Unconstrained Optimization Algorithms

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My goal is to give you practical tools for your research

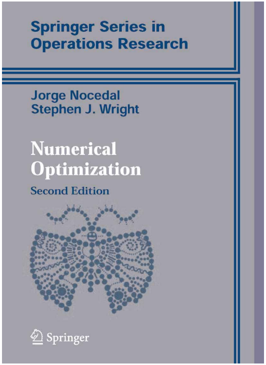
1. Unconstrained optimization preliminaries
2. Unconstrained optimization algorithms
3. Demo on LQR policy optimization

I will cover material from

- Boyd & Vandenberghe's textbook "Convex Optimization" [1]
- Nocedal & Wright's textbook "Numerical Optimization" [2]
- Assorted papers

I can't cover everything today

- See the extended notes
- Take MATH 6321



Intro

So far you have focused on

- Modeling & formulating optimization problems
- Studying & certifying convexity properties

Convexity **decouples** modeling & algorithm design...

- You can *use* convex optimization without *knowing* how solvers work under the hood
  - e.g. CVX, YALMIP

...but knowing how solvers work is important too!

- **Discern** which solver is right for your problem
- **Choose** solver settings in a principled way
- **Predict** how long problems will take to solve
- **Invent** new algorithms

Bonus - algorithms work on some nonconvex problems too!

Unconstrained Optimization Preliminaries

Unconstrained Optimization Problem (hard version)

Find a point x^* that solves

$$x^* = \operatorname*{argmin}_x f(x)$$

where $f : \mathbb{R}^n \to \mathbb{R}$ is called the **objective function**

If such a solution x^* exists, it is called a **global minimizer** and satisfies

$$f(x^*) \leq f(x) \text{ for all } x \in \mathbb{R}^n$$

For some f the problem is **ill-posed or too difficult**

- Settle for a solution to an easier problem
- **(Optional)** Impose mild restrictions on f so the easy and hard problem solutions coincide

What are we trying to do?

Unconstrained Optimization Problem (easy version)

Assume f is **smooth** and has a **local minimizer** x^*. Find x^*.

"Smooth"

- $\nabla f(x)$ exists
- $\nabla f(x)$ continuous
- $\nabla^2 f(x)$ exists
- $\nabla^2 f(x)$ continuous

$\nabla f(x)$ is the **gradient**,
$\nabla^2 f(x)$ is the **Hessian**

"Local minimizer"

There exists a nonempty open ball $\mathcal{N} = \{x : \|x - x^*\| < \varepsilon\}$ for which

$$f(x^*) \leq f(x) \text{ for all } x \in \mathcal{N}$$

Question: How do we know if we have found a minimizer?

Answer: Check optimality conditions.

First-order optimality conditions

First-order necessary condition (FONC) (Theorem 2.2 of [2])

If f has a local minimizer x^* and f is continuously differentiable in a neighborhood of x^*, then

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

Such a point is called a **stationary point**.

Proof: See [2]

Most optimization algorithms **search for a stationary point**

- FONC $\rightarrow$ only stationary points can be local minimizers

First-order optimality conditions

Global differentiable strict first-order sufficient condition (GD-SFOSC)

Suppose f is continuously differentiable and there exists x^* such that

$$\nabla f(x)^\intercal (x - x^*) \geq 0 \text{ for all } x \text{ with equality only when } x = x^*.$$

Then x^* is the unique stationary point and unique global minimizer of f.

Proof: See extended version of these lecture notes.

Note: The GD-SFOSC is **not necessary** (except in 1D) for f to have a unique stationary point and unique global minimizer

- **Counterexample**: Rosenbrock function

Second-order optimality conditions

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Second-order necessary condition (SONC) (Theorem 2.3 of [2])

If f has a local minimizer x^* and $\nabla^2 f$ exists and is continuous in a neighborhood of x^*, then

$$\nabla f(x^*) = 0 \quad \text{and} \quad \nabla^2 f(x^*) \succeq 0.$$

Proof: See [2]

Second-order sufficient condition (SOSC) (Theorem 2.4 of [2])

Suppose that $\nabla^2 f$ is continuous in a neighborhood of a point x^*, and

$$\nabla f(x^*) = 0 \quad \text{and} \quad \nabla^2 f(x^*) \succ 0.$$

then x^* is a strict local minimizer of f.

Proof: See [2]

Note: **SOSC implies SFOSC [3].**

We want slope conditions on f to certify that
all stationary points are global minimizers

Most slope conditions have a strict version which certifies that
a unique stationary point is the unique global minimizer

We already saw a special case - the GD-SFOSC

$$\nabla f(x)^\intercal (x - x^*) \geq 0 \text{ for all } x \text{ with equality only when } x = x^*.$$

implies **the stationary point x^* is the unique global minimizer**

The most well-known and well-studied slope condition is **convexity**

- As you are very familiar with by now!

