

SDS 385: Stat Models for Big Data

Lecture 3: GD and SGD cont.

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Scalability concerns

- You have to calculate the gradient every iteration.
- Take ridge regression.
- You want to minimize $1/n \left((\mathbf{y} - \mathbf{X}\boldsymbol{\beta})^T (\mathbf{y} - \mathbf{X}\boldsymbol{\beta}) - \lambda \boldsymbol{\beta}^T \boldsymbol{\beta} \right)$
- Take a derivative: $(-2\mathbf{X}^T (\mathbf{y} - \mathbf{X}\boldsymbol{\beta}) - 2\lambda \boldsymbol{\beta})/n$
- Grad descent update takes $\boldsymbol{\beta}_{t+1} \leftarrow \boldsymbol{\beta}_t + \alpha (\mathbf{X}^T (\mathbf{y} - \mathbf{X}\boldsymbol{\beta}_t) + \lambda \boldsymbol{\beta}_t)$
- What is the complexity?
 - Trick: first compute $\mathbf{y} - \mathbf{X}\boldsymbol{\beta}$.
 - np for matrix vector multiplication, $\text{nnz}(\mathbf{X})$ for sparse matrix vector multiplication.
 - Remember the examples with humongous n and p ?

What will you need for this class

- Stuff you should know from the last lecture.
- The knowledge of conditional expectation.
- Law of total expectation, which is also known as the tower property.

So what to do?

- For $t = 1 : T$
 - Draw σ_t with replacement from n
 - $\beta_{t+1} = \beta_t - \alpha \nabla f(x_{\sigma_t}; \beta_t)$
- In expectation (over the randomness of the index you chose), for a fixed β ,

$$E[\nabla f(x_{\sigma_t}; \beta)] = \frac{\sum_i \nabla f(x_i; \beta)}{n}$$

- Does this also converge?

Convergence

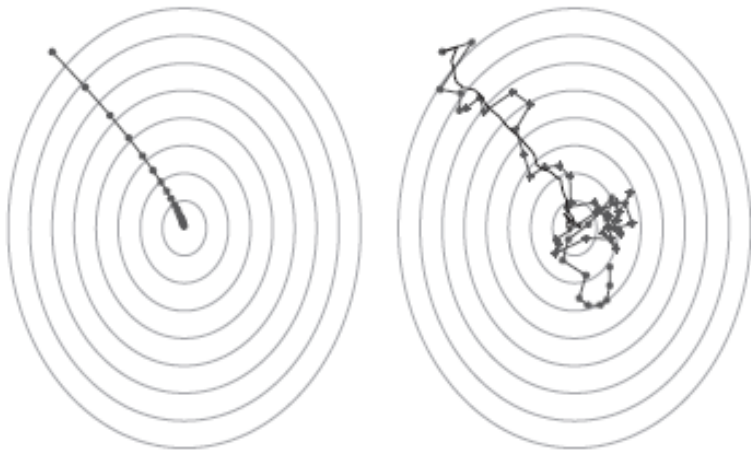


Figure 1: Gradient descent vs Stochastic gradient descent

Convergence

- Let $\nabla f(X; \beta)$ be the full derivative.

$$\begin{aligned}\beta_{t+1} - \beta^* &= \beta_t - \beta^* - \alpha \nabla f(x_{\sigma_t}; \beta_t) \\ &= \beta_t - \beta^* - \alpha (\nabla f(X; \beta_t) - \nabla f(X; \beta^*)) + \alpha (\nabla f(X; \beta_t) - \nabla f(x_{\sigma_t}; \beta_t)) \\ &= \underbrace{(I - \alpha H(z_t))(\beta_t - \beta^*)}_{g(\beta_t)} + \alpha \underbrace{(\nabla f(X; \beta_t) - \nabla f(x_{\sigma_t}; \beta_t))}_{h(\sigma_t, \beta_t)}\end{aligned}$$

- Take the expected squared length:

$$E[\|\beta_{t+1} - \beta^*\|^2 | \beta_t] = \underbrace{\|g(\beta_t)\|^2}_{\text{Same as before}} + \alpha^2 \underbrace{E[\|h(\sigma_t, \beta_t)\|^2 | \beta_t]}_{\text{variance of gradient update at a random point}}$$

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$$\begin{aligned} E[\|h(\sigma_t, \beta_t)\|^2 | \beta_t] &= E_X E_\sigma [\|h(\sigma_t, \beta_t)\|^2 | \beta_t] \\ &= E_X E_\sigma [\|\nabla f(x_{\sigma_t}; \beta_t) - \nabla f(X; \beta_t)\|^2 | \beta_t] \\ &= E_X \frac{1}{n} \sum_i [\|\nabla f(x_i; \beta_t) - \nabla f(X; \beta_t)\|^2 | \beta_t] \\ &= E_X [\|\nabla f(x_i; \beta_t) - \nabla f(X; \beta_t)\|^2 | \beta_t] =: M \end{aligned}$$

- So by total expectation rule,

$$E[\|\beta_{t+1} - \beta^*\|^2] \leq (1 - \alpha\mu)^2 E[\|\beta_t - \beta^*\|^2] + \alpha^2 M$$
$$\lim_{t \rightarrow \infty} E[\|\beta_{t+1} - \beta^*\|^2] \leq \frac{\alpha M}{2\mu - \alpha\mu^2}$$

- So SGD is converging to a noise ball.
- How to remedy this?

