Optimization and Gradient Descent[a]

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[a] based on slides by Eleni Triantafillou, Ladislav Rampasek, Jake Snell, Kevin Swersky, Shenlong Wang and others

Optimization

What is optimization?

Informally:
Minimizing (or maximizing) some quantity of interest.

Example Applications

- Engineering: Minimize fuel consumption of an automobile.
- Economics: Maximize returns on an investment.
- Supply Chain Logistics: Minimize time taken to fulfill an order.
- Life: Maximize happiness.

Formal definition of Optimization

Goal: find $\theta^* = \arg\min_\theta f(\theta)$, (possibly subject to constraints on θ).

- $\theta \in \mathbb{R}^n$: optimization variable
- $f : \mathbb{R}^n \to \mathbb{R}$: objective function

Maximizing $f(\theta)$ is equivalent to minimizing $-f(\theta)$, so we can treat everything as a minimization problem.

Assumptions

We make some assumptions to find the best method for solving an optimization problem:

- Is θ discrete or continuous?
- What form do constraints on θ take (if any)?
- Is f "well-behaved" (linear, differentiable, convex, etc.)?

Optimization for Machine Learning

Often in machine learning, we are interested in learning the parameters, θ of a model.
Goal: minimize some loss function.

- If we have data (x, y), we may want to maximize the probability $P(y|x, \theta)$.
- Equivalently, we can minimize $-P(y|x, \theta)$.

We can solve the same optimization problem equivalently by applying any monotonic transformation to the objective function.

- So equivalently, we can minimize $-\log P(y|x, \theta)$.
- Taking $\log$ can help for numerical reasons.

Gradient Descent

Gradient Descent is one method for solving an optimization problem.

Gradient Descent: Motivation

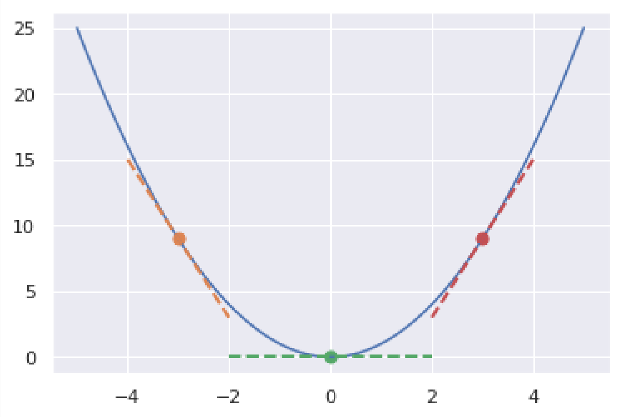
From calculus, we know that the minimum of f must lie at a point where its derivative vanishes, i.e. $\frac{\partial f(\theta^*)}{\partial \theta} = 0$.

- Sometimes, we can solve this equation analytically for θ.
- Mostly, we are not so lucky and must resort to iterative methods.

Recall the Gradient:

$$\nabla_\theta f = \left[\frac{\partial f(\theta)}{\partial \theta_1}, \frac{\partial f(\theta)}{\partial \theta_2}, \ldots, \frac{\partial f(\theta)}{\partial \theta_n}\right]$$

Gradient Descent: Motivation



Gradient Descent Algorithm Review

Let η be the learning rate and T be the number of iterations:

- Initialize θ_0 randomly.
- For $t = 1 : T$
  - $\delta_t = -\eta \nabla_{\theta_{t-1}} f$
  - $\theta_t \leftarrow \theta_{t-1} + \delta_t$

Choice of learning rate matters:

- Too big: the objective function will blow up.
- Too small: the algorithm with take a long time to converge.

Gradient Descent with Line Search

Let η be the learning rate and T be the number of iterations:

- Initialize θ_0 randomly.
- For $t = 1 : T$
  - Find a step size η_t such that $f(\theta_t - \eta_t \nabla_{\theta_{t-1}}) < f(\theta_t)$
  - $\delta_t = -\eta_t \nabla_{\theta_{t-1}} f$
  - $\theta_t \leftarrow \theta_{t-1} + \delta_t$

Requires a line-search step at every iteration.

Let η be the learning rate and T be the number of iterations. We introduce a momentum coefficient $\alpha \in [0, 1)$ so that the updates have "memory":

- Initialize θ_0 randomly.
- For $t = 1 : T$
  - $\delta_t = -\eta \nabla_{\theta_{t-1}} f + \alpha \delta_{t-1}$
  - $\theta_t \leftarrow \theta_{t-1} + \delta_t$

Momentum is a nice trick that can help speed up convergence. Generally, it is useful to try values between 0.8 and 0.95, but the choice is problem dependent.

Convergence Criterion

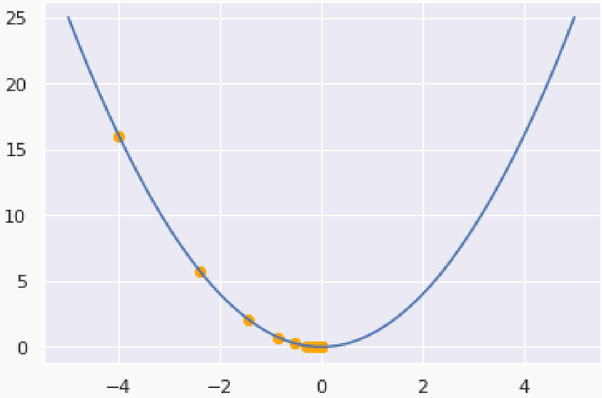
Instead of choosing a fixed number of iterations, we can define some convergence criterion, which is a condition upto which we would like to run the algorithm.