Invexity

Convexity is nice, but the class of functions for which **all stationary points are global minimizers** is much more broad.

In fact, the **broadest class** of such functions are those which are **invex**.

Definition of invexity (eq. (1) in [4])

The differentiable function $f : \mathbb{R}^n \to \mathbb{R}$ is **invex** if there exists a function $\eta : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}^n$ such that, for any $x, y \in \mathbb{R}^n$,

$$\nabla f(x)^\intercal \eta(x, y) \geq f(x) - f(y).$$

Convexity implies invexity by taking $\eta(x, y) = x - y$.

Characterization of invexity (Theorem 1 in [4])

The differentiable function $f : \mathbb{R}^n \to \mathbb{R}$ is **invex** if and only if **all stationary points are global minimizers**.

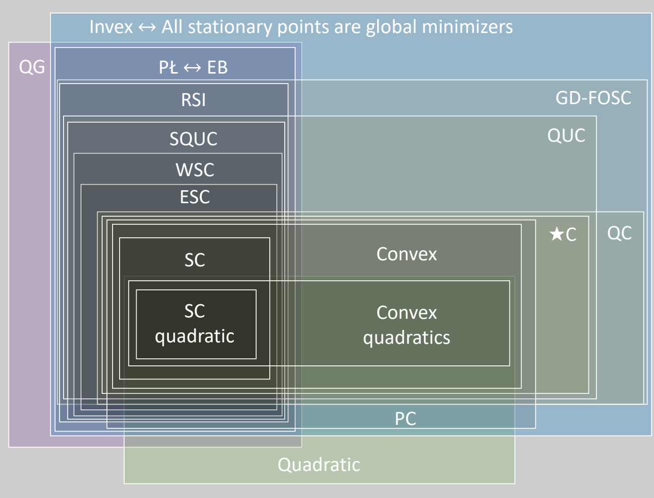


Figure 1: Slope condition nesting diagram when f is continuously differentiable and uniquely minimized. *Caveat emptor - check your assumptions and the literature before claiming an implication / non-implication.*

The zoo of slope conditions

Examples of functions in **control theory** that satisfy slope conditions:

SC quadratic	Finite-horizon LQR cost as function of the state-input sequence
Convex	Lyapunov-based control design objectives [5]
Invex	Rosenbrock function
Polyak-Łojasiewicz inequality	Infinite-horizon LQR cost as function of gain matrix [6] (w/ multiplicative noise [7])
Weakly quasiconvex	"Idealized risk" in learning linear systems [8]

Key takeaways up to this point

- Seek a stationary point x^* where $\nabla f(x^*) = 0$
- If we find x^*, we solved the "easy" problem
- If f continuously differentiable and invex or GD-SFOSC, then x^* is a global minimizer of f, and we solved the "hard" problem

Unconstrained Optimization Algorithms

What are we *really* trying to do?

Nesterov's thought experiment (Chapter 1.1.2 of [9])

1. Suppose our goal was just to **solve a particular problem** $\mathcal{P}_0$
2. Suppose somehow we managed to solve it and find x^*
3. At this point, we already have the best "algorithm" to solve $\mathcal{P}_0$, which is to **simply report** x^*
    - i.e. if we had to solve $\mathcal{P}_0$ again, we would just mindlessly blab x^*
4. But what happens if we **have a different problem** $\mathcal{P}_1 \neq \mathcal{P}_0$?
5. Unless we get exceptionally lucky, our old "algorithm" will give a **wrong answer**
6. We don't really care about the solution to a **particular problem**
7. We really want an algorithm to solve an **entire class of problems**
    - The faster it solves, the better
    - The less sensitive it is to numerical errors, the better

Algorithm 1 Generic descent

Input: Initial guess x_0

while $\|\nabla f(x_k)\| > \varepsilon$ **do**

$x_{k+1} = x_k + \mathsf{update}(f(x_k), \nabla f(x_k), \nabla^2 f(x_k); \mathsf{parameters})$

$k \leftarrow k+1$

Output: $x_k \approx x^*$

Iterative descent

Each iteration is designed to decrease the function value

Oracle model

Only require evaluations of $f(x)$, $\nabla f(x)$, $\nabla^2 f(x)$ at particular points x

- No explicit knowledge of the entire objective function f

Broad categories

Categories

1. Line-search methods
2. Trust-region methods
3. Accelerated gradient methods

Distinctions between line-search and trust-region are blurry!

