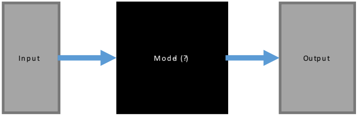
Selected Topics in Optimization

Some slides borrowed from
http://www.stat.cmu.edu/~ryantibs/convexopt/

Overview

- Optimization problems are almost everywhere in statistics and machine learning.



$\min_x f(x)$

Idea/model

Optimization problem: inference model x

Example

- In a regression model, we want the model to minimize deviation from the dependent variable.
- In a classification model, we want the model to minimize classification error.
- In a generative model, we want to maximize the likelihood to produce the observed data.
- …

Gradient descent

Consider unconstrained, smooth convex optimization

$$\min_x \; f(x)$$

i.e., f is convex and differentiable with $\mathrm{dom}(f) = \mathbb{R}^n$. Denote the optimal criterion value by $f^\star = \min_x \; f(x)$, and a solution by $x^\star$

Gradient descent: choose initial point $x^{(0)} \in \mathbb{R}^n$, repeat:

$$x^{(k)} = x^{(k-1)} - t_k \cdot \nabla f(x^{(k-1)}), \quad k = 1, 2, 3, \ldots$$

Stop at some point

Gradient descent interpretation

At each iteration, consider the expansion

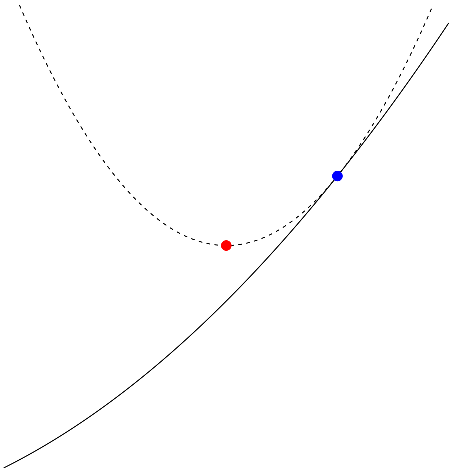
$$f(y) \approx f(x) + \nabla f(x)^T (y - x) + \frac{1}{2t}\|y - x\|_2^2$$

Quadratic approximation, replacing usual Hessian $\nabla^2 f(x)$ by $\frac{1}{t}I$

$f(x) + \nabla f(x)^T (y - x)$	linear approximation to f
$\frac{1}{2t}\|y - x\|_2^2$	proximity term to x, with weight $1/(2t)$

Choose next point $y = x^+$ to minimize quadratic approximation:

$$x^+ = x - t\nabla f(x)$$

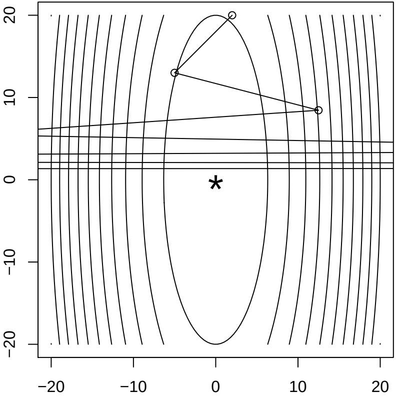


Blue point is x, red point is

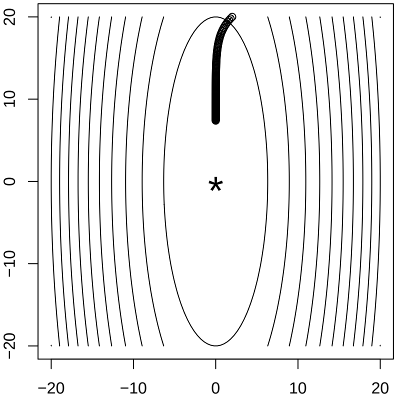
$$x^+ = \underset{y}{\operatorname{argmin}} \; f(x) + \nabla f(x)^T (y - x) + \frac{1}{2t}\|y - x\|_2^2$$

Fixed step size

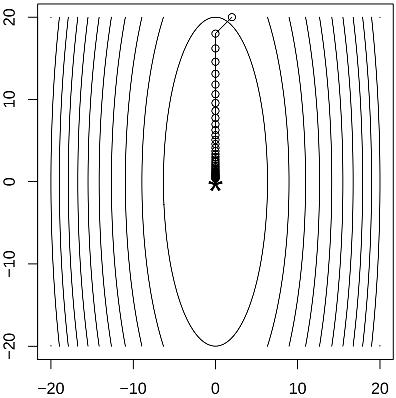
Simply take $t_k = t$ for all $k = 1, 2, 3, \ldots$, can diverge if t is too big. Consider $f(x) = (10x_1^2 + x_2^2)/2$, gradient descent after 8 steps:



Can be slow if t is too small. Same example, gradient descent after 100 steps:



Converges nicely when t is "just right". Same example, gradient descent after 40 steps:



Convergence analysis later will give us a precise idea of "just right"

Backtracking line search

One way to adaptively choose the step size is to use backtracking line search:

- First fix parameters $0 < \beta < 1$ and $0 < \alpha \leq 1/2$
- At each iteration, start with $t = t_{\text{init}}$, and while

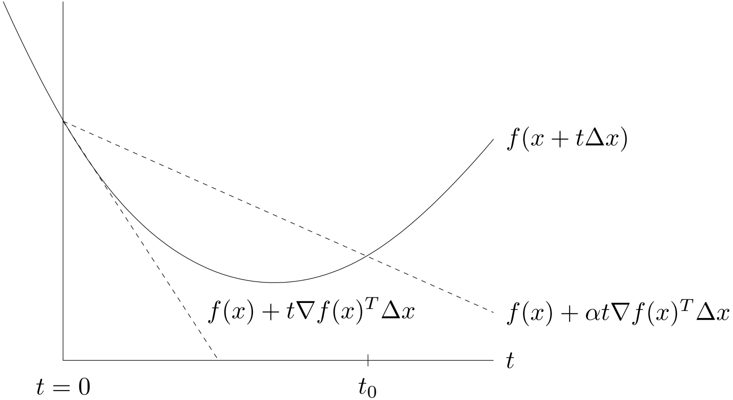
  $$f(x - t\nabla f(x)) > f(x) - \alpha t \|\nabla f(x)\|_2^2$$

  shrink $t = \beta t$. Else perform gradient descent update

  $$x^+ = x - t\nabla f(x)$$

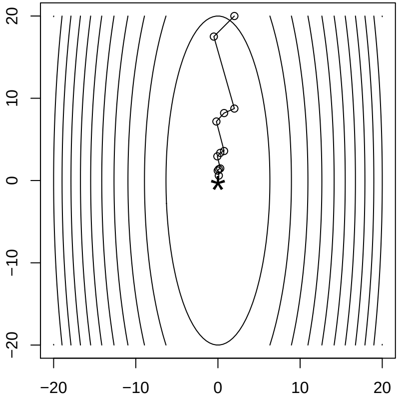
Simple and tends to work well in practice (further simplification: just take $\alpha = 1/2$)

Backtracking interpretation



For us $\Delta x = -\nabla f(x)$

Backtracking picks up roughly the right step size (12 outer steps, 40 steps total):



Here $\alpha = \beta = 0.5$

Practicalities

Stopping rule: stop when $\|\nabla f(x)\|_2$ is small

- Recall $\nabla f(x^\star) = 0$ at solution $x^\star$
- If f is strongly convex with parameter m, then

$$\|\nabla f(x)\|_2 \le \sqrt{2m\epsilon} \implies f(x) - f^\star \le \epsilon$$

Pros and cons of gradient descent:

- Pro: simple idea, and each iteration is cheap (usually)
- Pro: fast for well-conditioned, strongly convex problems
- Con: can often be slow, because many interesting problems aren't strongly convex or well-conditioned
- Con: can't handle nondifferentiable functions

Stochastic gradient descent

Consider minimizing a sum of functions

$$\min_x \sum_{i=1}^m f_i(x)$$

As $\nabla \sum_{i=1}^m f_i(x) = \sum_{i=1}^m \nabla f_i(x)$, gradient descent would repeat:

$$x^{(k)} = x^{(k-1)} - t_k \cdot \sum_{i=1}^m \nabla f_i(x^{(k-1)}), \quad k = 1, 2, 3, \ldots$$

In comparison, stochastic gradient descent or SGD (or incremental gradient descent) repeats:

$$x^{(k)} = x^{(k-1)} - t_k \cdot \nabla f_{i_k}(x^{(k-1)}), \quad k = 1, 2, 3, \ldots$$

where $i_k \in \{1, \ldots m\}$ is some chosen index at iteration k

Two rules for choosing index i_k at iteration k:

- Cyclic rule: choose $i_k = 1, 2, \ldots m, 1, 2, \ldots m, \ldots$
- Randomized rule: choose $i_k \in \{1, \ldots m\}$ uniformly at random

Randomized rule is more common in practice

What's the difference between stochastic and usual (called batch) methods? Computationally, m stochastic steps $\approx$ one batch step. But what about progress?

