Optimization Lecture 9

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Outline

Terminology and assumptions

Unconstrained minimization

- unconstrained minimization problem

$$\text{minimize } f(x)$$

- we assume
- f convex, twice continuously differentiable (hence $\operatorname{dom} f$ open)
- optimal value $p^\star = \inf_x f(x)$ is attained at $x^\star$ (not necessarily unique)
- optimality condition is $\nabla f(x) = 0$
- minimizing f is the same as solving $\nabla f(x) = 0$ (a set of n equations with n unknowns)

Quadratic functions

- convex quadratic: $f(x) = (1/2)x^T Px + q^T x + r, P \geq 0$
- we can solve exactly via linear equations

$$\nabla f(x) = Px + q = 0$$

- very important since a function can be approximated by quadratic locally.
- $argminf(x) = ? minf(x) = ?$

Iterative methods

- for most non-quadratic functions, we use iterative methods
- these produce a sequence of points $x^{(k)} \in \operatorname{dom} f, k = 0, 1, \ldots$
- $x^{(0)}$ is the initial point or **starting point**
- $x^{(k)}$ is the k th iterate
- we hope that the method converges, i.e.,

$$f\left(x^{(k)}\right) \to p^{\star}, \quad \nabla f\left(x^{(k)}\right) \to 0$$

Initial point and sublevel set

- iterative algorithms require a starting point $x^{(0)}$ such that
  - $x^{(0)} \in \mathbf{dom}\, f$
  - sublevel set $S = \{x \mid f(x) \leq f(x^{(0)})\}$ is closed
- 2nd condition is
  - equivalent to condition that $\mathbf{epi}\, f$ is closed
  - true if $\mathbf{dom}\, f = \mathbf{R}^n$
  - true if $f(x) \to \infty$ as $x \to \mathbf{bd}\,\mathbf{dom}\, f$
- examples of differentiable functions with closed sublevel sets:

$$f(x) = \log\left(\sum_{i=1}^{m} \exp\left(a_i^T x + b_i\right)\right), \quad f(x) = -\sum_{i=1}^{m} \log\left(b_i - a_i^T x\right)$$

Strong convexity and implications

- f is **strongly convex** on S if there exists an $m > 0$ such that

$$\nabla^2 f(x) \succeq mI \text{ for all } x \in S$$

- same as $f(x) - (m/2)\|x\|_2^2$ is convex
- if f is strongly convex, for $x, y \in S$,

$$f(y) \geq f(x) + \nabla f(x)^T (y - x) + \frac{m}{2}\|x - y\|_2^2$$

- hence, S is bounded
- we conclude $p^\star > -\infty$, and for $x \in S$,

$$f(x) - p^\star \leq \frac{1}{2m}\|\nabla f(x)\|_2^2$$

  (how to prove?)
- useful as stopping criterion (if you know m, which usually you do not)

Generic descent method

Descent methods

- descent methods generate iterates as

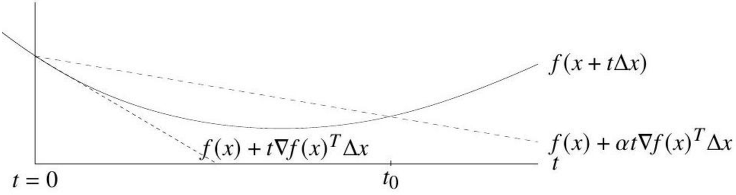
$$x^{(k+1)} = x^{(k)} + t^{(k)} \Delta x^{(k)}$$

with $f\left(x^{(k+1)}\right) < f\left(x^{(k)}\right)$ (hence the name)

- other notations: $x^{+} = x + t\Delta x, x := x + t\Delta x$
- $\Delta x^{(k)}$ is the step, or search direction
- $t^{(k)} > 0$ is the step size, or step length
- from convexity, $f\left(x^{+}\right) < f(x)$ implies $\nabla f(x)^T \Delta x < 0$ (why)
- this means Δx is a descent direction

Line search types

- exact line search: $t = \text{argmin}_{t>0} f(x + t\Delta x)$
- backtracking line search (with parameters $\alpha \in (0, 1/2), \beta \in (0, 1)$ why?)
- starting at $t = 1$, repeat $t := \beta t$ until $f(x + t\Delta x) < f(x) + \alpha t \nabla f(x)^T \Delta x$
- graphical interpretation: reduce t (i.e., backtrack) until $t \leq t_0$



The obtained t satisfies $\beta t_0 \leq t \leq 1$

Generic decent method

Generic descent method
given a starting point $x \in \operatorname{dom} f$.
repeat
1. Determine a descent direction Δx.
2. Line search. Choose a step size $t > 0$.
3. Update. $x := x + t\Delta x$.

until stopping criterion is satisfied.