Line Search Methods

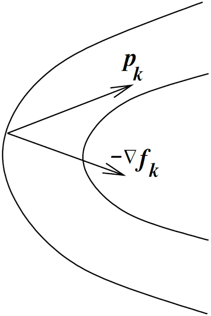
The **line-search method** uses updates of the form

$$x_{k+1} = x_k + \alpha_k p_k$$

where

- $x_k \in \mathbb{R}^n$ is the **current iterate**
- $\alpha_k \in \mathbb{R}$ is the **step size**, also called the **step length** in [2]
- $p_k \in \mathbb{R}^n$ is the **search direction**
- $x_{k+1} \in \mathbb{R}^n$ is the **next iterate**

Idea: Choose α_k and p_k so that $f(x_{k+1}) < f(x_k)$



A **descent direction** of f at x is any vector p that satisfies

$$\nabla f(x)^\intercal p < 0$$

i.e. the angle between $\nabla f(x)$ and p is less than 90 degrees
"p points downhill"

Descent directions

Question: Why does $\nabla f(x)^\intercal p < 0$ ensure descent is possible?

From Taylor's theorem we have a first-order expansion

$$f\left(x+\alpha p\right) = f\left(x\right) + \alpha \nabla f(x)^\intercal p + \mathcal{O}\left(\alpha^2\right)$$

$\nabla f(x)^\intercal p < 0$ implies

$$f\left(x+\alpha p\right) < f\left(x\right)$$

for all $\alpha > 0$ sufficiently small

(the linear term dominates the quadratic term for small α)

Search directions

Use search directions of the form:

$$p_k = -B_k^{-1} \nabla f_k$$

$$\begin{aligned} \textbf{Gradient method} \quad & B_k = I \\ \textbf{Newton method} \quad & B_k = \nabla^2 f_k \\ \textbf{Quasi-Newton method} \quad & B_k \approx \nabla^2 f_k \end{aligned}$$

Each of these p_k is a descent direction under mild assumptions

Motivation 1

Minimize a first-order Taylor series model of f around x_k on a trust region of radius $\|\nabla f(x)\|$

$$\begin{aligned} \underset{p}{\text{minimize}} \quad & f_k + \nabla f_k^\intercal p \qquad \approx f(x_k + p) \\ \text{subject to} \quad & \|p\| \leq \|\nabla f_k\| \end{aligned}$$

Solution is precisely the negative gradient $p_k = -\nabla f_k$

Motivation 2

$-\nabla f_k$ is a descent direction away from stationary points

Assume x_k is not a stationary point so $\nabla f_k \neq 0$
(i.e. we have not solved the problem yet)

Then

$$\nabla f_k^\intercal p_k = -\nabla f_k^\intercal \nabla f_k < 0$$

Newton method ($p_k = -\nabla^2 f_k^{-1} \nabla f_k$)

Motivation 1

Minimize a second-order Taylor series model of f around x_k

$$\underset{p}{\text{minimize}} \quad f_k + \nabla f_k^\intercal p + \frac{1}{2} p^\intercal \nabla^2 f_k p \qquad \approx f(x_k + p)$$

Solution is precisely the Newton direction $p_k = -\nabla^2 f_k^{-1} \nabla f_k$

Motivation 2

$-\nabla^2 f_k^{-1} \nabla f_k$ is a descent direction in regions of positive curvature

Assume $\nabla f_k \neq 0$. Also assume $\nabla^2 f_k \succ 0$ due to either

1. f is strictly convex
2. x_k is close enough to a local minimizer where the SOSC holds

Then

$$\nabla f_k^\intercal p_k = -\nabla f_k^\intercal \nabla^2 f_k^{-1} \nabla f_k < 0$$

Motivation 1

Minimize an approximate second-order Taylor series model of f around x_k

$$\underset{p}{\text{minimize}} \quad f_k + \nabla f_k^\intercal p + \frac{1}{2} p^\intercal B_k p \qquad \approx f(x_k + p)$$

Solution is precisely the quasi-Newton direction $p_k = -B_k^{-1} \nabla f_k$

Motivation 2

$-B_k^{-1} \nabla f_k$ is a descent direction for positive definite B_k

Assume $\nabla f_k \neq 0$ and choose $B_k \succ 0$

Then

$$\nabla f_k^\intercal p_k = -\nabla f_k^\intercal B_k^{-1} \nabla f_k < 0$$

Step size selection

Idea: Use a **constant step size**

$$\alpha_k = \alpha$$

- Advantage: Simple to implement
- Advantage: Simple to analyze
- Disadvantage: Cannot adapt to changing f_k, ∇f_k, $\nabla^2 f_k$ over iterations
  - If α too big, might get oscillations, divergence
  - If α too small, convergence will take forever
- Disadvantage: Choice of proper α depends on f and x_0
  - Might be difficult or impossible to verify in practice
- Not covered in [2], we'll skip these for now

Idea: Use a **varying history-dependent step size**

$$\alpha_k = \alpha\left(\{x_j, f_j, \nabla f_j, \nabla^2 f_j\}_{j=0}^{k}\right)$$

