CME 252: Gradient Descent

AJ Friend
ICME, Stanford University

Gradient Descent

Outline

Introduction

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

- initial assumptions on f:
  - convex
  - twice differentiable
  - unconstrained; domain of f is $\mathbf{R}^n$
  - assume min is attained: $p^\star = \inf_x f(x)$

Iterative Methods

- iterative methods produce a sequence of points, x^k for $k = 1, 2, \ldots$ such that

$$f(x^k) \to p^\star$$

- also consider the algebraic problem of finding $x^\star$ such that

$$\nabla f(x^\star) = 0$$

Optimization Master Algorithm

- solve “hard” problem via sequence of “easier” problems
  - approximate locally as “easier” problem
  - solve easy problem
  - move to new point
  - repeat until “solved”
- quadratic optimization problems via linear algebra
- unconstrained convex opt. via quadratic opt.
- constrained convex opt. via unconstrained convex opt.
- nonconvex opt. via convex opt.

Gradients

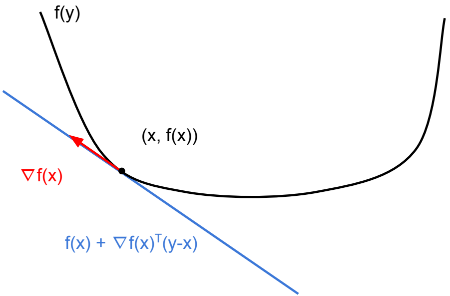
- $f(x) : \mathbf{R}^n \to \mathbf{R}$
- gradient $\nabla f(x) : \mathbf{R}^n \to \mathbf{R}^n$ given by

$$\nabla f(x) = \begin{bmatrix} \frac{\partial f}{\partial x_1} \\ \vdots \\ \frac{\partial f}{\partial x_n} \end{bmatrix}$$

- **intuition**: $\nabla f(x)$ points in direciton of steepest **ascent**

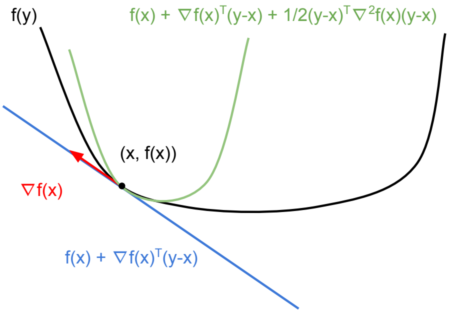
Affine Underestimator

- f is convex if and only if $\mathbf{dom}(f)$ is convex and
$$f(y) \geq f(x) + \nabla f(x)^T (y - x)$$
for all $x, y \in \mathbf{dom}(f)$
- first-order Taylor approximation is a **global underestimator** of f



Quadratic Estimator

- second-order Taylor $f(y) \approx f(x) + \nabla f(x)^T(y-x) + 1/2(y-x)\nabla^2 f(x)(y-x)$ may not be over- or under-estimator
- estimator is convex as $\nabla^2 f(x) \succeq 0$



Positive semidefinite matrices

- a matrix $A \in \mathbf{R}^{n \times n}$ is **positive semidefinite** $(A \succeq 0)$ if
  - A is **symmetric**: $A = A^T$
  - $x^T A x \geq 0$ for all $x \in \mathbf{R}^n$
- $A \succeq 0$ if and only if all **eigenvalues** of A are nonnegative
- intuition: graph of **convex** $f(x) = x^T A x$ looks like a bowl
- example: ρI for any $\rho \geq 0$ is PSD
- if $A = 100I$, $\{x \mid x^T A x \leq 1\}$ is a ball of radius 0.1
- if $A = 0.01I$, $\{x \mid x^T A x \leq 1\}$ is a ball of radius 10

Computing Gradients

- $f(x) = a^T x$
  - $\nabla f(x) = a$
- $f(x) = x^T B x$
  - $\nabla f(x) = (B + B^T)x$
  - $\nabla f(x) = 2Bx$ (if B symmetric)
  - $\nabla^2 f(x) = (B + B^T)$ (symmetric part of B)
- chain rule: $f(x) = g(Ax + b) : \mathbf{R}^n \to \mathbf{R}$
  - $\nabla f(x) = A^T \nabla g(Ax + b)$
  - $\nabla^2 f(x) = A^T \nabla^2 g(Ax + b) A$
- reference: "The Matrix Cookbook"

