Gradient and Stochastic Gradient Descent

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Linear Least Squares Regression

Setup

- Input space $\mathcal{X} = \mathbf{R}^d$
- Output space $\mathcal{Y} = \mathbf{R}$
- Action space $\mathcal{Y} = \mathbf{R}$
- Loss: $\ell(\hat{y}, y) = \frac{1}{2}(y - \hat{y})^2$
- **Hypothesis space:** $\mathcal{F} = \left\{ f : \mathbf{R}^d \to \mathbf{R} \mid f(x) = w^T x,\, w \in \mathbf{R}^d \right\}$

- Given data set $\mathcal{D}_n = \{(x_1, y_1), \ldots, (x_n, y_n)\}$,
  - Let's find the ERM $\hat{f} \in \mathcal{F}$.

Linear Least Squares Regression

Objective Function: Empirical Risk

The function we want to minimize is the empirical risk:

$$\hat{R}_n(w) = \frac{1}{n}\sum_{i=1}^{n}\left(w^T x_i - y_i\right)^2,$$

where $w \in \mathbf{R}^d$ parameterizes the hypothesis space $\mathcal{F}$.

Unconstrained Optimization

Setting

Objective function $f : \mathbf{R}^d \to \mathbf{R}$ is *differentiable.*
Want to find

$$x^* = \underset{x \in \mathbf{R}^d}{\arg\min}\, f(x)$$

The Gradient

Let $f : \mathbf{R}^d \to \mathbf{R}$ be differentiable at $x_0 \in \mathbf{R}^d$.

Definition

The **gradient** of f at the point x_0, denoted $\nabla_x f(x_0)$, is the direction to move in for the **fastest increase** in $f(x)$, when starting from x_0.

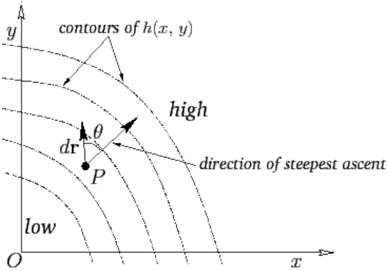


Figure A.111 from Newtonian Dynamics, by Richard Fitzpatrick.

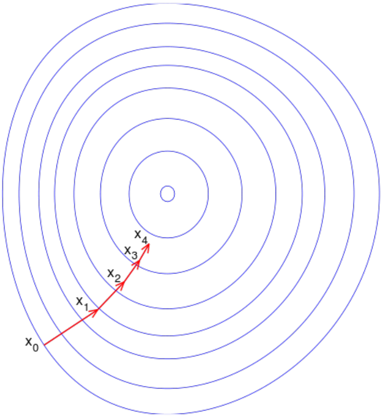
Gradient Descent

Gradient Descent

- Initialize $x = 0$
- repeat
    - $x \leftarrow x - \underbrace{\eta}_{\text{step size}} \nabla f(x)$
- until stopping criterion satisfied

Gradient Descent Path

Gradient Descent for a nice (convex) function



Gradient Descent - Details

Step Size

- Empirically $\eta = 0.1$ often works well
- **Better**: Optimize at every step (e.g. backtracking line search)

Stopping Rule

- Could use a maximum number of steps (e.g. 100)
- Wait until $\|\nabla f(x)\| \leqslant \varepsilon$.
- Wait until decreases in $f(x)$ become very slow.
- Test performance on holdout data (in learning setting)

Gradient Descent for Linear Regression

Gradient of Objective Function:

The gradient of the objective is

$$\begin{aligned}\nabla_w \hat{R}_n(w) &= \nabla_w \left[\frac{1}{n}\sum_{i=1}^{n}\left(w^T x_i - y_i\right)^2\right] \\ &= \frac{2}{n}\sum_{i=1}^{n}\underbrace{\left(w^T x_i - y_i\right)}_{i\text{th residual}} x_i\end{aligned}$$

Gradient Descent: Does it scale?

- At every iteration, we compute the gradient at current w:

$$\nabla_w \hat{R}_n(w) = \frac{2}{n} \sum_{i=1}^{n} \underbrace{\left(w^T x_i - y_i\right)}_{i\text{th residual}} x_i$$

- We have to touch all n training points to take a single step. $[O(n)]$
  - Will this scale to "big data"?
- Can we make progress without looking at all the data?

