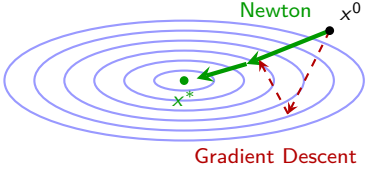
Newton step:

$$\Delta x_{\text{nt}} = -[\nabla^2 f(x^k)]^{-1} \nabla f(x^k)$$

Step size choices:

- **Pure Newton:** $\eta = 1$
- **Line search:** $\eta^* = \arg\min_\eta f(x^k + \eta \Delta x_{\text{nt}})$
- **Backtracking:** Armijo's rule

Isaac Newton (1643–1727)



Why Newton's Method?

Key idea: Use **second-order Taylor expansion** around x^k:

$$f(y) \approx f(x) + \nabla f(x)^T(y-x) + \frac{1}{2}(y-x)^T\nabla^2 f(x)(y-x)$$

Find y that minimizes the approximation:

$$\nabla f(x) + \nabla^2 f(x)(y-x) = 0 \quad \Rightarrow \quad y^* = x - [\nabla^2 f(x)]^{-1}\nabla f(x)$$

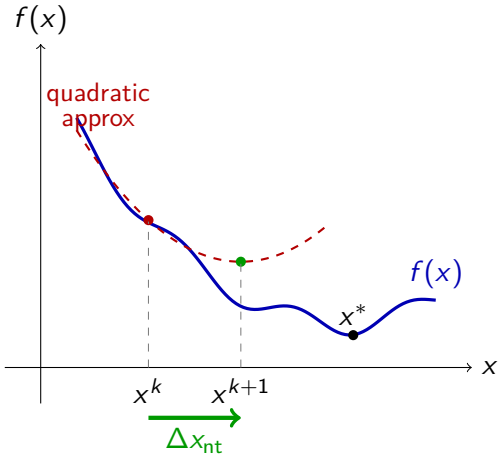
Properties of 2nd order Taylor model:

- **Exact** for quadratic functions
- **Good approximation** locally

Key Insight

Pure Newton step ($\eta = 1$) lands at the **exact minimum of the quadratic approximation**

Why Newton's Method? – Geometric View



Newton minimizes the local quadratic model, then repeats. For quadratic f, one step suffices!

Newton's Decrement

Q: *How much improvement do we expect from one Newton step?*

Newton's decrement: Substitute $y^* = x + \Delta x_{\text{nt}}$ into Taylor expansion:

$$f(x) - f(y^*) \approx \frac{1}{2}\nabla f(x)^T[\nabla^2 f(x)]^{-1}\nabla f(x) \triangleq \frac{1}{2}\lambda^2(x)$$

Definition (Newton Decrement)

$$\lambda(x) = \sqrt{\nabla f(x)^T[\nabla^2 f(x)]^{-1}\nabla f(x)}$$

Stopping Criterion

Stop when $\lambda^2(x)/2 \leq \epsilon$ (expected improvement is small)

Newton's Method with Backtracking

Algorithm 3 *

Newton's Method with Backtracking

Input: tolerance ϵ, $\alpha \in (0, 0.5)$, $\beta \in (0, 1)$, initial x^0
for $k = 0, 1, 2, \ldots$ **do**
  Solve $\nabla^2 f(x^k)\Delta x = -\nabla f(x^k)$; $\lambda^2 \leftarrow -\nabla f(x^k)^T \Delta x$
  if $\lambda^2/2 \leq \epsilon$ **then return** x^k
  end if
  $\eta \leftarrow 1$
  while $f(x^k + \eta\Delta x) > f(x^k) - \alpha\eta\lambda^2$ **do** $\eta \leftarrow \beta\eta$
  end while
  $x^{k+1} \leftarrow x^k + \eta\Delta x$
end for

Typical parameters:

- $\alpha = 0.25$, $\beta = 0.5$
- $\epsilon = 10^{-6}$

Per iteration cost:

- $O(n^2)$: compute Hessian
- $O(n^3)$: solve linear system

Complexity of Newton's Method

Cost breakdown per iteration:

Operation	Cost	Comment
Compute gradient $\nabla f(x^k)$	$O(n)$ to $O(n^2)$	depends on f
Compute Hessian $\nabla^2 f(x^k)$	$O(n^2)$	storage + computation
Solve $\nabla^2 f(x^k)\Delta x = -\nabla f(x^k)$	$O(n^3)$	Cholesky factorization
Line search	$O(1)$	typically few steps

Main Bottleneck: $O(n^3)$ per iteration

- Manageable for n up to $\sim 10^4$
- Prohibitive for $n \sim 10^6 \Rightarrow$ use first-order methods
- Can exploit sparsity in Hessian for structured problems

Convergence of Newton's Method

Theorem (Two-Phase Convergence)

Suppose f is m-strongly convex, M-smooth, with H-Lipschitz Hessian. Then Newton with backtracking converges in two phases:

Phase 1 (Damped):

- When $\|\nabla f(x^k)\|$ is large
- **Linear convergence**
- Step size $\eta < 1$ (damped)

Iterations: $O\left(\frac{f(x^0)-f^*}{\gamma}\right)$
where γ depends on α, β, m, M

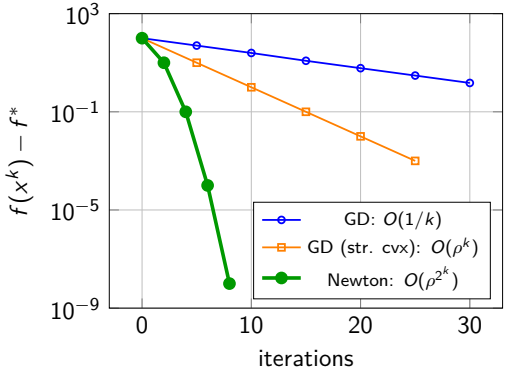
Phase 2 (Pure Newton):

- When $\|\nabla f(x^k)\|$ is small
- **Quadratic convergence**
- Step size $\eta = 1$ accepted

Iterations: $O(\log\log(1/\epsilon))$
Error halves *its exponent* each step!

Total: $O(1) + O(\log\log(1/\epsilon))$ iterations to reach ϵ-accuracy

Quadratic Convergence: Doubling Digits of Accuracy



Quadratic convergence:
Error at step $k+1$:

$$\epsilon_{k+1} \approx C \cdot \epsilon_k^2$$

Digits double each step:

$$\begin{aligned} \epsilon &= 10^{-2} \\ &\to 10^{-4} \\ &\to 10^{-8} \\ &\to 10^{-16} \end{aligned}$$

Machine precision in 3-4 Newton steps once in Phase 2!

amazon

Newton's Method is Affine Invariant

Key property: Newton's method is **independent of coordinate system**

Affine transformation: $y = Ax$ for invertible A, define $g(y) = f(A^{-1}y)$

Newton step in y-coordinates:

$$\begin{aligned}\Delta y &= -[\nabla^2 g(y)]^{-1}\nabla g(y) \\ &= -[A^{-T}\nabla^2 f(x)A^{-1}]^{-1}A^{-T}\nabla f(x) \\ &= A \cdot \underbrace{[-\nabla^2 f(x)]^{-1}\nabla f(x)}_{\Delta x} = A\Delta x\end{aligned}$$

Affine Invariance

Newton produces **identical iterates** (up to transformation) in any coordinate system!

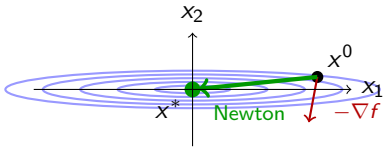
Contrast with GD: Gradient descent is **not** affine invariant — suffers from poor conditioning. Newton automatically adapts to the local geometry via the Hessian.