- Assume you are far away from the noise ball.
- $\|\beta_t - \beta^*\|^2 \geq 2\alpha M/\mu$.
- Then,

$$\begin{aligned} E[\|\beta_{t+1} - \beta^*\|^2 | \beta_t] &\leq (1 - \alpha\mu)^2 \|\beta_t - \beta^*\|^2 + \frac{\alpha\mu}{2} \|\beta_t - \beta^*\|^2 \\ &\leq \left(1 - \frac{\alpha\mu}{2}\right) \|\beta_t - \beta^*\|^2 \quad \text{If } \alpha\mu < 1 \\ E[\|\beta_T - \beta^*\|^2] &\leq e^{-\alpha\mu T/2} C, \end{aligned}$$

- C is the initial loss
- It takes $2/\alpha\mu \log M$ steps to achieve M factor contraction.

- Recall that the size of the noise ball is

$$\lim_{t \rightarrow \infty} E[\|\beta_{t+1} - \beta^*\|^2] \leq \frac{\alpha M}{2\mu - \alpha\mu^2}$$

- So the size is $O(\alpha)$, i.e. for larger α we converge to a larger noise ball.
- But convergence time is $2/\alpha\mu \log M$, i.e. inversely proportional to step size α .
- So there is a tradeoff.

What if we allow the step size to vary

- We will set the stepsize as $1/t$, and check the following by induction.

Theorem

If we use $\alpha_t = a/t$, for $a > 1/\mu$ we have:

$$E[\|\beta_t - \beta_0\|^2] \leq \frac{\max(\|\beta_1 - \beta^*\|^2, Y)}{t}$$

where $Y = \frac{Ma^2}{a\mu - 1}$.

Proof.

We will do this by induction. First note Step 1 is obviously true. Now assume that the above holds for t . We will show that it holds for $t + 1$. □

What if we allow the step size to vary

- Let $C = \max(\|\beta_1 - \beta^*\|^2, Y)$
- Recall that we have:

$$\begin{aligned} E[\|\beta_{t+1} - \beta^*\|^2] &\leq (1 - \alpha_t \mu) E\|\beta_t - \beta^*\|^2 + \alpha_t^2 M \\ &\leq (1 - a\mu/t) \frac{Y}{t} + \frac{Ma^2}{t^2} \\ &= \frac{Y}{t} - \frac{a}{t^2} (\mu Y - Ma) \end{aligned}$$

- Set $a(Y\mu - Ma) = Y$, i.e. $Y = \frac{Ma^2}{a\mu - 1}$
- So

$$E[\|\beta_{t+1} - \beta^*\|^2] \leq Y \left(\frac{1}{t} - \frac{1}{t(t+1)} \right) = \frac{Y}{t+1}$$

What if we allow the step size to vary

- $\beta_{t+1} = \beta_t - \alpha_t \nabla f(x_i; \beta_t)$
- How do we choose this optimally?
- Recall our bound, and assume $\alpha_t \mu < 1$

$$\begin{aligned} E[\|\beta_{t+1} - \beta^*\|^2] &\leq (1 - \alpha_t \mu)^2 E[\|\beta_t - \beta^*\|^2] + \alpha_t^2 M \\ &\leq (1 - \alpha_t \mu) E[\|\beta_t - \beta^*\|^2] + \alpha_t^2 M \end{aligned}$$

- Define $d_t := E[\|\beta_{t+1} - \beta^*\|^2]$
- Differentiate and set to zero. This gives,

$$-\mu d_t + 2\alpha_t M = 0 \rightarrow \alpha_t = \frac{\mu d_t}{2M}$$

Varying step size

$$\begin{aligned}d_{t+1} &\leq (1 - \mu^2 d_t / 2M) d_t + \mu^2 d_t^2 / 4M \\&= d_t - \mu^2 d_t^2 / 4M \\ \frac{1}{d_{t+1}} &\geq \frac{1}{d_t} \frac{1}{1 - \mu^2 d_t / 4M} \\&\geq \frac{1}{d_t} \left(1 + \frac{\mu^2 d_t}{4M} \right) \\&= \frac{1}{d_t} + \frac{\mu^2}{4M}\end{aligned}$$

- If you think of $1/d_t$ to be analogous to the accuracy of the score, then this is saying at each iteration the accuracy is increasing by some increment.

