# CSC411: Optimization for Machine Learning

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

# 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 $\theta$).

- $\theta \in \mathbb{R}^n$: *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 $\theta$ discrete or continuous?
- What form do constraints on $\theta$ 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 $\theta$ 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 $\theta$.
- 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 $\eta$ is the learning rate and $T$ is the number of iterations:

- Initialize $\theta_0$ 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 $\eta$ 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 $\theta_0$ randomly
- Initialize $\delta_0$ 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 $\alpha$ between 0.8 and 0.95, but this is problem dependent

# Outline of Gradient Descent Algorithm

Where $\eta$ is the learning rate and $T$ is the number of iterations:

- Initialize $\theta_0$ randomly
- Do:
  - $\delta_t \leftarrow -\eta \nabla_{\theta_{t-1}} f$
  - $\theta_t \leftarrow \theta_{t-1} + \delta_t$
- Until convergence

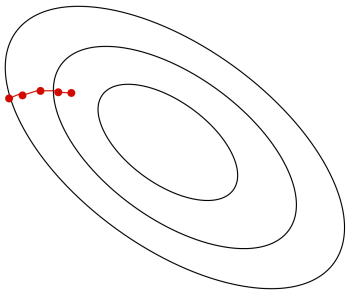
Setting a convergence criteria.

# Some convergence criteria

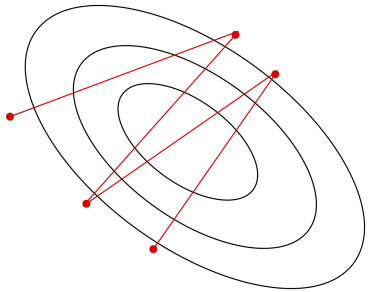
- Change in objective function value is close to zero: $|f(\theta_{t+1}) - f(\theta_t)| < \epsilon$
- Gradient norm is close to zero: $\|\nabla_\theta f\| < \epsilon$
- Validation error starts to increase (this is called *early stopping*)

# Learning Rate (Step Size)

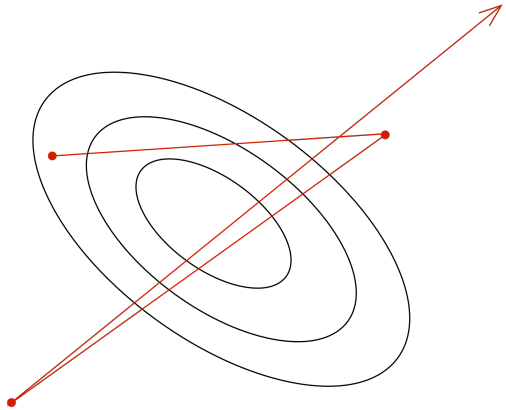
- In gradient descent, the learning rate $\alpha$ is a hyperparameter we need to tune. Here are some things that can go wrong:



$\alpha$ too small:
slow progress



$\alpha$ too large:
oscillations



$\alpha$ much too large:
instability

- Good values are typically between 0.001 and 0.1. You should do a grid search if you want good performance (i.e. try $0.1, 0.03, 0.01, \ldots$).

# Checkgrad

- When implementing the gradient computation for machine learning models, it's often difficult to know if our implementation of $f$ and $\nabla f$ 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

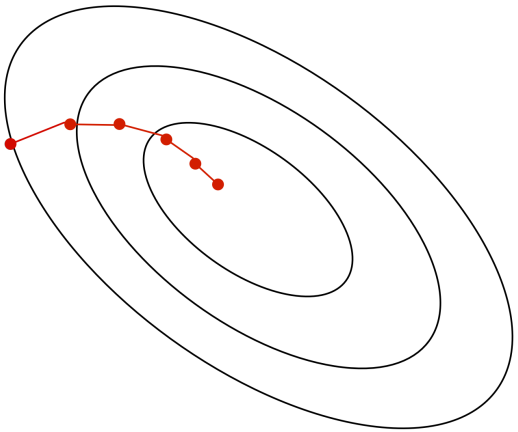
- Any iteration of a gradient descent (or quasi-Newton) method requires that we sum over the entire dataset to compute the gradient.
- SGD idea: at each iteration, sub-sample a small amount of data (even just 1 point can work) and use that to estimate the gradient.
- Each update is noisy, but very fast!
- 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

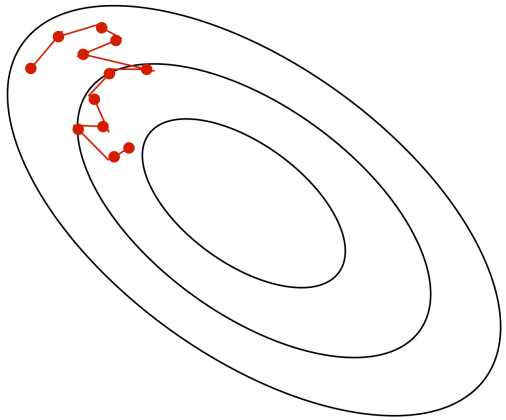
- The reason SGD works is because similar data yields similar gradients, so if there is enough redundancy in the data, the noise from subsampling won't be so bad.
- SGD is very easy to implement compared to other methods, but the step sizes need to be tuned to different problems, whereas batch learning 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).