Example: Newton vs Gradient Descent

Problem: $f(x) = x_1^2 + 100x_2^2$ (condition number $\kappa = 100$)

Gradient and Hessian:

$$\nabla f = \begin{bmatrix} 2x_1 \\ 200x_2 \end{bmatrix}, \quad \nabla^2 f = \begin{bmatrix} 2 & 0 \\ 0 & 200 \end{bmatrix}$$



Newton step at $x^0 = [1, 1]^T$:

$$\Delta x = -\begin{bmatrix} 1/2 & 0 \\ 0 & 1/200 \end{bmatrix} \begin{bmatrix} 2 \\ 200 \end{bmatrix} = \begin{bmatrix} -1 \\ -1 \end{bmatrix}$$

Hessian inverse rescales gradient to point directly at x^*

$\Rightarrow$ **One step to optimum!**

GD would need $O(\kappa) = O(100)$ iterations

Newton with Equality Constraints

Problem: minimize$_x$ $f(x)$ subject to $Ax = b$

Idea: Use KKT to find Newton step that is feasible (use Taylor approx.)

KKT system for Newton step:

$$\begin{bmatrix} \nabla^2 f(x) & A^T \\ A & 0 \end{bmatrix} \begin{bmatrix} \Delta x \\ \nu \end{bmatrix} = \begin{bmatrix} -\nabla f(x) \\ 0 \end{bmatrix}$$

Variables:

- $\Delta x \in \mathbb{R}^n$: Newton step (primal)
- $\nu \in \mathbb{R}^p$: Lagrange multipliers (dual)

For feasibility we require:

$$\begin{cases} Ax^k = b \\ Ax^{k+1} = Ax^k + A\Delta x = b \end{cases} \Rightarrow A\Delta x = 0$$

Cost: Solve $(n + p) \times (n + p)$ linear system per iteration

Interior Point Methods: Motivation

Problem: $\min_x f(x) \quad \text{s.t.} \quad g_i(x) \leq 0, \quad i = 1, \ldots, m$

Reformulation with indicator:

$$\min_x \; f(x) + \sum_{i=1}^{m} I(g_i(x))$$

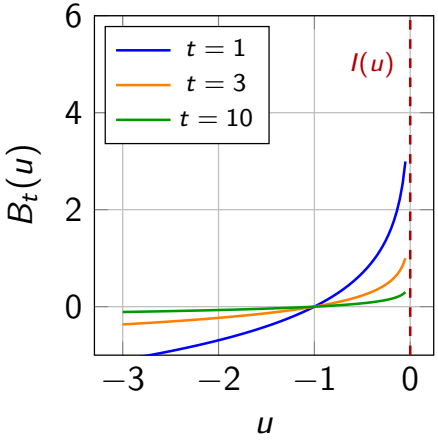
where $I(u) = \begin{cases} 0 & u \leq 0 \\ +\infty & u > 0 \end{cases}$

Problem: non-smooth, non-differentiable!

Idea: Approximate $I(.)$ with a smooth function:

$$B_t(u) = -\frac{1}{t}\log(-u)$$

✓ Smooth, convex, and $B_t(u) \to I(u)$ as $t \to \infty$



Barrier Problem Formulation

Original problem:

$$\underset{x}{\text{minimize}} \;\; f(x) \text{ subject to } g_i(x) \leq 0, \quad i = 1, \ldots, m$$

Barrier problem: (unconstrained!)

$$\underset{x}{\text{minimize}} \quad t \cdot f(x) + \phi(x)$$

where the **log barrier** is:

$$\phi(x) = -\sum_{i=1}^{m} \log(-g_i(x))$$

Properties:

- Domain: $\{x : g_i(x) < 0 \; \forall i\}$
- Barrier $\to \infty$ at boundary
- Solution approaches optimum as $t \to \infty$

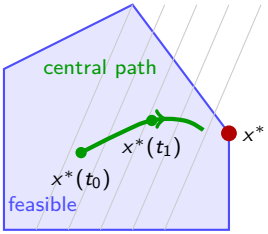
Key insight:

- Unconstrained problem!
- Can solve with Newton's method
- **Gradually increase** t

The Central Path

Definition: The **central path** is $\{x^*(t) : t > 0\}$ for increasing t where $x^*(t)$ solves:

$$\underset{x}{\text{minimize}} \quad t \cdot f(x) + \phi(x)$$



Properties:

- Path stays **strictly inside**
- As $t \to \infty$: $x^*(t) \to x^*$
- Smooth path (easy to follow)

