CSC 411 Tutorial: Optimization for Machine Learning

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

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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 $\theta_0$ randomly
for $t = 1 : T$:
    Finding a step size $\eta_t$ 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!
- It can be shown that this method produces an unbiased estimator of the true gradient.
- 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?

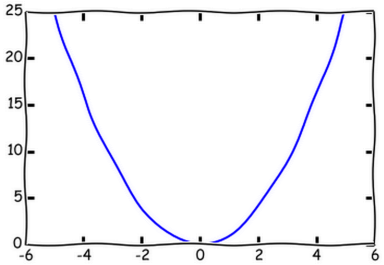
- Any local minimum is a global minimum.
- This makes optimization a lot easier because we don't have to worry about getting stuck in a local minimum.

Examples of Convex Functions

Quadratics

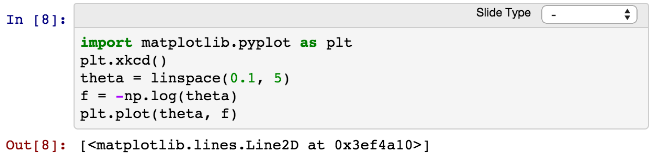
```
In [6]: import matplotlib.pyplot as plt
        plt.xkcd()
        theta = linspace(-5, 5)
        f = theta**2
        plt.plot(theta, f)
```

```
Out[6]: [<matplotlib.lines.Line2D at 0x3ceae90>]
```



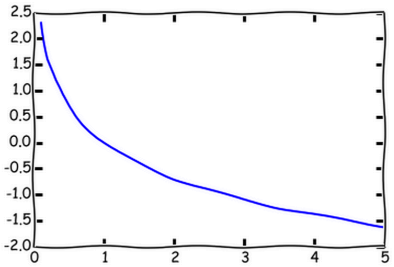
Examples of Convex Functions

Negative logarithms



```
In [8]:  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>]
```

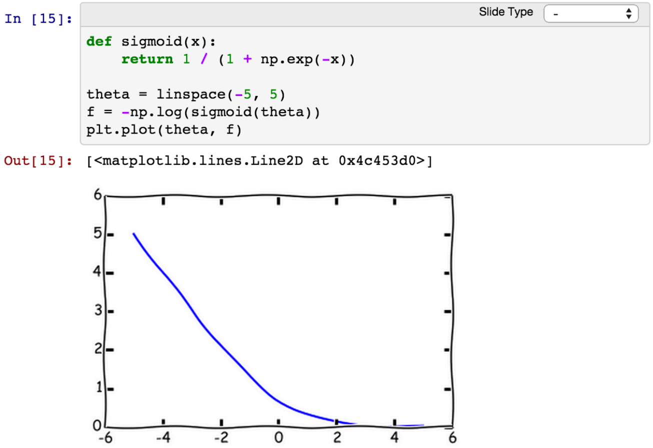


Convexity for logistic regression

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]:
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

- *Automatic Differentiation* Modern technique (used in libraries like tensorflow, pytorch, etc) to efficiently compute the gradients required for optimization. A survey of these techniques can be found here: https://arxiv.org/pdf/1502.05767.pdf
- *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