Recitation 2

Gradient Descent and Stochastic Gradient Descent

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Agenda

- Gradient Descent
  - Adaptive Learning Rate
- Stochastic Gradient Descent
- Application
  - Linear Regression
  - Logistic Regression

Gradient Descent Recap

Gradient Descent

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

- Choosing the step size is the key in gradient descent
- A fixed step size will work, eventually, as long as it's small enough

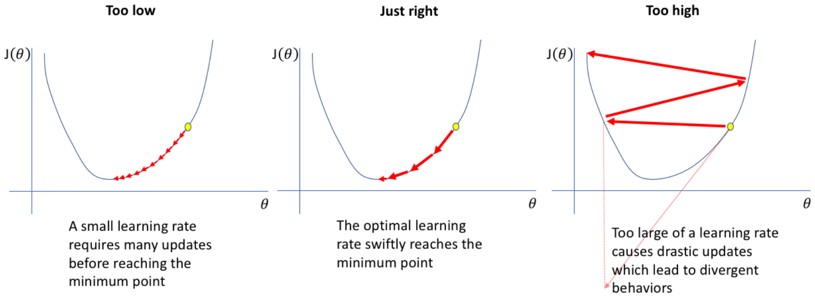
Gradient Descent

Gradient Descent Algorithm

- Goal: find $\theta^* = \arg\min_\theta J(\theta)$
- $\theta^0 :=$ [initial condition]
- $i := 0$
- while not [termination condition]:
  - compute $\nabla J(\theta_i)$
  - $\epsilon_i :=$ [choose learning rate at iteration i]
  - $\theta^{i+1} := \theta^i - \epsilon_i \nabla J(\theta_i)$
  - $i = i + 1$
- return θ^i

Gradient Descent

- How to initialize θ^0?
  - sample from some distribution
  - compose θ^0 using some heuristics
- How to choose termination conditions?
  - run for a fixed number of iteration
  - the value of $f(\theta)$ stabilizes
  - θ^i converges
- What is a good learning rate?



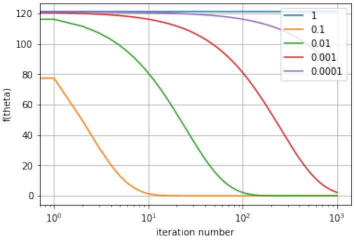
Learning Rate

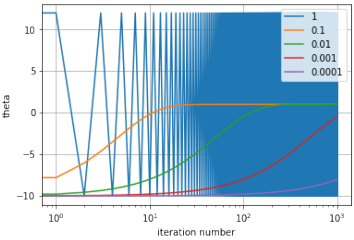
Application

Suppose we would like to find $\theta^* \in \mathbb{R}$ that minimizes $f(\theta) = \theta^2 - 2\theta + 1$. The gradient (in this case, the derivative) $\nabla f(\theta) = 2\theta - 2$. We can easily see that $\theta^* = \operatorname{argmin}_\theta f(\theta) = 1$.

Learning Rate

- We applied gradient descent for 1000 iterations on $f(\theta) = \theta^2 - 2\theta + 1$ with varying learning rate $\epsilon \in \{1, 0.1, 0.01, 0.001, 0.0001\}$
- When the learning rate is too large $(\epsilon = 1)$, $f(\theta)$ does not decrease through iterations. The value of θ_i at each iteration significantly fluctuates.
- When the learning rate is too small $(\epsilon = 0.0001)$, $f(\theta)$ decreases very slowly.





Adaptive Learning Rate

- Instead of using a fixed learning rate through all iterations, we can adjust our learning rate in each iteration using a simple algorithm.
- At each iteration i:
  - $\tilde{\theta} := \theta_{i-1} - \epsilon_{i-1} \nabla f\left(\theta_{i-1}\right)$
  - $\delta := f\left(\theta_{i-1}\right) - f(\tilde{\theta})$
  - if $\delta \geq$ threshold:
    - we achieve a satisfactory reduction on $f(\theta)$
    - $\theta_i = \bar{\theta}$
    - maybe we can consider increasing the learning rate for next iteration $\epsilon_j := 2\epsilon_{i-1}$
  - else:
    - the reduction is unsatisfactory
    - $\theta_i = \theta_{i-1}$
    - the learning rate is too large, so we reduce the learning rate
    - $\epsilon_i := \frac{1}{2}\epsilon_{i-1}$

Adaptive Learning Rate

How to decide a proper threshold for $f(\theta_{i-1}) - f(\tilde{\theta})$

Armijo rule

If learning rate ϵ satisfies

$$f(\theta_{i-1}) - f(\tilde{\theta}) \geq \frac{1}{2}\epsilon \left\|\nabla f(\theta_{i-1})\right\|^2$$

then $f(\theta)$ is guaranteed to converge to a (local) minimum under certain technical assumptions.