Gradient Descent on the Risk

1. Real goal is to minimize the risk (expected loss)

   $$R(f) = \mathbb{E}\left[\ell(f(X), Y)\right]$$

   over a hypothesis space $\mathcal{F}$.
2. Say hypothesis space $\mathcal{F}$ is parameterized by $w \in \mathbf{R}^d$.
3. Can we do anything with

   $$\nabla_w \mathbb{E}\left[\ell(f(X), Y)\right]?$$

Gradient Descent on the Risk

- We have

$$\text{Gradient(Risk)} = \nabla_w \mathbb{E}\left[\ell(f(X), Y)\right]$$

- Switching ∇_w and $\mathbb{E}$ we can write the gradient of risk as

$$\text{Gradient(Risk)} = \mathbb{E}\left[\nabla_w \ell(f(X), Y)\right]$$

- Can we approximate this expectation?

Gradient Descent on the Risk

- Let's approximate Gradient(Risk)

$$\nabla_w R(f) = \mathbb{E}\left[\nabla_w \ell(f(X), Y)\right]$$

with an average over the data:

$$\widehat{\nabla_w R(f)} = \frac{1}{n} \sum_{i=1}^{n} \left[\nabla_w \ell(f_w(x_i), y_i)\right]$$

Three things to note about of $\widehat{\nabla_w R(f)}$ as an estimator of $\nabla_w R(f)$:

1. **Unbiased**: $\mathbb{E}\widehat{\nabla_w R(f)} = \nabla_w R(f)$.
2. **Consistent:** $\lim_{n\to\infty} \widehat{\nabla_w R(f)} = \nabla_w R(f)$. (Law of large numbers.)
3. It's exactly the gradient of the emprical risk $\nabla \hat{R}(f)$.

Gradient Descent on the Risk

- We want Gradient(Risk)
- Estimate it using sample of size n.
  - (Our standard procedure when we see an expectation.)
- Bigger $n \implies$ Better estimate
- Bigger $n \implies$ Touching more data (slower!)
- But how big an n do we need?

Gradient Descent on the Risk [approximately]

- Gradient descent takes a bunch of steps whether we use
    - the perfect step direction $\nabla R(w)$,
    - an empirical estimate using all training data $\nabla \hat{R}_n(w)$, or
    - an empirical estimate using a random subset of data $\nabla \hat{R}_m(w)$ ($m \ll n$)
- What about $m = 1$?
- Even with a sample of size 1, the estimate

$$\nabla_w \ell(f_w(x_i), y_i)$$

is still **unbiased for Gradient(Risk).**

Terminology for Gradient Descent Risk Minimization

- **Gradient descent** or **"batch" gradient descent**
  - Use full data set of size n to determine step direction
- **Minibatch gradient descent**
  - Use a random subset of size m to determine step direction
  - Yoshua Bengio says[1]:
    - m is typically between 1 and few hundred
    - $m = 32$ is a good default value
    - With $m \geqslant 10$ we get computational speedup (per datum touched)
- **Stochastic gradient descent**
  - Minibatch with $m = 1$.
  - Use a single randomly chosen point to determine step direction.

[1] See Yoshua Bengio's "Practical recommendations for gradient-based training of deep architectures" http://arxiv.org/abs/1206.5533.

Minibatch Gradient Descent

Minibatch Gradient Descent (minibatch size m)

- initialize $w = 0$
- repeat
  - randomly choose m points $\{(x_i, y_i)\}_{i=1}^{m} \subset \mathcal{D}_n$
  - $w \leftarrow w - \eta \left[\frac{1}{m} \sum_{i=1}^{m} \nabla_w \ell(f_w(x_i), y_i) \right]$
- until stopping criteria met

Stochastic Gradient Descent (SGD)

Stochastic Gradient Descent

- initialize $w = 0$
- repeat
  - randomly choose training point $(x_i, y_i) \in \mathcal{D}_n$
  - $w \leftarrow w - \eta \underbrace{\nabla_w \ell(f_w(x_i), y_i)}_{\text{Grad(Loss on i'th example)}}$
- until stopping criteria met

Step Size

- Let η_t be the step size at the t'th step.
- What should should first step size be?
- How should η_t's decrease with each step?

Robbins-Monro Conditions

Many classical convergence results depend on the following two conditions:

$$\sum_{t=1}^{\infty} \eta_t^2 < \infty \qquad \sum_{t=1}^{\infty} \eta_t = \infty$$

- As fast as $\eta_t = O\left(\frac{1}{t}\right)$ would satisfy this... but should be faster than $O\left(\frac{1}{\sqrt{t}}\right)$.
- A useful reference for practical techniques: Leon Bottou's "Tricks": http://research.microsoft.com/pubs/192769/tricks-2012.pdf