Gradient Example

- log-sum-exp function $g(y) : \mathbf{R}^n \to \mathbf{R}$ with

$$g(y) = \log \sum_{i=1}^{n} e^{y_i}, \quad \nabla g(y) = \frac{1}{\sum_{i=1}^{n} e^{y_i}} \begin{bmatrix} e^{y_1} \\ \vdots \\ e^{y_n} \end{bmatrix}$$

- $f(x) = g(Ax + b)$
- let $z_i = \exp(a_i^T x + b_i)$ (a_i^T: ith row of A)

$$\nabla f(x) = A^T \nabla g(Ax + b) = \frac{1}{\mathbf{1}^T z} A^T z$$

Least-squares Example

- minimize $f(x) = \|Ax - b\|_2^2$ for $A \in \mathbf{R}^{m \times n}$
- possibly no x such that $Ax = b$
- A "skinny", $m \geq n$, and full rank (least-squares has unique solution)
- note:

$$\|Ax - b\|_2^2 = (Ax - b)^T (Ax - b) = x^T A^T Ax - 2(A^T b)^T x + b^T b$$

- solution via the **normal equations**
- i.e., $\nabla f(x^\star) = 0$ implies

$$A^T Ax^\star = A^T b$$

- call a linear system solver to find $x^\star$

Convex Quadratic Problems

- least-squares is an example of an unconstrained **convex quadratic** problem

$$\text{minimize} \quad 1/2x^TQx + b^Tx,$$

  where $Q \succeq 0$ (find lowest point in a bowl)
- prototypical convex function/problem
- without linear algebra software, how would you solve?

Gradient Descent:

- $-\nabla f(x)$ is a **descent direction**
- repeatedly move a little bit in that direction

$$x^{k+1} = x^k - \alpha^k \nabla f(x^k)$$

- α^k is a stepsize (to be chosen)
- repeat until "solved" (when?)

Stopping Criteria

assume $f(x^\star) = p^\star$ is attained

- $\|\nabla f(x^k)\| \leq \epsilon$
- $\|f(x) - p^\star\| \leq \epsilon$ (if known or estimatted)
- $\|x - x^\star\|_2 \leq \epsilon$ (if known or estimated)

Gradient Descent in Python

with α^k fixed:

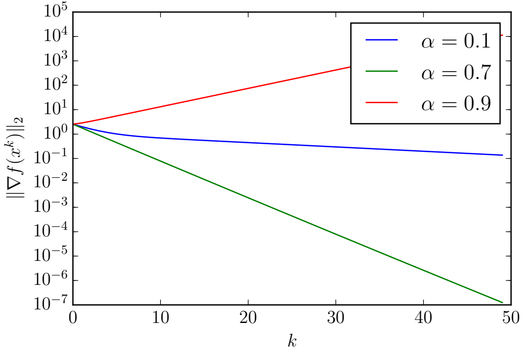
```python
def f(x):
    return x.dot(A).dot(x)/2 - b.dot(x)

def g(x):
    return A.dot(x) - b

for i in range(100):
    gr = g(x)
    x = x - alpha*gr
```

Gradient Descent Example

- quadratic problem: minimize $1/2xAx - b^T x$, $A \succ 0$



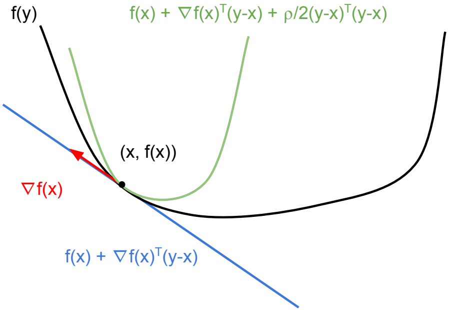
- how to choose α^k without hand-tuning?