- Initialize θ_0 randomly.
- Until convergence criterion is satisfied
  - $\delta_t = -\eta \nabla_{\theta_{t-1}} f$
  - $\theta_t \leftarrow \theta_{t-1} + \delta_t$

Example Convergence Criteria

- Change in objective function value is close to zero (or less than some threshold): $|f(\theta_{t+1}) - f(\theta_t)| < \epsilon$.
- Gradient norm is smaller than some threshold: $||\nabla_\theta f|| < \epsilon$.
- Validation error starts to increase: also known as Early Stopping.

Gradient Descent Updates



Exercise: Gradient Exercise Intuition

Suppose we are trying to optimize the loss function $f(x) = \frac{1}{2}x^T Ax$, where $x \in \mathbb{R}^2$. Let $A = \begin{bmatrix} 4 & 0 \\ 0 & 1 \end{bmatrix}$ and $x_0 = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$. What are the first two iterates of gradient descent, with a learning rate $\eta = 0.1$?

(Solution: We have

$$\begin{aligned} x_{n+1} &= x_n - \eta \nabla f(x_n) \\ &= x_n - \eta A x_n \\ &= (I - \eta A)x_n \\ &= \begin{bmatrix} 1 - 4\eta & 0 \\ 0 & 1 - \eta \end{bmatrix} x_n \end{aligned}$$

So in general:

$$x_n = \begin{bmatrix} (1 - 4\eta)^n & 0 \\ 0 & (1 - \eta)^n \end{bmatrix} x_0$$

giving us $x_1 = \begin{bmatrix} 0.6 \\ 0.9 \end{bmatrix}$ and $x_2 = \begin{bmatrix} 0.36 \\ 0.81 \end{bmatrix}$.)

Stochastic Gradient Descent (SGD)

- Each iteration of Gradient Descent requires that we sum over the entire dataset to compute the gradient.
- SGD idea: at each iteration, sub-sample a small (mini-)batch of data (even just 1 point can work) and use that to estimate the gradient.
- Each update is noisy, but very fast!
- It can be shown that this method produces an unbiased estimate of the true gradient.

Stochastic Gradient Descent (SGD)

- Batch-learning: computing gradients using the full dataset (which can be a huge, very high-dimensional matrix, e.g. 1 million images of size $224 \times 224 \times 3$).
- Mini-batch learning: computing gradients using subsets of data at every iteration.

SGD Intuition

- SGD works because similar data yields similar gradients.
- If there is enough redundancy in the data, the noise from subsampling isn't too bad.

Tips:

- Step sizes need to be tuned to different problems.
- Divide the log-likelihood estimate by the mini-batch size. Then learning rate is invariant to mini-batch size.
- Subsample without replacement so that each point is visited during an epoch of training.

Convexity

Convexity

A function f is convex if for any two points θ_1 and θ_2 and any $t \in [0, 1]$,

$$f(t\theta_1 + (1-t)\theta_2) \leq tf(\theta_1) + (1-t)f(\theta_2)$$

Geometric Intuition: If you draw a line segment between the two points and it lies above the function curve, then the function is said to be convex.

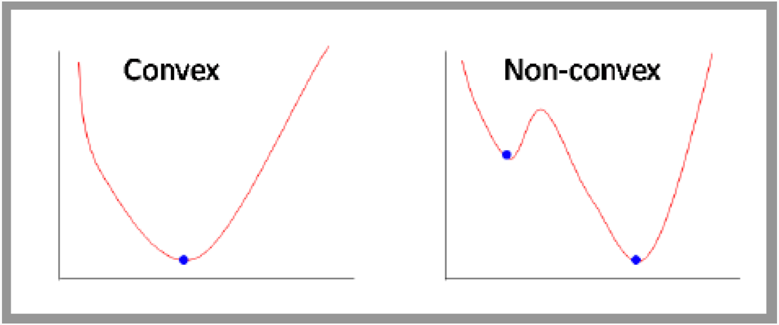
Compositions of Convex Functions

We can compose convex functions such that the resulting function is also convex:

- If f is convex, then so is αf for $\alpha \geq 0$.
- If f_1 and f_2 are both convex, then so is $f_1 + f_2$.

Why do we care about convexity?

- Any local minimum is a global minimum.
- This makes optimization a lot easier because we don't have to worry about getting stuck in a local minimum.



Examples of Convex Functions

- Quadratic Functions
- Negative Logarithms
- Cross-entropy Loss Function

Check out the colab!

Exercise: Sum of Convex Functions

Prove that the sum of two convex functions is convex.
(Solution: Let f and g be convex functions. Consider $h = f + g$. We have

$$\begin{aligned} h(\lambda x + (1-\lambda)y) &= f(\lambda x + (1-\lambda)y) + g(\lambda x + (1-\lambda)y) \\ &\leq \lambda f(x) + (1-\lambda)f(y) + \lambda g(x) + (1-\lambda)g(y) \\ &= \lambda h(x) + (1-\lambda)h(y) \end{aligned}$$

for all x, y and $\lambda \in (0,1)$. So h is convex.)