Gradient Descent Method

Gradient descent method

- general descent method with $\Delta x = -\nabla f(x)$

given a starting point $x \in \mathbf{dom}\, f$.
repeat

1. $\Delta x := -\nabla f(x)$.
2. Line search. Choose step size t via exact or backtracking line search.
3. Update. $x := x + t\Delta x$.

until stopping criterion is satisfied.

- stopping criterion usually of the form $\|\nabla f(x)\|_2 \leq \epsilon$
- convergence result: for strongly convex f,

$$f\left(x^{(k)}\right) - p^\star \leq c^k \left(f\left(x^{(0)}\right) - p^\star\right)$$

$c \in (0,1)$ depends on $m, x^{(0)}$, line search type (how to prove it?)

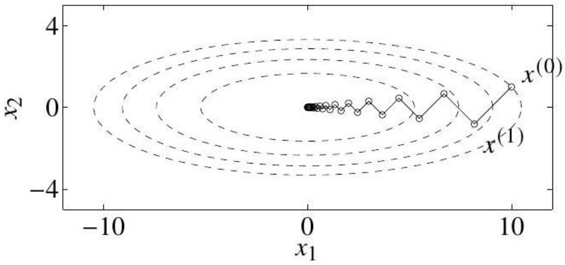
- very simple, but can be very slow

Example: Quadratic function on $\mathbf{R}^2$

- take $f(x) = (1/2)\left(x_1^2 + \gamma x_2^2\right)$, with $\gamma > 0$
- with exact line search, starting at $x^{(0)} = (\gamma, 1)$:

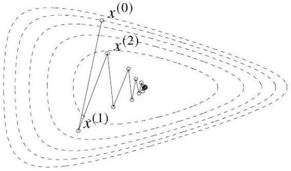
$$x_1^{(k)} = \gamma \left(\frac{\gamma - 1}{\gamma + 1}\right)^k, \quad x_2^{(k)} = \left(-\frac{\gamma - 1}{\gamma + 1}\right)^k$$

  - very slow if $\gamma \gg 1$ or $\gamma \ll 1$ (condition number $\gg 1$)
  - example for $\gamma = 10$ at right
  - called zig-zagging

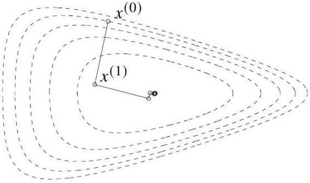


Example: Nonquadratic function on $\mathbf{R}^2$

$$f(x_1, x_2) = e^{x_1+3x_2-0.1} + e^{x_1-3x_2-0.1} + e^{-x_1-0.1}$$



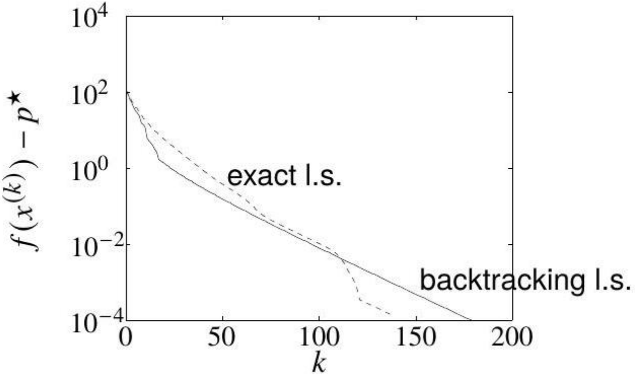
backtracking line search



exact line search

Example: A problem in $\mathbf{R}^{100}$

- $f(x) = c^T x - \sum_{i=1}^{500} \log\left(b_i - a_i^T x\right)$



- linear convergence, i.e., a straight line on a semilog plot
- exercise: do it using cvx.