Re-interpret Gradient Descent

- what if you were given a **quadratic upper-bound** on f?
- at x^k had **guarantee** that

$$f(y) \le q(y) = f(x^k) + \nabla f(x^k)^T (y - x^k) + 1/2(y - x^k)(\rho I)(y - x^k),$$

  for some $\rho > 0$
- what could you do with it?



Quadratic Over-estimator

- $f(y) \le q(y)$ everywhere
- $f(x^k) = q(x^k)$
- $\nabla f(x^k) = \nabla q(x^k) \neq 0$
- move to the minimum of $q(y)$

$$x^{k+1} = \operatorname{argmin} q(y)$$

- guaranteed descent: $f(x^{k+1}) \le q(x^{k+1}) < q(x^k) = f(x^k)$

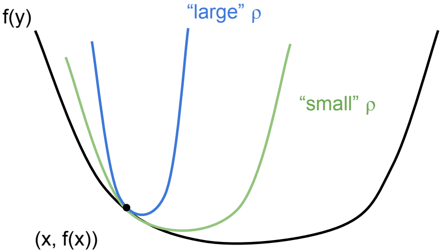
Gradient Step

$$q(y) = f(x^k) + \nabla f(x^k)^T (y - x^k) + 1/2(y - x^k)(\rho I)(y - x^k)$$

- move to
$$x^{k+1} = \operatorname*{argmin}_y q(y)$$
- solve algebraically: $\nabla q(y) = \nabla f(x^k) + \rho(y - x^k) = 0$ implies
$$x^{k+1} = y = x^k - \frac{1}{\rho}\nabla f(x^k)$$
- **exactly** the gradient step with $\alpha^k = 1/\rho$

Gradient Step

- gradient descent is equivalent to minimizing a quadratic upper bound on f
- "small" ρ: low curvature, large step $\alpha^k = 1/\rho$
- "large" ρ: high curvature, more conservative step



Quadratic Upper Bound

- how to **guarantee** quadratic upper bound?
- Taylor theorem: for all $x, y \in \mathbf{dom}(f)$

  $$f(y) = f(x) + \nabla f(x)^T (y - x) + 1/2(y - x)\nabla^2 f(z)(y - x)$$

  for some z
- if some $M > 0$ such that $\nabla^2 f(x) \preceq MI$ for all x then

  $$f(y) \leq f(x) + \nabla f(x)^T (y - x) + M/2\|y - x\|_2^2$$

  is an upper bound

Quadratic Upper Bound

intuition for $\nabla^2 f(x) \preceq MI$:

- $MI - \nabla^2 f(x)$ is PSD (all nonnegative eigenvalues)
- M larger than any eigenvalue of $\nabla^2 f(x)$
- MI has stronger curvature than $\nabla^2 f(x)$ in every direction
- change in gradient is bounded:

$$\|\nabla f(x^{k+1}) - \nabla f(x^k)\|_2 \leq M\|x^{k+1} - x^k\|_2$$

if you know M:

- take $\alpha^k = 1/M$
- taking smallest possible M gives larger steps and potentially faster convergence

Other Over-estimators

- anything special about our quadratic over-estimator?
- not really; just that minimizing it was easy
- other estimators are possible
  - collect many gradients instead of just one (bundle methods)
  - other convex functions to over-estimate or just estimate
- leads to other methods, but minimizing at each step may be harder
- recurring theme: approximate "hard" problem with simple model; solve; repeat

Line Search

- M usually not known in practice, so how to choose α^k?
- line search!
- exact: $\alpha^k = \mathrm{argmin}_t\, f(x^k - t\nabla f(x^k))$ (usually expensive)
- approximate quadratic model search (assuming $\nabla^2 f(x) \preceq MI$ exists)
  - $y = x^k - t\nabla f(x^k)$
  - start with some M
  - decrease t (increase $M = 1/t$) until $f(x^{k+1}) \leq q(x^{k+1})$
  - that is, until quadratic upper bound "looks" accurate
  - but how to keep the step size from getting too small?
  - re-estimate M as $\|\nabla f(x^{k+1}) - \nabla f(x^k)\|/\|x^{k+1} - x^k\|$
- many other line search options