You can find more details at **this link**

Stochastic Gradient Descent

Stochastic Gradient Descent

- Initialize w = 0
- Repeat:
  - randomly choose training point $(x_i, y_i) \in \mathcal{D}_n$
  - $w \leftarrow w - \eta \underbrace{\nabla_w \ell\left(f_w\left(x_i\right), y_i\right)}_{\text{Grad(Loss on i'th example)}}$
- Until stopping criterion satisfied

- Equivalent to Minibatch Gradient Descent with batch size $N = 1$.
- Use a single randomly chosen point to determine step direction.

Minibatch Gradient Descent

Minibatch Gradient Descent (minibatch size N)

- Initialize w = 0
- Repeat:
    - randomly choose N points $\{(x_i, y_i)\}_{i=1}^{N} \subset \mathcal{D}_n$
    - $w \leftarrow w - \eta \left[\frac{1}{N}\sum_{i=1}^{N} \nabla_w \ell\left(f_w\left(x_i\right), y_i\right)\right]$
- Until stopping criterion satisfied

- Minibatch gradient is an unbiased estimate of full-batch gradient: $\mathbb{E}\left[\nabla \hat{R}_N(w)\right] = \nabla \hat{R}_n(w)$
- Use a random subset of size N to determine step direction
    - Bigger N: Better estimate of the gradient, but slower (more data to touch)
    - Smaller N: Worse estimate of the gradient, but faster

Gradient Descent for Linear Regression

Linear Least Squares Regression Setup

- **Data**: Inputs are feature vectors of dimension d. Outputs are continuous scalars.

$$\mathcal{D} = \left\{ \mathbf{x}^{(i)}, y^{(i)} \right\}_{i=1}^{n} \text{ where } \mathbf{x} \in \mathbb{R}^d \text{ and } y \in \mathbb{R}$$

- **Hypothesis Space**: $\mathcal{F} = \left\{ f : \mathbf{R}^d \to \mathbf{R} \mid f(x) = \theta^T x, \theta \in R^d \right\}$
- **Action**: Our prediction is a linear function of the inputs

$$\hat{y} = f_\theta(\mathbf{x}) = \theta_1 x_1 + \theta_2 x_2 + \ldots + \theta_d x_d \qquad \text{(We assume } x_1 \text{is 1)}$$
$$\hat{y} = f_\theta(\mathbf{x}) = \boldsymbol{\theta}^T \boldsymbol{x}$$

- **Loss**: $\ell(\hat{y}, y) = (y - \hat{y})^2$

Gradient Descent for Linear Regression

- **Goal**: Finding the set of parameters that minimize the empirical risk:

$$\hat{R}_n(\theta) = \frac{1}{n}\sum_{i=1}^{n}\left(\theta^T x^{(i)} - y^{(i)}\right)^2$$

  where $\theta \in R^d$ parameterizes the hypothesis space $\mathcal{F}$

- Set our cost function:

$$J(\boldsymbol{\theta}) = \frac{1}{2}\sum_{i=1}^{n}\left(\boldsymbol{\theta}^T \mathbf{x}^{(i)} - y^{(i)}\right)^2$$

Three Approach to solving $\theta^* = \underset{\theta}{\text{argmin}} J(\theta)$

- **Approach 1**: Closed Form Solution (set derivatives equal to zero and solve for parameters)
  - pros: one shot algorithm!
  - cons: does not scale to large datasets (matrix inverse is bottleneck)
- **Approach 2**: Gradient Descent (take larger, more certain steps toward the negative gradient)
  - pros: conceptually simple, guaranteed convergence
  - cons: batch, often slow to converge
- **Approach 3**: Stochastic Gradient Descent (take many small, quick steps opposite the gradient)
  - pros: memory efficient, fast convergence, less prone to local optima
  - cons: convergence in practice requires tuning and fancier variants

Approach 1: Close-Form Solution

- Transform the cost function in matrix form

$$J(\theta) = \frac{1}{2}\sum_{i=1}^{n}\left(\mathbf{x}_i^T\theta - y_i\right)^2$$
$$= \frac{1}{2}(X\theta - \bar{y})^T(X\theta - \bar{y}) \quad = \frac{1}{2}\|X\theta - y\|_2^2$$

- To minimize $J(\theta)$, take derivative and set to zero:

$$\nabla J(\theta) = \left(X^T X\theta - X^T y\right) = X^T(X\theta - y) = 0$$

$$\Rightarrow \hat{\theta} = \left(\mathbf{X}^\top \mathbf{X}\right)^{-1}\mathbf{X}^T\mathbf{y}$$

  - Ensure invertibility of $\mathbf{X}^\top\mathbf{X}$
  - What if X has less than full column rank?