- Advantage: Adaptive, can accelerate convergence
- Advantage: State-of-the-art in training huge neural networks
- Disadvantage: Hyperparameter settings require careful tuning
- Disadvantage: Most are heuristics w/o convergence guarantees
- Examples: Accelerated gradient methods mentioned later
- Not covered in [2], we'll skip these for now
- See the survey

Idea: Use a varying step size that solves the 1D **line search** problem

$$\alpha_k = \operatorname*{argmin}_{\alpha} f(x_k + \alpha p_k)$$

- Advantage: Adaptive, maximizes greedy one-step benefit
- Advantage: Guarantees descent if p_k is a descent direction
- Advantage: Formal convergence guarantees
- Disadvantage: Requires extra function evaluations, usually have to settle for an approximate solution

Wolfe conditions

Usually we cannot solve the line search problem exactly

- Need conditions to **certify quality** of inexact line search solutions

Wolfe conditions

The **Wolfe conditions** require

$$f\left(x_k + \alpha_k p_k\right) \leq f\left(x_k\right) + c_1 \alpha_k \nabla f_k^T p_k \qquad \text{(Sufficient decrease)}$$
$$\nabla f\left(x_k + \alpha_k p_k\right)^T p_k \geq c_2 \nabla f_k^T p_k \qquad \text{(Curvature condition)}$$

for some constants $0 < c_1 < c_2 < 1$.

Practically, Wolfe conditions are used to select step sizes that ensure

- The function value decreases enough (in a relative sense)
- The iterates make reasonable progress

Theoretically, Wolfe conditions are used to prove convergence and rates

Backtracking line search

Backtracking Line Search (Algo. 3.1 in [2], Algo. 9.2 in [1])

Choose $\bar{\alpha} > 0$, $\rho \in (0, 1)$, $c \in (0, 1)$; Set $\alpha \leftarrow \bar{\alpha}$;
repeat until $f(x_k + \alpha p_k) \leq f(x_k) + c\alpha \nabla f_k^T p_k$
$\quad \alpha \leftarrow \rho\alpha$;
end (repeat)
Terminate with $\alpha_k = \alpha$.

Ensures α_k is never smaller than it needs to be

Terminates after a finite number of trials

- Eventually α shrinks enough that the sufficient decrease holds (since p_k is a descent direction)

Note: Backtracking line search satisfies sufficient decrease,
but **not the curvature Wolfe condition!**

- Rules out some theoretical results in [2]

More sophisticated **Wolfe line search**

- Solve the line search problem more exactly
- Guarantee satisfaction of the Wolfe conditions
- Use interpolation polynomials, bracketing and selection phases
- Tedious to code from scratch
- Implemented in scipy.optimize
- See Chapter 3.5 of [2]

Rates of convergence

Q-order convergence

The sequence $\{x_k\}$ is

- **Q-linearly convergent** if there exists a constant $r \in (0,1)$ such that

$$\frac{\|x_{k+1} - x^*\|}{\|x_k - x^*\|} \leq r \text{ for all } k \text{ sufficiently large.}$$

- **Q-superlinearly convergent** if

$$\lim_{k \to \infty} \frac{\|x_{k+1} - x^*\|}{\|x_k - x^*\|} = 0.$$

- **Q-quadratically convergent** if there exists a constant $M > 0$ such that

$$\frac{\|x_{k+1} - x^*\|}{\|x_k - x^*\|^2} \leq M \text{ for all } k \text{ sufficiently large.}$$

Note: Q-quadratic $\Rightarrow$ Q-superlinear $\Rightarrow$ Q-linear

Rates of convergence

Convergence of line search methods

Under mild assumptions, the iterates x_k converge to x^* according to

Method	Rate	Reference
Gradient	Linear	Theorem 3.4 in [2]
Quasi-Newton	Superlinear	Theorem 3.5 in [2]
Newton	Quadratic	Theorem 3.6 in [2]

Rate constants depend on slope properties of f

Constant step size?