- Cyclic rule, m steps: $x^{(k+m)} = x^{(k)} - t \sum_{i=1}^m \nabla f_i(x^{(k+i-1)})$
- Batch method, one step: $x^{(k+1)} = x^{(k)} - t \sum_{i=1}^m \nabla f_i(x^{(k)})$
- Difference in direction is $\sum_{i=1}^m [\nabla f_i(x^{(k+i-1)}) - \nabla f_i(x^{(k)})]$

So SGD should converge if each $\nabla f_i(x)$ doesn't vary wildly with x

Rule of thumb: SGD thrives far from optimum, struggles close to optimum ... (we'll revisit in just a few lectures)

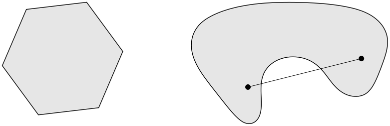
References and further reading

- D. Bertsekas (2010), "Incremental gradient, subgradient, and proximal methods for convex optimization: a survey"
- S. Boyd and L. Vandenberghe (2004), "Convex optimization", Chapter 9
- T. Hastie, R. Tibshirani and J. Friedman (2009), "The elements of statistical learning", Chapters 10 and 16
- Y. Nesterov (1998), "Introductory lectures on convex optimization: a basic course", Chapter 2
- L. Vandenberghe, Lecture notes for EE 236C, UCLA, Spring 2011-2012

Convex sets and functions

Convex set: $C \subseteq \mathbb{R}^n$ such that

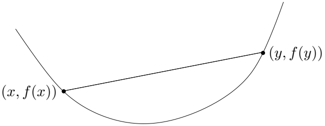
$$x, y \in C \implies tx + (1-t)y \in C \text{ for all } 0 \le t \le 1$$



Convex function: $f : \mathbb{R}^n \to \mathbb{R}$ such that $\mathrm{dom}(f) \subseteq \mathbb{R}^n$ convex, and

$$f(tx + (1-t)y) \le tf(x) + (1-t)f(y) \quad \text{for } 0 \le t \le 1$$

and all $x, y \in \mathrm{dom}(f)$



Convex optimization problems

Optimization problem:

$$\begin{aligned} \min_{x \in D} \quad & f(x) \\ \text{subject to} \quad & g_i(x) \le 0,\ i = 1, \dots m \\ & h_j(x) = 0,\ j = 1, \dots r \end{aligned}$$

Here $D = \mathrm{dom}(f) \cap \bigcap_{i=1}^m \mathrm{dom}(g_i) \cap \bigcap_{j=1}^p \mathrm{dom}(h_j)$, common domain of all the functions

This is a convex optimization problem provided the functions f and $g_i, i = 1, \dots m$ are convex, and $h_j, j = 1, \dots p$ are affine:

$$h_j(x) = a_j^T x + b_j, \quad j = 1, \dots p$$

Local minima are global minima

For convex optimization problems, local minima are global minima

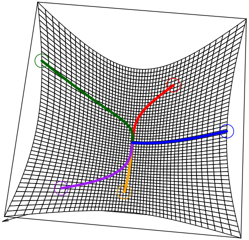
Formally, if x is feasible—$x \in D$, and satisfies all constraints—and minimizes f in a local neighborhood,

$$f(x) \leq f(y) \text{ for all feasible } y, \; \|x - y\|_2 \leq \rho,$$

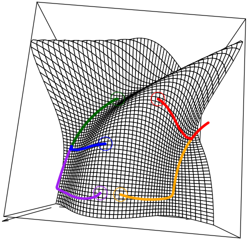
then

$$f(x) \leq f(y) \text{ for all feasible } y$$

This is a very useful fact and will save us a lot of trouble!



Convex



Nonconvex

Nonconvex Problem

- Convex problem: convex objective function, convex constraints, convex domain
- Non-convex problem: not all above conditions are met.
- Usually find approximations or local optimum.

Summary

- GD/SGD: both simple implementation
  - SGD: fewer iterations of the whole dataset, fast especially when data size is large; more able to get over local optimums for non-convex problems.
  - GD: less tricky stepsize tuning.

- Second-order methods (e.g. Newton methods, L-BFGS):
  - Simple stepsize tuning; closer to optimum for non-convex problems.
  - More memory cost.