Duality gap bound:

$$f(x^*(t)) - f^* \leq \frac{m}{t}$$

where $m = \#$ constraints

Double $t \Rightarrow$ halve the gap

The Barrier Method Algorithm

Algorithm 4 *

Barrier Method

1: **Input:** strictly feasible x^0, initial $t > 0$, growth factor $\mu > 1$, tolerance ϵ
2: **while** $m/t > \epsilon$ **do**
3: **Centering:** Starting from x, solve via Newton:

$$x \leftarrow \arg\min_x \{t \cdot f(x) + \phi(x)\}$$

4: **Increase:** $t \leftarrow \mu \cdot t$
5: **end while**
6: **return** x

Typical parameters:

- $\mu = 10$ to 20
- Initial t: moderate centering cost

Trade-off in μ:

- Large μ: fewer outer, more Newton
- Small μ: more outer, fewer Newton

Warm start: Previous $x^*(t)$ is excellent initial point for $x^*(\mu t)$

From KKT to Interior Point Methods

Original problem: $\min_x f(x) \quad \text{s.t.} \quad g_i(x) \leq 0, \quad i = 1, \ldots, m$

KKT conditions:

1. $\nabla f(x^*) + \sum_{i=1}^m \lambda_i^* \nabla g_i(x^*) = 0$
2. $g_i(x^*) \leq 0$ (primal feas.)
3. $\lambda_i^* \geq 0$ (dual feas.)
4. $\lambda_i^* g_i(x^*) = 0$ (compl. slack.)

Problem: Condition 4 is **non-smooth** — either $\lambda_i = 0$ or $g_i = 0$, discrete choice!

Relaxed KKT conditions:

1. $\nabla f(x) + \sum_{i=1}^m \lambda_i \nabla g_i(x) = 0$
2. $g_i(x) < 0$ (strictly feas.)
3. $\lambda_i > 0$ (strictly dual feas.)
4. $\lambda_i(-g_i(x)) = 1/t$ (relaxed!)

✓ Condition 4 is now **smooth** — can solve with Newton's method!

As $t \to \infty$: relaxed condition $\lambda_i(-g_i) = 1/t \to 0$
$\Rightarrow$ recover exact complementary slackness!

Relaxed KKT $\Leftrightarrow$ Barrier Optimality

Step 1: Invert relaxed complementary slackness to get λ_i

$$\lambda_i(-g_i(x)) = \frac{1}{t} \qquad \Longrightarrow \qquad \boxed{\lambda_i = \frac{1}{-t \cdot g_i(x)}}$$

Step 2: Substitute into stationarity condition

$$\nabla f(x) + \sum_{i=1}^{m} \lambda_i \nabla g_i(x) = 0 \qquad \Longrightarrow \qquad \nabla f(x) + \sum_{i=1}^{m} \frac{\nabla g_i(x)}{-t \cdot g_i(x)} = 0$$

Step 3: Multiply by t and recognize the gradient

$$t\nabla f(x) - \sum_{i=1}^{m} \frac{\nabla g_i(x)}{g_i(x)} = 0 \qquad \Longrightarrow \qquad \boxed{\nabla \left(t \cdot f(x) - \sum_{i=1}^{m} \log(-g_i(x)) \right) = 0}$$

Result: Relaxed KKT = optimality conditions for **barrier problem**!

$$\min_x \; t \cdot f(x) + \left(-\sum_{i=1}^{m} \log(-g_i(x)) \right)$$

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IPM Complexity: Derivation

Barrier method: At outer iteration k, solve $\min_x \; t_k f(x) + \phi(x)$, where $\phi(x) = -\sum_{i=1}^{m} \log(-f_i(x))$

Step 1: Suboptimality from central path
The minimizer $x^*(t)$ satisfies (from duality):

$$f(x^*(t)) - f^* \leq \frac{m}{t}$$

So to achieve $f - f^* \leq \epsilon$, we need $t_{\text{final}} \geq m/\epsilon$.