Varying step size

$$\begin{aligned}d_{t+1} &\leq (1 - \mu^2 d_t / 2M) d_t + \mu^2 d_t^2 / 4M \\&= d_t - \mu^2 d_t^2 / 4M \\ \frac{1}{d_{t+1}} &\geq \frac{1}{d_t} \frac{1}{1 - \mu^2 d_t / 4M} \\&\geq \frac{1}{d_t} \left(1 + \frac{\mu^2 d_t}{4M} \right) \\&= \frac{1}{d_t} + \frac{\mu^2}{4M}\end{aligned}$$

- If you think of $1/d_t$ to be analogous to the accuracy of the score, then this is saying at each iteration the accuracy is increasing by some increment.

Varying step size

- So $\frac{1}{d_T} \geq \frac{1}{d_0} + \frac{\mu^2 T}{4M}$
- Take $\alpha_t = \frac{\mu d_t}{2M} = \frac{\mu \left(\frac{1}{d_0} + \frac{\mu^2 T}{4M} \right)^{-1}}{2M} \approx 1/t$

Mini batch Stochastic Gradient Descent

- SGD uses one data-point at a time.
 - Number of iterations to reach ϵ error is $1/\epsilon$
 - Work per iteration $O(p)$
 - Total work p/ϵ
- GD uses all data-points at a time.
 - Number of iterations to reach ϵ error is $\log(1/\epsilon)$
 - Work per iteration $O(np)$
 - Total work $np \log(1/\epsilon)$

A compromise

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- Pick B_t without replacement from $\{1, \dots, n\}$ with $|B_t| = b$
- $\beta_{t+1} = \frac{1}{b} \sum_{i \in B_t} \nabla f(x_i; \beta_t)$
- $b \ll N$

- Takes b times more time than Stochastic Gradient Descent
- Hopefully converges **sooner**?

Convergence

$$\begin{aligned}\beta_{t+1} - \beta^* &= \beta_t - \beta^* - \alpha \frac{1}{b} \sum_{i \in B_t} \nabla f(x_i; \beta_t) \\ &= \beta_t - \beta^* - \alpha(\nabla f(X; \beta_t) - \nabla f(X; \beta^*)) + \alpha(\nabla f(X; \beta_t) - \nabla f(x_{\sigma_t}; \beta_t)) \\ &= \beta_t - \beta^* - \alpha(\nabla f(X; \beta_t) - \nabla f(X; \beta^*)) - \alpha \left(\frac{1}{b} \sum_{i \in B_t} \nabla f(x_i; \beta_t) - \nabla f(X; \beta_t) \right)\end{aligned}$$

Lets look at the variance of

$$\text{var} \left(\frac{1}{b} \sum_{i \in B_t} \nabla f(x_i; \beta_t) - \nabla f(X; \beta_t) \right)$$

Variance reduction

- Let $\Delta_i := f(x_i; \beta_t) - \nabla f(X; \beta_t)$
- Let $Y_i \in \{0, 1\}$ be a random variable that denotes whether $i \in B_t$ or not.
- Expectation:

$$E \left[\frac{1}{b} \sum_{i \in B_t} \nabla f(x_i; \beta_t) - \nabla f(X; \beta_t) \right] = E \left[\frac{1}{b} \sum_i Y_i \nabla f(x_i; \beta_t) - \nabla f(X; \beta_t) \right] = 0$$

- Let $\Delta_i = \nabla f(x_i; \beta_t) - \nabla f(X; \beta_t)$
- Variance:

$$\begin{aligned} E \left[\frac{1}{b} \sum_{i \in B_t} \nabla f(x_i; \beta_t) - \nabla f(X; \beta_t) \right]^2 &= E \left[\frac{1}{b} \sum_i Y_i \Delta_i \right]^2 \\ &= \sum_{ij} \Delta_i \Delta_j E(Y_i Y_j) / b^2 \end{aligned}$$

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$$\begin{aligned}\sum_{ij} \Delta_i \Delta_j E(Y_i Y_j) &= \sum_{i \neq j} \frac{b(b-1)}{n(n-1)} \Delta_i \Delta_j + \sum_i \frac{b}{n} \Delta_i^2 \\&= \frac{b}{n} \left(\frac{b-1}{n-1} \sum_{i \neq j} \Delta_i \Delta_j + \sum_i \Delta_i^2 \right) \\&= \frac{b}{n} \left(\frac{b-1}{n-1} (\sum_i \Delta_i)^2 + \sum_i \Delta_i^2 (1 - \frac{b-1}{n-1}) \right) \\&= \frac{b}{n} \sum_i \Delta_i^2 (1 - \frac{b-1}{n-1})\end{aligned}$$

- So

$$E_{X, B_t} \left[\frac{1}{b} \sum_{i \in B_t} \nabla f(x_i; \beta_t) - \nabla f(X; \beta_t) | \beta_t \right]^2 \leq \sum_i E_X [\Delta_i^2] / bn \leq M/b$$

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