- Similar results
- Easier analysis
- Worse rate constants

Gradient descent on strongly convex functions

Gradient descent on strongly convex functions (eq. (9.18) in [1])

Suppose $f(x)$ is strongly convex with

$$mI \preceq \nabla^2 f(x) \preceq MI \quad \forall x$$

Gradient descent with exact line search leads to linear convergence

$$\frac{f(x_{k+1}) - f(x^*)}{f(x_k) - f(x^*)} \leq \frac{\kappa - 1}{\kappa}$$

- $\kappa = M/m$ is the **condition number**

Special cases

- $\kappa = 1$, then $\frac{\kappa-1}{\kappa} = 0$ so minimum found in **one iteration**
- $\kappa \to \infty$, then $\frac{\kappa-1}{\kappa} \to 1$ so convergence gets **arbitrarily slow**

Preconditioning

Trick: Use change-of-variables to reduce condition number of $\nabla^2 f(x)$

Example

Before	Change-of-variables	After
$f(x) = 4x_1^2 + 100x_2^2$	$y_1 = 2x_1$	$g(y) = y_1^2 + y_2^2$
so $\kappa = 100/4 = 25$	$y_2 = 10x_2$	so $\kappa = 1/1 = 1$

Note: Not straightforward in practice

- Non-quadratic $\rightarrow$ Hessian eigenvalues change over domain
  - Always stuck with poor conditioning on some parts of the domain
- May not be easy to find a good scaling
- **Rule-of-thumb**: Use units that make the decision variables have the same order-of-magnitude on the domain of interest

Newton method

Not hard to show that Newton method is **affine invariant**

- Affine change-of-variables has no effect on the convergence rate
- See Chapter 9.5 of [1]

Per-iteration cost of Newton method is high

- Requires storing $\mathcal{O}(n^2)$ entries of $\nabla^2 f_k$
- Requires solving n linear equations $\nabla^2 f_k \cdot (x_{k+1} - x_k) = -\nabla f_k$
  - $\mathcal{O}(n^3)$ operations using basic techniques if $\nabla^2 f_k$ full
  - Fewer operations if $\nabla^2 f_k$ banded, sparse, low rank
    - Chapter 9.7 of [1]
  - Fewer operations if approximate solver e.g. conjugate gradient used
    - Chapter 5, 7.1 of [2]

Example: Strongly convex function (9.20) from [1]

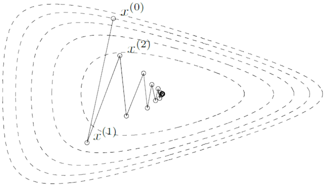


Figure 2: Gradient descent with backtracking line search

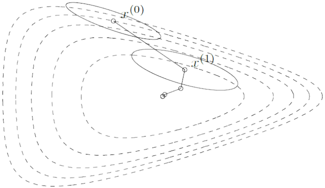


Figure 3: Newton method with backtracking line search

Quasi-Newton Methods

Motivation:
Newton method converges fast... but Hessians are expensive!

Idea: Approximate Hessian with gradient information at multi-points

- In **finite-differencing**, the multi-points are chosen close to x_k i.e. $\{x_k + \varepsilon e_i\}$ where e_i are unit vectors, $0 < \varepsilon << 1$
  - Chapter 8 of [2]
- In **model-based derivative-free methods** the multi-points are spread out over a large trust-region centered on x_k
  - Chapter 9.2 of [2]
- In **quasi-Newton methods**, the multi-points are chosen as the iterates themselves $\{x_0, x_1, \dots, x_k\}$
  - Chapter 6 of [2]

Idea: Approximate the true objective f with a quadratic model m_k

$$f(x_k + p) \approx m_k(p) := f_k + \nabla f_k^\intercal p + \frac{1}{2} p^\intercal B_k p$$

Idea: Update quadratic model from m_k to m_{k+1} at each iteration:

$$m_{k+1}(p) = f_{k+1} + \nabla f_{k+1}^\intercal p + \frac{1}{2} p^\intercal B_{k+1} p$$

Question: How to choose B_{k+1} given all prior information?

Answer:

1. Make the gradient of m_{k+1} match the gradient of f at x_{k+1}
2. Make the gradient of m_{k+1} match the gradient of f at x_k
3. Make B_{k+1} symmetric positive definite
4. Make B_{k+1} similar to B_k

DFP and BFGS methods

Davidon-Fletcher-Powell (DFP) update

$$B_{k+1} = \left(I - \frac{s_k y_k^\intercal}{y_k^\intercal s_k}\right)^\intercal B_k \left(I - \frac{s_k y_k^\intercal}{y_k^\intercal s_k}\right) + \frac{y_k y_k^\intercal}{y_k^\intercal s_k}$$

Broyden-Fletcher-Goldfarb-Shanno (BFGS) update

$$B_{k+1} = B_k - \frac{B_k s_k s_k^\intercal B_k}{s_k^\intercal B_k s_k} + \frac{y_k y_k^\intercal}{y_k^\intercal s_k}$$

Concepts

- B_{k+1} is a **rank-2 update** from B_k
  - Based on most recent iterate x_k and gradient ∇f_k information
- B_k encodes information about curvature from **all previous updates**
- DFP and BFGS are **duals**
- BFGS typically outperforms DFP

SR1 method

Idea: Instead of a rank-2 update like BFGS or DFP, use a **symmetric rank-1 (SR1)** update

$$B_{k+1} = B_k + \frac{(y_k - B_k s_k)(y_k - B_k s_k)^\mathsf{T}}{(y_k - B_k s_k)^\mathsf{T} s_k}$$

