ESE 402/542 Recitation 8: Gradient Descent

Outline

1. Starting in 1-D
2. Introducing gradient descent
3. When is gradient descent guaranteed to work?
4. Examples in data science

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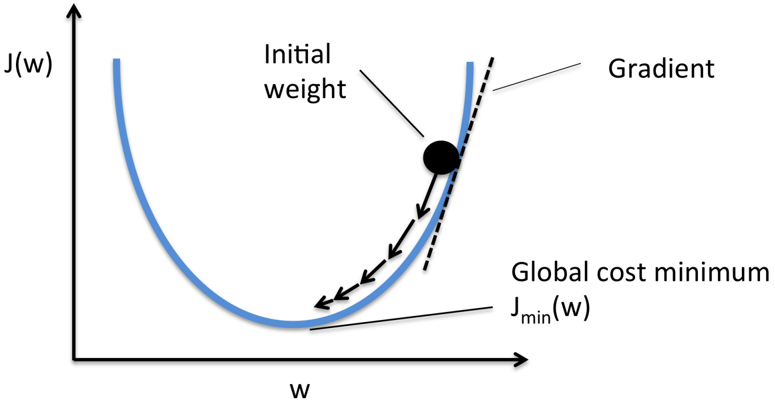
- Notice in general, we get $x_{t+1} = (1 - 2\eta)x_t$, which implies recursively $x_{t+1} = (1 - 2\eta)^{t+1}x_0$. Iterates decay exponentially toward 0.

Starting in 1-D



Introducing Gradient Descent

- Following intuition from previous part, let $f(\vec{x}) : \mathbb{R}^n \to \mathbb{R}$ be a scalar function that brings a vector in $\mathbb{R}^n$ to $\mathbb{R}$. Simple example extending 1-D case: $f(x) = x_1^2 + x_2^2 + \cdots + x_n^2$.

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- What is gradient (at a point)? Simply vector in $\mathbb{R}^n$ whose entries are the partial derivatives evaluated at a point:

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- Base algorithm is the same: $t = 0, \ldots, N$, $x_{t+1} = x_t - \eta \nabla f(x_t)$. $\eta > 0$ is step-size hyperparameter.

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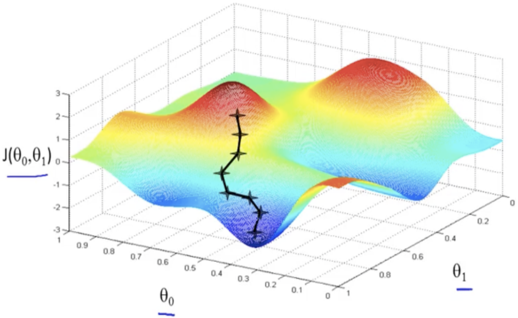

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- In English: function value evaluated anywhere along the line between any two points x, y is always lower than the accordingly weighted function values at the end points.
- Gradient naturally requires differentiability.
- Can show that for convex, differentiable functions, minimizer x^* satisfies $\nabla f(x^*) = \vec{0}$.

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Intuitively, gradient descent converges on continuously differentiable functions because it goes toward the minimizer x^*, and thus $\nabla f(x_t) \to_t \vec{0}$.

Every caveat is important to guarantee convergence of GD:

- Convex, but not continuously differentiable.
- Continuously differentiable, but not convex.
- Bad choice of step-size.

$$f(x) = x^2. \quad x_{t+1} = x_t - f'(x_t), \quad \eta = 1.$$

When is GD guaranteed to work?

That being said, variants of GD are used heavily in practice when aforementioned hypotheses are violated, e.g. neural net optimization. Deep theory to understand why this is OK; even if we don't have theory, GD is often a good starting algorithm.

Data Science Example 1: Least-Squares

- Recall that least-squares solves $\min_{\boldsymbol{\beta}} \|\boldsymbol{y} - \boldsymbol{X}\beta\|_2^2$
- Objective $f(\boldsymbol{\beta}) = \|\boldsymbol{y} - \boldsymbol{X}\beta\|_2^2$ is convex in $\boldsymbol{\beta}$
- $\nabla_{\boldsymbol{\beta}} f(\boldsymbol{\beta}) = \nabla_{\boldsymbol{\beta}}(\boldsymbol{y} - \boldsymbol{X}\beta)^\top(\boldsymbol{y} - \boldsymbol{X}\beta) =$
  $\nabla_{\boldsymbol{\beta}}(\boldsymbol{y}^\top\boldsymbol{y} - 2\boldsymbol{\beta}^\top\boldsymbol{X}^\top\boldsymbol{y}^\top + \boldsymbol{\beta}^\top\boldsymbol{X}^\top\boldsymbol{X}\beta) = -2\boldsymbol{X}^\top\boldsymbol{y} + 2\boldsymbol{X}^\top\boldsymbol{X}\beta$
- Gradient Descent: iterate $\boldsymbol{\beta}_{t+1} = \boldsymbol{\beta}_t - \eta(-2\boldsymbol{X}^\top\boldsymbol{y} + 2\boldsymbol{X}^\top\boldsymbol{X}\beta)$
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- If η small enough, will converge to $\boldsymbol{\beta}^*$
- Known closed form solution: $\boldsymbol{\beta}^* = (\boldsymbol{X}^\top\boldsymbol{X})^{-1}\boldsymbol{X}^\top\boldsymbol{y}$. Gradient descent not extremely useful in this case.

Data Science Example 2: Logistic Regression (HW5)

- MLE in logistic regression solves $\min_{\boldsymbol{\beta}} \sum_{i=1}^{n} \log(1 + e^{-y_i \boldsymbol{\beta}^\top \boldsymbol{x}_i})$
- Note: each $\boldsymbol{x}_i$ has a 1 appended to account for the bias term
- $\boldsymbol{\beta}^*$ does *not* have an easily attainable closed-form solution, must use gradient descent (HW5 Q2)
- Objective $f(\boldsymbol{\beta}) = \sum_{i=1}^{n} \log(1 + e^{-y_i \boldsymbol{\beta}^\top \boldsymbol{x}_i})$ is convex in $\boldsymbol{\beta}$
- $\nabla_{\boldsymbol{\beta}} f(\boldsymbol{\beta}) = \sum_{i=1}^{n} \nabla_{\boldsymbol{\beta}} \log(1 + e^{-y_i \boldsymbol{\beta}^\top \boldsymbol{x}_i}) = \sum_{i=1}^{n} \frac{e^{-y_i \boldsymbol{\beta}^\top \boldsymbol{x}_i}}{1 + e^{-y_i \boldsymbol{\beta}^\top \boldsymbol{x}_i}} y_i \boldsymbol{x}_i$
- Iterate $\boldsymbol{\beta}_{t+1} = \boldsymbol{\beta}_t - \eta \sum_{i=1}^{n} \frac{e^{-y_i \boldsymbol{\beta}^\top \boldsymbol{x}_i}}{1 + e^{-y_i \boldsymbol{\beta}^\top \boldsymbol{x}_i}} y_i \boldsymbol{x}_i$