CSC 411 Tutorial: Optimization for Machine Learning

Renjie Liao[1]

September 19, 2016

[1] Based on tutorials and slides by Ladislav Rampasek, Jake Snell, Kevin Swersky, Shenlong Wang and others

Contents

Overview of Optimization

An informal definition of optimization

Minimize (or maximize) some quantity.

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

More formally

Goal: find $\theta^* = \text{argmin}_\theta f(\theta)$, (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.

Optimization is a large area of research

The best method for solving the optimization problem depends on which assumptions we want to make:

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

- For example, if we have some data (x, y), we may want to maximize $P(y|x, \theta)$.
- Equivalently, we can minimize $-\log P(y|x, \theta)$.
- We can also minimize other sorts of loss functions

log can help for numerical reasons

Gradient Descent

Gradient Descent: Motivation

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

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

Review

- Gradient: $\nabla_\theta f = (\frac{\partial f}{\partial \theta_1}, \frac{\partial f}{\partial \theta_2}, ..., \frac{\partial f}{\partial \theta_k})$

Outline of Gradient Descent Algorithm

Where η is the learning rate and T is the number of iterations:

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

The learning rate shouldn't be too big (objective function will blow up) or too small (will take a long time to converge)

Gradient Descent with Line-Search

Where η is the learning rate and T is the number of iterations:

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

Require a line-search step in each iteration.

Gradient Descent with Momentum

We can introduce a momentum coefficient $\alpha \in [0, 1)$ so that the updates have "memory":

- Initialize θ_0 randomly
- Initialize δ_0 to the zero vector
- for $t = 1 : T$:
  - $\delta_t \leftarrow -\eta \nabla_{\theta_{t-1}} f + \alpha \delta_{t-1}$
  - $\theta_t \leftarrow \theta_{t-1} + \delta_t$

Momentum is a nice trick that can help speed up convergence. Generally we choose α between 0.8 and 0.95, but this is problem dependent

Outline of Gradient Descent Algorithm

Where η is the learning rate and T is the number of iterations:

- Initialize θ_0 randomly
- Do:
  - $\delta_t \leftarrow -\eta \nabla_{\theta_{t-1}} f$
  - $\theta_t \leftarrow \theta_{t-1} + \delta_t$
- Until convergence

Setting a convergence criteria.

Some convergence criteria

- Change in objective function value is close to zero: $|f(\theta_{t+1}) - f(\theta_t)| < \epsilon$
- Gradient norm is close to zero: $\|\nabla_\theta f\| < \epsilon$
- Validation error starts to increase (this is called *early stopping*)

Checkgrad

- When implementing the gradient computation for machine learning models, it's often difficult to know if our implementation of f and ∇f is correct.
- We can use finite-differences approximation to the gradient to help:

$$\frac{\partial f}{\partial \theta_i} \approx \frac{f((\theta_1, \ldots, \theta_i + \epsilon, \ldots, \theta_n)) - f((\theta_1, \ldots, \theta_i - \epsilon, \ldots, \theta_n))}{2\epsilon}$$

Why don't we always just use the finite differences approximation?

- slow: we need to recompute f twice for each parameter in our model.
- numerical issues

Stochastic Gradient Descent

- Any iteration of a gradient descent (or quasi-Newton) method requires that we sum over the entire dataset to compute the gradient.
- SGD idea: at each iteration, sub-sample a small amount of data (even just 1 point can work) and use that to estimate the gradient.
- Each update is noisy, but very fast!
- This is the basis of optimizing ML algorithms with huge datasets (e.g., recent deep learning).
- Computing gradients using the full dataset is called batch learning, using subsets of data is called mini-batch learning.

Stochastic Gradient Descent

- The reason SGD works is because similar data yields similar gradients, so if there is enough redundancy in the data, the noise from subsampling won't be so bad.
- SGD is very easy to implement compared to other methods, but the step sizes need to be tuned to different problems, whereas batch learning typically "just works".
- Tip 1: divide the log-likelihood estimate by the size of your mini-batches. This makes the learning rate invariant to mini-batch size.
- Tip 2: subsample without replacement so that you visit each point on each pass through the dataset (this is known as an epoch).

Demo

- Logistic regression

Convexity

Definition of Convexity

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

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

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 $f_1 + f_2$
- *etc.*, see http://www.ee.ucla.edu/ee236b/lectures/functions.pdf for more

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

Quadratics

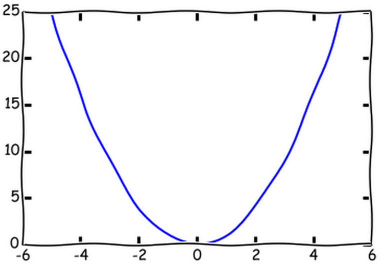
In [6]:

Slide Type -

```
import matplotlib.pyplot as plt
plt.xkcd()
theta = linspace(-5, 5)
f = theta**2
plt.plot(theta, f)
```

Out[6]:

```
[<matplotlib.lines.Line2D at 0x3ceae90>]
```



Examples of Convex Functions

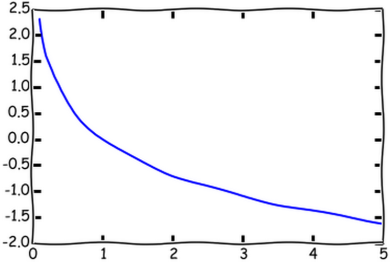
Negative logarithms

In [8]:

Slide Type -

```
import matplotlib.pyplot as plt
plt.xkcd()
theta = linspace(0.1, 5)
f = -np.log(theta)
plt.plot(theta, f)
```

Out[8]: [<matplotlib.lines.Line2D at 0x3ef4a10>]



Convexity for logistic regression

Cross-entropy objective function for logistic regression is also convex!

$$f(\theta) = -\sum_n t^{(n)} \log p(y = 1|x^{(n)}, \theta) + (1 - t^{(n)}) \log p(y = 0|x^{(n)}, \theta)$$

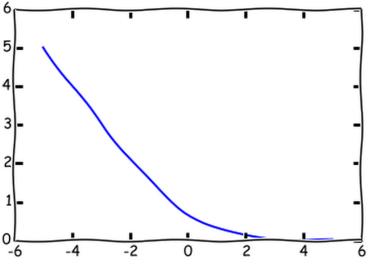
Plot of $-\log \sigma(\theta)$

In [15]: Slide Type -

```
def sigmoid(x):
    return 1 / (1 + np.exp(-x))

theta = linspace(-5, 5)
f = -np.log(sigmoid(theta))
plt.plot(theta, f)
```

Out[15]: [<matplotlib.lines.Line2D at 0x4c453d0>]



More on optimization

Convex Optimization by Boyd & Vandenberghe
Book available for free online at
http://www.stanford.edu/~boyd/cvxbook/
Numerical Optimization by Nocedal & Wright
Electronic version available from UofT Library