Issue: Unlike BFGS/DFP, the SR1 matrices often become **indefinite**

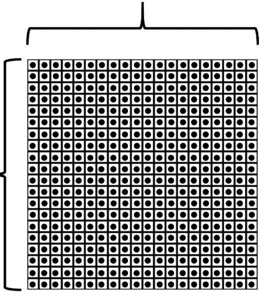
- Actually an **advantage** since true Hessian may be indefinite
- **Fix 1**: Make eigenvalues positive for **line-search** (not recommended by [2])
- **Fix 2**: Use indefinite B_k in a **modified trust-region method** (Algorithm 6.2 in [2])

Large-scale quasi-Newton methods

Motivation: Storing full $n \times n$ approximate Hessians can be intractable!

$n = 10{,}000{,}000$

$n = 10{,}000{,}000$



$(1e7)^2$ entries $\times$ 8 bytes / entry
$= 800$ TB

Full Hessian approximation captures gradient information from **all previous iterations**

Instead, just store $m << n$ pairs of length-n vectors associated with the **most recent few iterations**

Doing this uses **limited memory**

Special structure of B_k and BFGS updates allows efficient reconstruction of $p_k = -B_k^{-1} \nabla f_k$ **without explicitly constructing** B_k

Limited-memory BFGS (L-BFGS) is derived in Chapter 7.2 of [2]

Trust-Region Methods

Trust-region methods

Idea: Approximate the true objective f with a quadratic model m

$$f(x+p) \approx m(p) \coloneqq f(x) + \nabla f(x)^\intercal p + \frac{1}{2} p^\intercal \nabla^2 f(x) p$$

Idea: Only trust the model within a small radius Δ of x

$$\|p\| \leq \Delta$$

Together this yields the **trust-region subproblem**

$$\begin{aligned} \underset{p}{\text{minimize}} \quad & m(p) = f(x) + \nabla f(x)^\intercal p + \frac{1}{2} p^\intercal \nabla^2 f(x) p \\ \text{subject to} \quad & \|p\| \leq \Delta \end{aligned}$$

Trust-region methods (Figure 2.4 in [2])

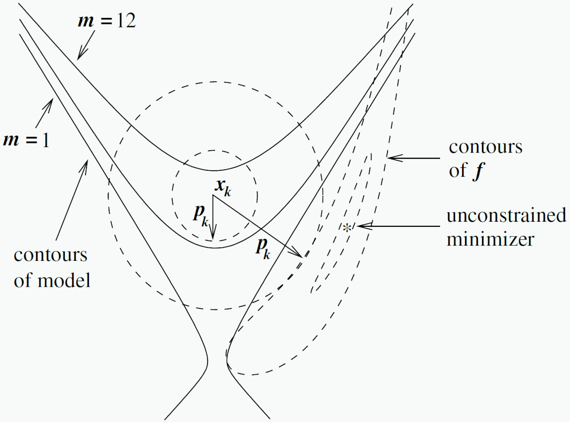


Figure 4: Two possible trust regions (circles) and their corresponding steps p_k. The solid lines are contours of the model function m_k

Trust-region subproblem

What happens to p as the trust radius Δ varies from 0 to ∞?

Case 1: $\Delta \to 0$
Solution is the **gradient step** $p = -\frac{\Delta}{\|\nabla f(x)\|} \nabla f(x)$

Case 2: $\Delta \to \infty$
Solution is the **Newton step** $p = -\nabla^2 f(x)^{-1} \nabla f(x)$

Case 3: $0 < \Delta < \infty$
Solution follows a **curved path**

Trust-region interpolates between gradient and Newton method in a principled way

Since $\nabla^2 f(x)$ may not be positive semidefinite, the trust-region subproblem is generally a **nonconvex** problem

However, we can still show that **strong duality** holds

- Best bound from the **Lagrange dual** is tight (zero **duality gap**)

Strong duality of the trust-region subproblem (Theorem 4.1 in [2])

The vector p^* is a global solution of the trust-region problem

$$\min_{p \in \mathbb{R}^n} m(p) = f + g^T p + \frac{1}{2} p^T B p, \quad \text{s.t. } \|p\| \le \Delta, \tag{4.7}$$

if and only if p^* is feasible and there is a scalar $\lambda \ge 0$ such that

$$(B + \lambda I) p^* = -g, \tag{4.8a}$$

$$\lambda(\Delta - ||p^*||) = 0, \tag{4.8b}$$

$$(B + \lambda I) \quad \text{is positive semidefinite.} \tag{4.8c}$$

- Direct proof - see Chapter 4.3 of [2]
- Proof using S-procedure - see Appendix B of [1]

How to solve the trust-region subproblem?