# Stochastic Gradient Descent

- Batch gradient descent moves directly downhill. SGD takes steps in a noisy direction, but moves downhill on average.



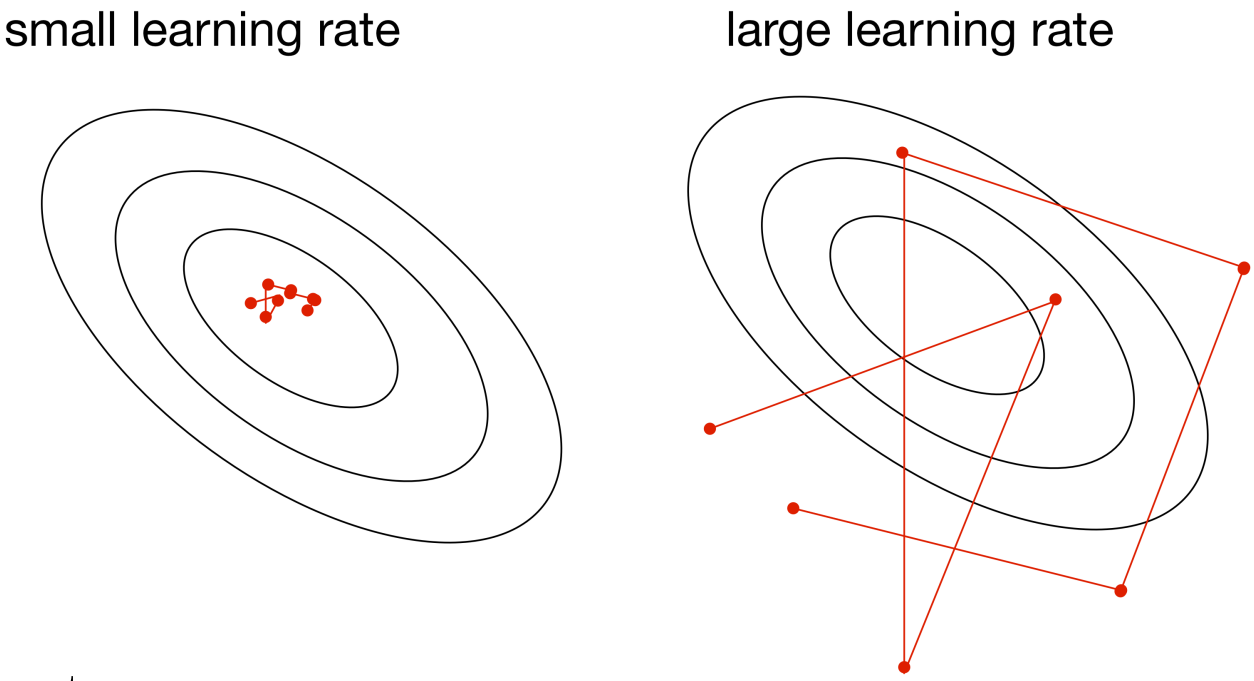
**batch gradient descent**



**stochastic gradient descent**

# SGD Learning Rate

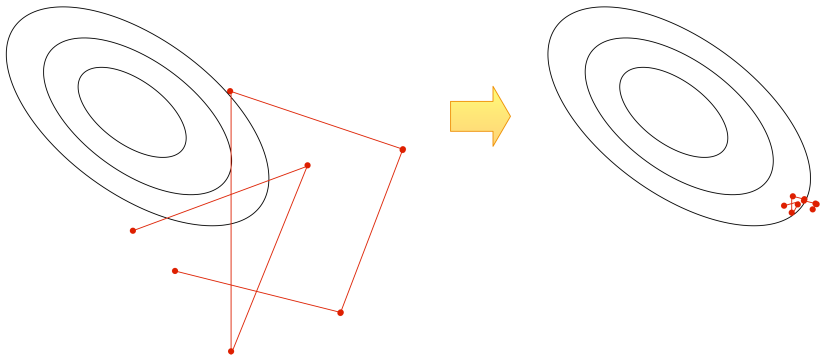
- In stochastic training, the learning rate also influences the fluctuations due to the stochasticity of the gradients.