Steepest descent method

Steepest descent method

- normalized steepest descent direction (at x, for norm $\|\cdot\|$):

$$\Delta x_{\mathrm{nsd}} = \operatorname{argmin}\left\{\nabla f(x)^T v \mid \|v\| = 1\right\}$$

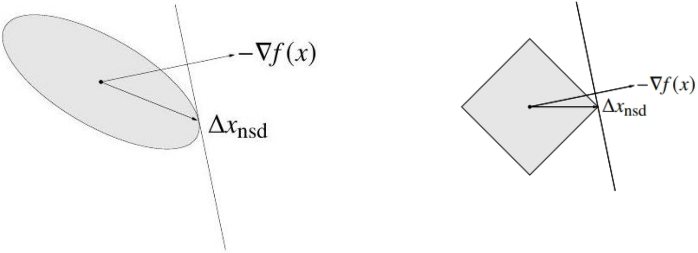
- interpretation: for small v, $f(x+v) \approx f(x) + \nabla f(x)^T v$;
- direction Δx_{nsd} is unit-norm step with most negative directional derivative
- (unnormalized) steepest descent direction: $\Delta x_{\mathrm{sd}} = \|\nabla f(x)\|_* \Delta x_{\mathrm{nsd}}$
- satisfies $\nabla f(x)^T \Delta x_{\mathrm{sd}} = -\|\nabla f(x)\|_*^2$

steepest descent method

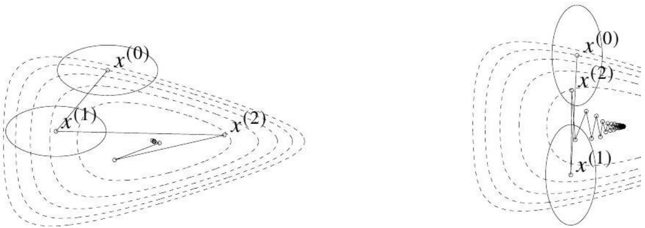
- general descent method with $\Delta x = \Delta x_{\mathrm{sd}}$
- convergence properties similar to gradient descent

Examples

- Euclidean norm: $\Delta x_{\mathrm{sd}} = -\nabla f(x)$
- quadratic norm
  $\|x\|_P = \left(x^T P x\right)^{1/2}$ $(P \in \mathbf{S}^n_{++})$: $\Delta x_{\mathrm{sd}} = -P^{-1}\nabla f(x)$
- ℓ_1-norm: $\Delta x_{\mathrm{sd}} = -\left(\partial f(x)/\partial x_i\right) e_i$, where $|\partial f(x)/\partial x_i| = \|\nabla f(x)\|_\infty$
- unit balls, normalized steepest descent directions for quadratic norm and ℓ_1-norm:



Choice of norm for steepest descent

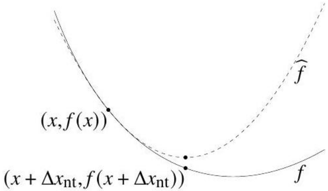


- steepest descent with backtracking line search for two quadratic norms
- ellipses show $\{x \mid \|x - x^{(k)}\|_P = 1\}$
- interpretation of steepest descent with quadratic norm $\|\cdot\|_P$: gradient descent after change of variables $\bar{x} = P^{1/2}x$
- shows choice of P has strong effect on speed of convergence
- Example "Quadratic function on R^2".

Newton's method

- Newton step is $\Delta x_{\mathrm{nt}} = -\nabla^2 f(x)^{-1} \nabla f(x)$
- interpretation: $x + \Delta x_{\mathrm{nt}}$ minimizes second order approximation

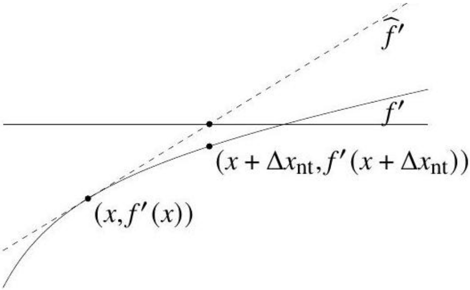
$$\widehat{f}(x+v) = f(x) + \nabla f(x)^T v + \frac{1}{2} v^T \nabla^2 f(x) v$$