- Form the Lagrange dual problem & solve in CVX (expensive)
- Use a specialized approximate solution (cheap)

Remember: We have to solve a new subproblem at each iteration, so we want to get "good enough" solutions quickly

Approximations effectively try to solve the KKT conditions

1. Dogleg method
2. 2d-subspace minimization
3. Conjugate gradient
4. Iterative solution via dual

Quadratic convergence of trust region (Theorem 4.9 in [2])

Under mild assumptions, using the trust region method with any of the approximate subproblem solutions leads to **quadratic convergence**.

Least-squares Methods

Least-squares problems

In **nonlinear least-squares** problems, the objective f takes the form

$$f(x) = \frac{1}{2}\|r(x)\|^2$$

where

- $r(x) : \mathbb{R}^n \to \mathbb{R}^m$ is a nonlinear **residual** function
- n is the number of **parameters** (e.g. in a prediction model)
- m is the number of **observations** (e.g. collected from experiments)

The **Jacobian** of the residuals is

$$J(x) = \left[\frac{\partial r_j}{\partial x_i}\right]_{j=1,2,\ldots,m} = \begin{bmatrix} \nabla r_1(x)^T \\ \nabla r_2(x)^T \\ \vdots \\ \nabla r_m(x)^T \end{bmatrix}$$

The gradient and Hessian of the objective are then

$$\nabla f(x) = J(x)^T r(x)$$
$$\nabla^2 f(x) = J(x)^T J(x) + \sum_{j=1}^{m} r_j(x) \nabla^2 r_j(x)$$

Idea: Approximate the Hessian as

$$\nabla^2 f(x) \approx J(x)^\mathsf{T} J(x)$$

Need to compute $J(x)$ for $\nabla f(x)$, so we get this for free!

Two cases when the Hessian approximation is good

- If $r(x)$ is small (model fits data well)
- If $\nabla^2 r_j(x)$ is small (residuals nearly affine in parameters)

Gauss-Newton algorithm

Gauss-Newton

- Line-search quasi-Newton using the Hessian approximation $B_k = J_k^\intercal J_k$

Can be solved very efficiently

- We only have to compute J_k
- The Newton equation is a **normal equation**

$$J_k^\intercal J_k p_k = -J_k r_k$$

  which can be solved with QR or SVD techniques

  - Chapter 10.2 of [2]

Levenberg-Marquadt

- Trust-region using the Hessian approximation $B_k = J_k^\intercal J_k$

Can be solved very efficiently because

- We only have to compute J_k
- The KKT conditions for the trust-region subproblem specialize and can be solved using linear algebra techniques
  - Chapter 10.3 of [2]

Accelerated Gradient Methods

Motivation

Large-scale machine learning objectives & gradients are expensive

- Only store a few iterates in memory / hard drive / cloud
- Only evaluate gradient once per iteration
- Use cheap noisy gradient estimates in place of exact gradients
- Use heuristics & tricks to get speedups for free

Too many accelerated gradient methods to cover right now

Here are some famous methods & references

- Polyak momentum [10] (Beautiful interactive explainer)
- Nesterov acceleration
  - Original paper (Russian) [11]
  - Nesterov's lecture notes [9]
  - Chapter 3.7 of Bubeck's book [12]
  - Sutskever paper [13]
- Conformal symplectic / relativistic acceleration [14]
  - Zhang et al. [15] question the connection between symplectic integration of the descent ODE and acceleration
- RMSprop (never published, only in Hinton's lecture notes)
- AdaGrad [16]
- Adam & AdaMax [17]

Optimization of Nonsmooth Functions

Optimization of nonsmooth functions

So far we only considered objective functions that are smooth

- We demanded the gradient $\nabla f(x)$ exist everywhere

But sometimes objective functions are not differentiable at certain points

- Ex. sparsity-promoting ℓ_1 regularization $\min f(x) + \|x\|_1$

What can we do?

Smoothing methods [Vandenberghe's notes]
Subgradient methods [Boyd's notes]
Proximal methods [Parikh & Boyd tutorial]

Calculating Derivatives

Let's face it, calculating derivatives by hand is tedious

Wouldn't it be great to get derivatives without the hassle?

Finite differences	Chapter 8.1 of [2]
Automatic differentiation	Chapter 8.2 of [2]
Symbolic differentiation	Chapter 8 intro of [2]

Constrained Optimization

So far we did not permit explicit constraints on decision variables

What can we do?

1. Form the Lagrangian dual problem & apply unconstrained algorithms
2. Use specialized algorithms that handle constraints natively
   - Simplex algorithm for LPs
   - Projected gradient
   - Proximal algorithms
   - Augmented Lagrangian
   - Alternating direction method of multipliers (ADMM)
   - Interior point methods

LQR Policy Optimization

Why use LQR policy optimization as a test case in optimization?