Step 2: How many outer iterations to reach t_{final}?
We multiply t by $\mu > 1$ each iteration: $t_k = \mu^k t_0$. Need $\mu^k t_0 \geq m/\epsilon$:

$$k \;\geq\; \frac{\log(m/(\epsilon\, t_0))}{\log \mu}$$

Step 3: The tension — how large can μ be?

	Large μ	**Small μ**
Outer iterations	Few	Many
Centering (Newton)	Many steps (cold start)	Few steps (warm start)

The optimal μ balances these two effects $\longrightarrow$

IPM Complexity: The $\sqrt{m}$ Barrier

Step 4: Newton decrement after t-update
After multiplying $t \to \mu\, t$, the centering problem changes. One can show:

$$\lambda(x^*(t)) \text{ for the new problem at } \mu\, t \;\leq\; \frac{\mu - 1}{\mu} \cdot \sqrt{m}$$

(The barrier ϕ has m terms, each contributing $\sim 1/\sqrt{m}$ to the decrement shift.)
For Newton's method to converge in $O(1)$ steps (warm start), we need $\lambda \leq \beta$ for some constant $\beta < 1$:

$$\frac{\mu - 1}{\mu}\sqrt{m} \leq \beta \quad\Longrightarrow\quad \mu \;\leq\; \frac{1}{1 - \beta/\sqrt{m}} \;\approx\; 1 + \frac{\beta}{\sqrt{m}}$$

Step 5: Combine everything
With $\mu = 1 + \frac{c}{\sqrt{m}}$ and $\log(1 + c/\sqrt{m}) \approx c/\sqrt{m}$:

$$k \;=\; \frac{\log(m/\epsilon)}{\log \mu} \;\approx\; \frac{\log(m/\epsilon)}{c/\sqrt{m}} \;=\; \boxed{\frac{\sqrt{m}}{c}\log\left(\frac{m}{\epsilon}\right)}$$

Each outer iteration: $O(1)$ Newton steps $\times$ $O(n^3)$ per Newton step.

$$\text{Total: } \underbrace{O(\sqrt{m})}_{\text{outer iters}} \times \underbrace{O(1)}_{\substack{\text{Newton per}\\ \text{centering}}} \times \underbrace{O(n^3)}_{\substack{\text{per Newton}\\ \text{step}}} \times \underbrace{\log(m/\epsilon)}_{\text{accuracy}} = O(n^3\sqrt{m}\log(m/\epsilon))$$

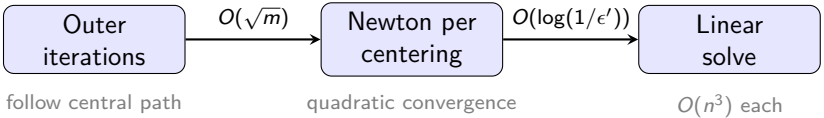
Insight: The $\sqrt{m}$ comes from how much the barrier shifts when t changes

Interior Point Method Complexity

Theorem (IPM Convergence)

The barrier method achieves $f(x) - f^* \leq \epsilon$ in $O\left(\sqrt{m}\log(m/\epsilon)\right)$ outer iterations, where $m =$ number of inequality constraints.

Complexity breakdown:



Total complexity:

$$O(n^3\sqrt{m}\log(m/\epsilon))$$

Polynomial in all parameters!

In practice:

- 20–50 Newton steps **total**
- Nearly independent of n, m
- Theoretically faster than simplex (in worst case)

Key: IPM solves LPs and convex programs in **polynomial time**

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Summary: Second-Order Methods

Method	Problem	Per-iter	Convergence
Newton	Unconstrained	$O(n^3)$	Quadratic
Equality Newton	$Ax = b$	$O((n+p)^3)$	Quadratic
Barrier/IPM	Inequalities	$O(n^3)$	$O(\sqrt{m}\log(1/\epsilon))$

Use second-order when:

- Moderate dimension ($n \leq 10^4$)
- High accuracy needed
- Hessian available/cheap
- Inequality constraints (IPM)

Use first-order when:

- Large scale ($n > 10^6$)
- Low-moderate accuracy OK
- Special structure (sparsity)
- Hessian unavailable/expensive

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