CSC 2515 Tutorial: Optimization for Machine Learning

Shenlong Wang[1]

January 20, 2015

[1]Modified based on Jake Snell's tutorial, with additional contents borrowed from Kevin Swersky and Jasper Snoek

Outline

- Overview
- Gradient descent
- Checkgrad
- Convexity
- Stochastic gradient descent

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)
- Are the observations noisy or not?
- Is f "well-behaved"? (linear, differentiable, convex, submodular, etc.)
- Some are specialized for the problem at hand (e.g. Dijkstra's algorithm for shortest path). Others are general black-box solutions for general algorithms (e.g. simplex algorithm).

Optimization for machine learning

Often in machine learning we are interested in learning **model parameters** θ with the goal of **minimizing error**.
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

Note:

- log can help for numerical reasons

Gradient descent

Review

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

Gradient descent

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.

Informal version:

- Start at some initial setting of the weights θ_0.
- Until **convergence** or reaching **maximum number of iterations**, repeatedly compute the gradient of our objective and move along that direction.
- Convergence can be measured by the norm of the gradient (0 at 'optimal' solution).

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 $t = 1 : T$:
  - $\delta_t \leftarrow -\eta((1-\beta)\nabla_{\theta_{t-1}} f + \beta\delta_{t-1})$
  - $\theta_t \leftarrow \theta_{t-1} + \delta_t$

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

Convergence

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:

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

- Usually $10^{-3} < \epsilon < 10^{-6}$ is sufficient.

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

Demo

- Linear regression
- Logistic regression

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.
- Many standard problems in machine learning are convex.

Examples of convex functions

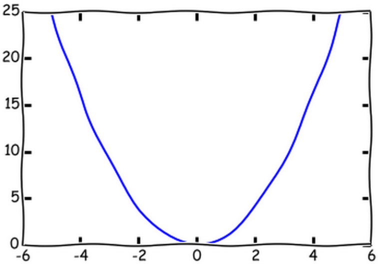
Quadratics

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>]



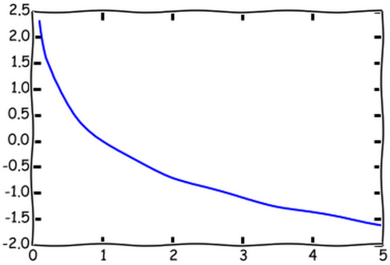
Examples of convex functions

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]:

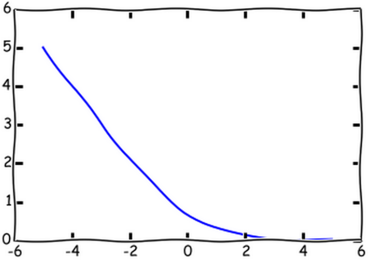
Slide Type -

```python
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>]
```



Stochastic gradient descent

The methods presented earlier have a few limitations.

- They require a full pass through the data to compute the gradient.
- When the dataset is large, computing the exact gradient is expensive.

Stochastic gradient descent

Let's recall gradient descent:

- Step size η, gradient function δf, initial weight θ_0, data $\{x_n\}_{n=1}^N$, number of iterations T.
- for $t = 1 : T$:
  - $\delta_t \leftarrow -\eta \nabla_{\theta_{t-1}} f(\{x_n\}_{n=1}^N)$
  - $\theta_t \leftarrow \theta_{t-1} + \delta_t$

Stochastic gradient descent

Stochastic gradient descent:

- Step size η, gradient function δf, initial weight θ_0, data $\{x_n\}_{n=1}^{N}$, number of iterations T.
- for $t = 1 : T$:
  - Randomly choose a training case x_n, $n \in \{1, ..., N\}$
  - $\delta_t \leftarrow -\eta \nabla_{\theta_{t-1}} f(x_n)$
  - $\theta_t \leftarrow \theta_{t-1} + \delta_t$

Stochastic gradient descent

- Now the function is noisy (even if it wasn't before) so it will take more iterations to converge.
- But each iteration is N times cheaper.
- On the whole this tends to give a huge win in terms of computation time, especially on large datasets.
- Mini-batch is a compromise.

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

Resources for MATLAB

- Tutorials are available on the course website at
  `http://www.cs.toronto.edu/~zemel/inquiry/matlab.php`

Resources for Python

- Official tutorial: http://docs.python.org/2/tutorial/
- Google's Python class: https://developers.google.com/edu/python/
- Zed Shaw's *Learn Python the Hard Way*: http://learnpythonthehardway.org/book/

NumPy/SciPy/Matplotlib

- Scientific Python bootcamp (with video!): http://register.pythonbootcamp.info/agenda
- SciPy lectures: http://scipy-lectures.github.io/index.html

Questions?