Another interpretation

- $x + \Delta x_{\mathrm{nt}}$ solves linearized optimality condition

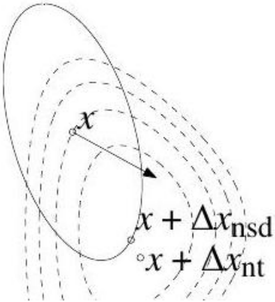
$$\nabla f(x+v) \approx \nabla \widehat{f}(x+v) = \nabla f(x) + \nabla^2 f(x) v = 0$$



And one more interpretation

- $\Delta x_{\rm nt}$ is steepest descent direction at x in local Hessian norm

$$\|u\|_{\nabla^2 f(x)} = \left(u^T \nabla^2 f(x) u\right)^{1/2}$$



- dashed lines are contour lines of f; ellipse is $\left\{x + v \mid v^T \nabla^2 f(x) v = 1\right\}$
- arrow shows $-\nabla f(x)$

Newton decrement

Newton decrement is $\lambda(x) = \left(\nabla f(x)^T \nabla^2 f(x)^{-1} \nabla f(x)\right)^{1/2}$

- a measure of the proximity of x to $x^\star$
- gives an estimate of $f(x) - p^\star$, using quadratic approximation $\widehat{f}$:

$$f(x) - \inf_y \widehat{f}(y) = \frac{1}{2}\lambda(x)^2$$

- equal to the norm of the Newton step in the quadratic Hessian norm

$$\lambda(x) = \left(\Delta x_{\mathrm{nt}}^T \nabla^2 f(x) \Delta x_{\mathrm{nt}}\right)^{1/2}$$

- directional derivative in the Newton direction:
  $\nabla f(x)^T \Delta x_{\mathrm{nt}} = -\lambda(x)^2$

Newton's method

given a starting point $x \in \operatorname{dom} f$, tolerance $\epsilon > 0$.
repeat

1. Compute the Newton step and decrement.

$$\Delta x_{\mathrm{nt}} := -\nabla^2 f(x)^{-1} \nabla f(x); \quad \lambda^2 := \nabla f(x)^T \nabla^2 f(x)^{-1} \nabla f(x)$$

2. Stopping criterion. quit if $\lambda^2/2 \leq \epsilon$.
3. Line search. Choose step size t by backtracking line search.
4. Update. $x := x + t\Delta x_{\mathrm{nt}}$.

- affine invariant, i.e., independent of linear changes of coordinates
  Newton iterates for $\tilde{f}(y) = f(Ty)$ with starting point $y^{(0)} = T^{-1}x^{(0)}$
  are $y^{(k)} = T^{-1}x^{(k)}$

Classical convergence analysis of Newton's method

Assumptions

- f strongly convex on S with constant m
- $\nabla^2 f$ is Lipschitz continuous on S, with constant $L > 0$:

$$\left\|\nabla^2 f(x) - \nabla^2 f(y)\right\|_2 \leq L\|x - y\|_2$$

(L measures how well f can be approximated by a quadratic function)
Outline: there exist constants $\eta \in \left(0, m^2/L\right), \gamma > 0$ such that

- if $\|\nabla f(x^k)\|_2 \geq \eta$, then $f\left(x^{(k+1)}\right) - f\left(x^{(k)}\right) \leq -\gamma$
- if $\|\nabla f(x^k)\|_2 < \eta$, then

$$\frac{L}{2m^2}\left\|\nabla f\left(x^{(k+1)}\right)\right\|_2 \leq \left(\frac{L}{2m^2}\left\|\nabla f\left(x^{(k)}\right)\right\|_2\right)^2$$

Damped Newton phase ($\|\nabla f(x)\|_2 \geq \eta$)

- most iterations require backtracking steps
- function value decreases by at least γ
- if $p^\star > -\infty$, this phase ends after at most $\left(f\left(x^{(0)}\right) - p^\star\right)/\gamma$ iterations

Quadratically convergent phase ($\|\nabla f(x)\|_2 < \eta$)