Approach 2: Iterative Method GD

Gradient Descent Algorithm

- $\theta^0 :=$ [initial condition]
- $i := 0$
- while not [termination condition]:
  - $\theta^{i+1} := \theta^i - \epsilon_i \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta})$
  - $i = i + 1$
- return θ^i

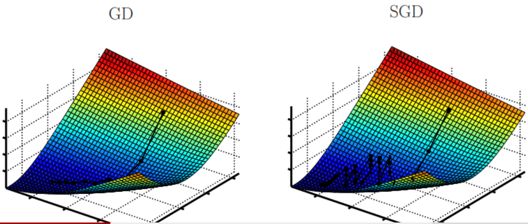
Recall:

$$\nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}) = \begin{bmatrix} \frac{d}{d\theta_1} J(\boldsymbol{\theta}) \\ \frac{d}{d\theta_2} J(\boldsymbol{\theta}) \\ \vdots \\ \frac{d}{d\theta_d} J(\boldsymbol{\theta}) \end{bmatrix}$$

Approach 3: Iterative Method SGD

Stochastic Gradient Descent Algorithm

- $\theta^0 :=$ [initial condition]
- $i := 0$
- while not [termination condition]:
  - For each training pair (x^j, y^j) (in random order)
  - $\theta^{i+1} := \theta^i - \epsilon_i \nabla_{\boldsymbol{\theta}} J^{(j)}(\boldsymbol{\theta}) \quad \{\text{with} \quad J^{(j)}(\boldsymbol{\theta}) = \frac{1}{2}\left(\boldsymbol{\theta}^T \mathbf{x}^{(j)} - y^{(j)}\right)^2\}$
  - $i = i + 1$
- return θ^i



Gradient Descent for Logistic Regression

Binary Classification Setup for Logistic Regression

- **Data**: Inputs are feature vectors of dimension d. Targets are class labels. $\mathcal{D} = \left\{\mathbf{x}^{(i)}, y^{(i)}\right\}_{i=1}^{n}$ where $\mathbf{x} \in \mathbb{R}^d$ and $y \in \{0, 1\}$
- **Action**: Our prediction is the probability of class label given linear signals

$$h_\theta(x) = g\left(\theta^T x\right) = \frac{1}{1+e^{-\theta^T x}} \quad \text{with} \quad g(z) = \frac{1}{1+e^{-z}}$$

  - Sigmoid Function $g(z)$: takes a real-valued number and maps it into the range [0,1] (Probability Interpretation)
- Assume

$$\begin{cases} P(y = 1 \mid x; \theta) = h_\theta(x) \\ P(y = 0 \mid x; \theta) = 1 - h_\theta(x) \end{cases}$$

  - More Compactly: $p(y \mid x; \theta) = (h_\theta(x))^y \left(1 - h_\theta(x)\right)^{1-y}$

Learning Logistic Regression

- Assumption: $(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_n, y_n)$ are independently generated
- **Likelihood**: The probability of getting the $y_1 \ldots\ldots, y_n$ in $\mathcal{D}$ from the corresponding $x_1, \ldots, x_n$

$$\begin{aligned} P(y_1, \ldots, y_n \mid \mathbf{x}_1, \ldots, \mathbf{x}_n) &= \prod_{i=1}^{n} p(y^{(i)} \mid x^{(i)}; \theta) \\ &= \prod_{i=1}^{n} (h_\theta(x^{(i)}))^{y^{(i)}} (1 - h_\theta(x^{(i)}))^{1-y^{(i)}} \end{aligned}$$

- **Goal**: maximize the log likelihood (Easier)

$$\ell(\theta) = \log L(\theta) \quad = \sum_{i=1}^{n} y^{(i)} \log h_\theta(x^{(i)}) + (1 - y^{(i)}) \log(1 - h_\theta(x^{(i)}))$$

  - Equivalent to minimize the objective function with logistic loss: $J(\theta) = \sum_{i=1}^{n} \ell\left(h_\theta\left(x^{(i)}\right), y^{(i)}\right)$ where $\ell(h(x), y) = -y \log(h_\theta(x)) - (1 - y) \log(h_\theta(x))$

Learning Logistic Regression

- Analytic solution won't work
- Find optimum using iterative methods: Gradient Ascent or Stochastic Gradient Ascent
  - Gradient ascent rule: $\theta := \theta + \alpha \nabla_\theta \ell(\theta)$
  - Stochastic gradient ascent rule: $\theta := \theta + \alpha \nabla_\theta \ell^{(i)}(\theta)$ for random training pair (x^i, y^i)
- For one training example (x, y), the partial derivative of log likelihood $\ell(\theta)$:

$$
\begin{aligned}
&= (y\frac{1}{g(\theta^T x)} - (1-y)\frac{1}{1-g(\theta^T x)})\frac{\partial}{\partial \theta_j} g(\theta^T x) \\
&= (y\frac{1}{g(\theta^T x)} - (1-y)\frac{1}{1-g(\theta^T x)}) g(\theta^T x)(1-g(\theta^T x))\frac{\partial}{\partial \theta_j}\theta^T x \\
&= (y(1-g(\theta^T x)) - (1-y)g(\theta^T x))x_j \\
&= (y - h_\theta(x)) \cdot x_j
\end{aligned}
$$

References

- DS-GA 1003 Machine Learning Spring 2021 & 2022
- Stanford CS229 Note1
- CMU 10-701 Linear Regression Slide