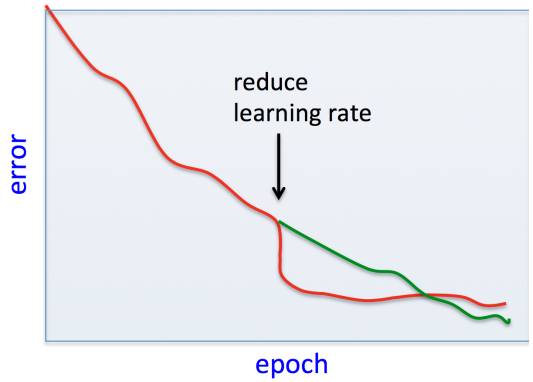



- Typical strategy:
  - Use a large learning rate early in training so you can get close to the optimum
  - Gradually decay the learning rate to reduce the fluctuations

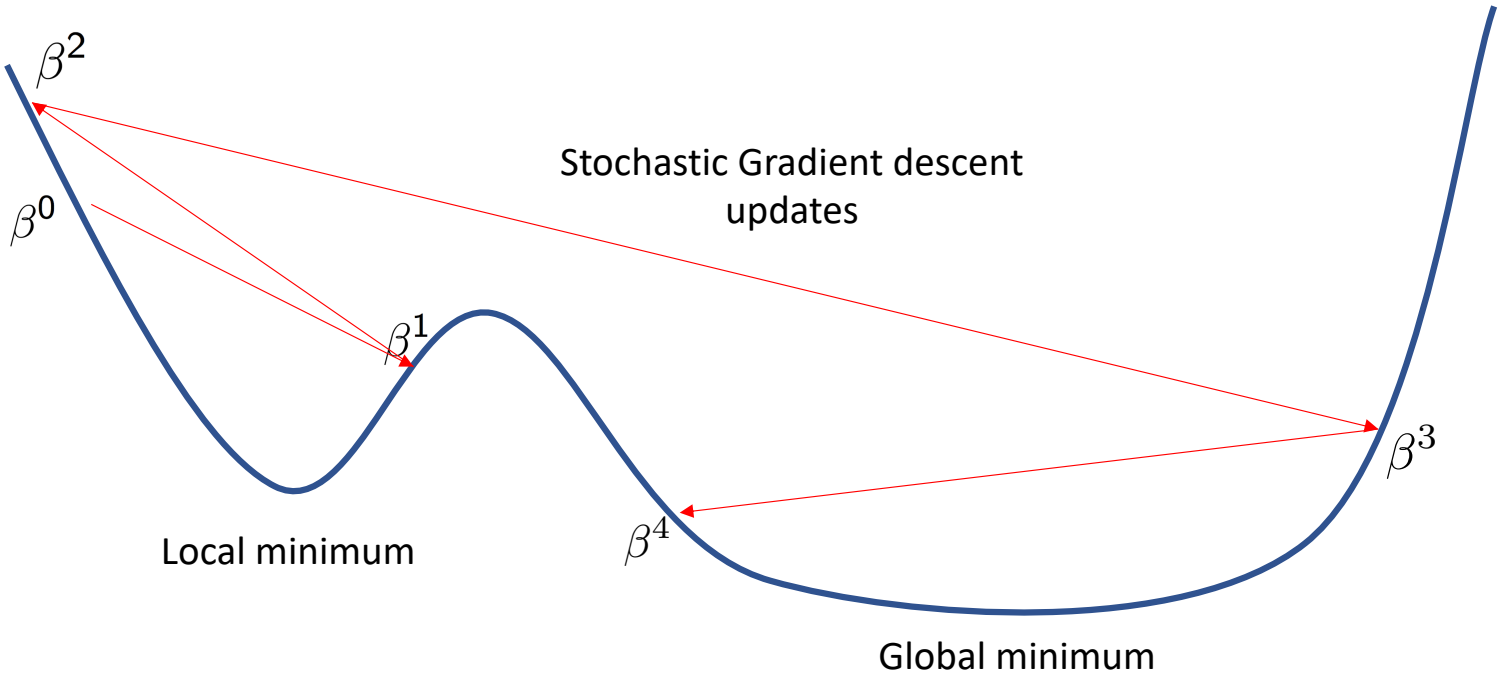
# SGD Learning Rate

- Warning: by reducing the learning rate, you reduce the fluctuations, which can appear to make the loss drop suddenly. But this can come at the expense of long-run performance.





# SGD and Non-convex optimization




- Stochastic methods have a chance of escaping from bad minima.
- Gradient descent with small step-size converges to first minimum it finds.