- all iterations use step size $t = 1$
- $\|\nabla f(x)\|_2$ converges to zero quadratically: if $\left\|\nabla f\left(x^{(k)}\right)\right\|_2 < \eta$, then

$$\frac{L}{2m^2}\left\|\nabla f\left(x^l\right)\right\|_2 \leq \left(\frac{L}{2m^2}\left\|\nabla f\left(x^k\right)\right\|_2\right)^{2^{l-k}} \leq \left(\frac{1}{2}\right)^{2^{l-k}}, \quad l \geq k$$

Remember:

$$f(x) - p^\star \leq \frac{1}{2m}\|\nabla f(x)\|_2^2$$

Then

$$f(x^{(l)}) - p^\star \leq \frac{2m^3}{L^2}(1/2)^{2^{l-k+1}}$$

Roughly, the number of correct digits doubles at each generation (quadratic convergence)

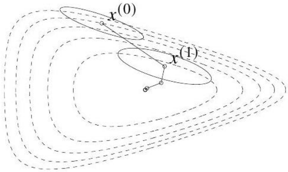
Conclusion: number of iterations until $f(x) - p^\star \leq \epsilon$ is bounded above by

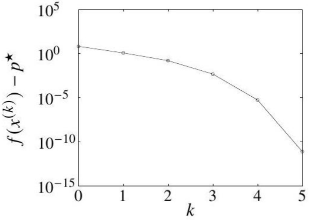
$$\frac{f\left(x^{(0)}\right) - p^\star}{\gamma} + \log_2 \log_2 (\epsilon_0 / \epsilon)$$

- γ, ϵ_0 are constants that depend on $m, L, x^{(0)}$
- second term is small (of the order of 6) and almost constant for practical purposes
- in practice, constants m, L (hence γ, ϵ_0) are usually unknown
- provides qualitative insight in convergence properties (i.e., explains two algorithm phases)

Example: $\mathbf{R}^2$

- $f(x) = c^T x - \sum_{i=1}^{500} \log\left(b_i - a_i^T x\right)$

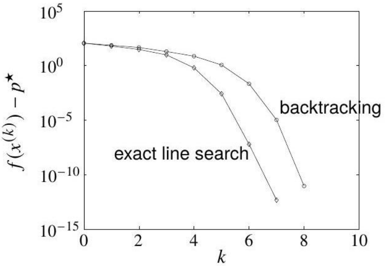


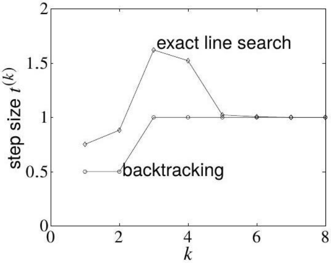


- backtracking parameters $\alpha = 0.1, \beta = 0.7$
- converges in only 5 steps
- quadratic local convergence

Example in $\mathbf{R}^{100}$

- $f(x) = c^T x - \sum_{i=1}^{500} \log\left(b_i - a_i^T x\right)$



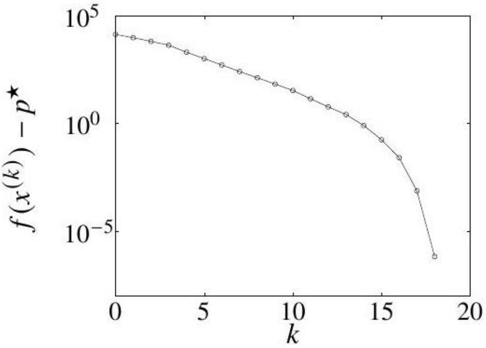


- backtracking parameters $\alpha = 0.01, \beta = 0.5$
- backtracking line search almost as fast as exact l.s. (and much simpler)
- clearly shows two phases in algorithm

Example in $\mathbf{R}^{10000}$

(with sparse a_i)

$$f(x) = -\sum_{i=1}^{10000} \log\left(1 - x_i^2\right) - \sum_{i=1}^{100000} \log\left(b_i - a_i^T x\right)$$



- backtracking parameters $\alpha = 0.01, \beta = 0.5$.
- performance similar as for small examples

Self-concordance functions

Why self-concordance

Shortcomings of classical convergence analysis

- depends on unknown constants $(m, L, \ldots)$
- bound is not affinely invariant, although Newton's method is

convergence analysis via self-concordance (Nesterov and Nemirovski)