- Attractive theoretical properties
  - Nontrivial slope characteristics
  - Baseline solution from control theoretic techniques
- Practical utility
  - Fundamental problem in control theory
  - Design useful controllers automatically
- Springboard for harder problem classes, algorithms, & analysis
  - Nonlinear systems
  - Model-free reinforcement learning

$$\begin{aligned} \underset{K}{\text{minimize}} \quad & \mathbb{E}_{x_0} \sum_{t=0}^{\infty} \begin{bmatrix} x_t \\ u_t \end{bmatrix}^\intercal \begin{bmatrix} Q_{xx} & Q_{xu} \\ Q_{ux} & Q_{uu} \end{bmatrix} \begin{bmatrix} x_t \\ u_t \end{bmatrix} \\ \text{subject to} \quad & x_{t+1} = Ax_t + Bu_t \\ & u_t = Kx_t \\ & x_0 \sim \mathcal{D}(0, X_0) \end{aligned}$$

Decision variable: K

Problem data: (A, B, Q, X_0)

Assumptions:

- (A, B) controllable
- (A, Q_{xx}) observable
- $Q \succ 0$
- $X_0 \succ 0$

You already know how to solve LQR using convex programming (from past homework)

$$\begin{aligned} \underset{P}{\text{maximize}} \quad & \operatorname{trace}(PX_0) \\ \text{subject to} \quad & \begin{bmatrix} -P + Q_{xx} + A^\intercal PA & Q_{xu} + A^\intercal PB \\ Q_{ux} + B^\intercal PA & Q_{uu} + B^\intercal PB \end{bmatrix} \succeq 0, \\ & P \succeq 0 \end{aligned}$$

- Form a linear matrix inequality (LMI) constraint
  - Schur complement of algebraic Riccati inequality (ARI)
- Put the semidefinite program (SDP) into CVX and hit run
- Optimal gain $K^* = -(Q_{uu} + B^\intercal PB)^{-1}(Q_{ux} + B^\intercal PA)$

What's wrong with solving LQR via SDP?

- Requires knowledge of problem data (A, B, Q)
- In reinforcement learning, we do not know (A, B, Q)
- But we can estimate objective, gradient, Hessian from observed data
- (A, B, Q) not exposed explicitly in objective, gradient, Hessian

Eliminate constraints to obtain the equivalent problem

$$\underset{K}{\text{minimize}} \quad f(K) = \begin{cases} \text{trace}(P_K X_0) & \text{if } \rho(A_K) < 1 \\ \infty & \text{else} \end{cases}$$

where P_K is the solution to the **discrete-time Lyapunov equation**

$$P_K = A_K^\intercal P_K A_K + Q_K$$

equivalently

$$\mathrm{vec}(P_K) = (I - A_K^\intercal \otimes A_K^\intercal)^{-1} \,\mathrm{vec}(Q_K)$$

where

$$\begin{aligned} A_K &= A + BK \\ Q_K &= \begin{bmatrix} I \\ K \end{bmatrix}^\intercal Q \begin{bmatrix} I \\ K \end{bmatrix} \end{aligned}$$

Under the given assumptions, the analysis of [18] shows

- f is a **real analytic** function over its domain
  - Implies f has **continuous derivatives of arbitrary order** over its domain
- f is **gradient dominated**, thus invex
- f has a **unique stationary point and global minimizer** K^*

Takeaway

Descent methods will solve the LQR policy optimization problem

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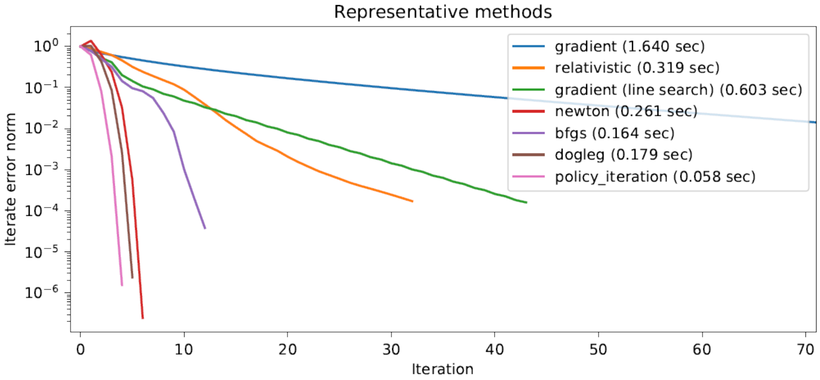
Notice that $f(K)$ is expressed with linear algebraic operations

Takeaway

Use automatic differentiation to compute gradients and Hessians

Grab the Python code



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