- does not depend on any unknown constants
- gives affine-invariant bound
- applies to special class of convex functions ('self-concordant' functions)
- developed to analyze polynomial-time interior-point methods for convex optimization

Def of Self-concordant functions

definition

- convex $f : \mathbf{R} \rightarrow \mathbf{R}$ is self-concordant if $|f'''(x)| \leq 2f''(x)^{3/2}$ for all $x \in \mathrm{dom}\, f$
- $f : \mathbf{R}^n \rightarrow \mathbf{R}$ is self-concordant if $g(t) = f(x + tv)$ is self-concordant for all $x \in \mathrm{dom}\, f$, $v \in \mathbf{R}^n$

Examples on R

- linear and quadratic functions
- negative logarithm $f(x) = -\log x$
- negative entropy plus negative logarithm: $f(x) = x \log x - \log x$

affine invariance: if $f : \mathbf{R} \rightarrow \mathbf{R}$ is s.c., then $\tilde{f}(y) = f(ay + b)$ is s.c.:

$$\tilde{f}'''(y) = a^3 f'''(ay + b), \quad \tilde{f}''(y) = a^2 f''(ay + b)$$

Self-concordant calculus

properties

- preserved under positive scaling $\alpha \geq 1$, and sum
- preserved under composition with affine function
- if g is convex with $\mathbf{dom}\, g = \mathbf{R}_{++}$ and $|g'''(x)| \leq 3g''(x)/x$ then

$$f(x) = \log(-g(x)) - \log x$$

is self-concordant

examples: properties can be used to show that the following are s.c.

- $f(x) = -\sum_{i=1}^{m} \log\left(b_i - a_i^T x\right)$ on $\left\{x \mid a_i^T x < b_i, i = 1, \ldots, m\right\}$
- $f(X) = -\log\det X$ on $\mathbf{S}_{++}^n$
- $f(x) = -\log\left(y^2 - x^T x\right)$ on $\{(x, y) \mid \|x\|_2 < y\}$

Convergence analysis for self-concordant functions

Summary: there exist constants $\eta \in (0, 1/4], \gamma > 0$ such that

- if $\lambda(x) > \eta$, then

$$f\left(x^{(k+1)}\right) - f\left(x^{(k)}\right) \leq -\gamma$$

- if $\lambda(x) \leq \eta$, then

$$2\lambda\left(x^{(k+1)}\right) \leq \left(2\lambda\left(x^{(k)}\right)\right)^2$$

(η and γ only depend on backtracking parameters α, β)
complexity bound: number of Newton iterations bounded by

$$\frac{f\left(x^{(0)}\right) - p^\star}{\gamma} + \log_2 \log_2(1/\epsilon)$$

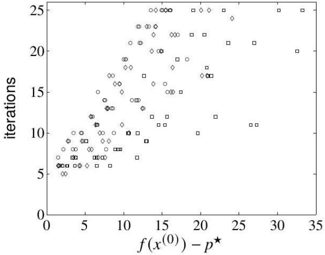
for $\alpha = 0.1, \beta = 0.8, \epsilon = 10^{-10}$, bound $= 375\left(f\left(x^{(0)}\right) - p^\star\right) + 6$

Numerical example

150 randomly generated instances of

$$\text{minimize } f(x) = -\sum_{i=1}^{m} \log\left(b_i - a_i^T x\right)$$

$\circ$: $m = 100, n = 50$
$\square$: $m = 1000, n = 500$
$\diamond$: $m = 1000, n = 50$



- number of iterations much smaller than $375\left(f\left(x^{(0)}\right) - p^\star\right) + 6$
- bound of the form $c\left(f\left(x^{(0)}\right) - p^\star\right) + 6$ with smaller c (empirically) valid

Implementation

Implementation

main effort in each iteration: evaluate derivatives and solve Newton system

$$H\Delta x = -g$$

where $H = \nabla^2 f(x), g = \nabla f(x)$
via Cholesky factorization

$$H = LL^T, \quad \Delta x_{\mathrm{nt}} = -L^{-T}L^{-1}g, \quad \lambda(x) = \left\|L^{-1}g\right\|_2$$

- cost $(1/3)n^3$ flops for unstructured system
- cost $\ll (1/3)n^3$ if H sparse, banded