

# 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  $p$ ?

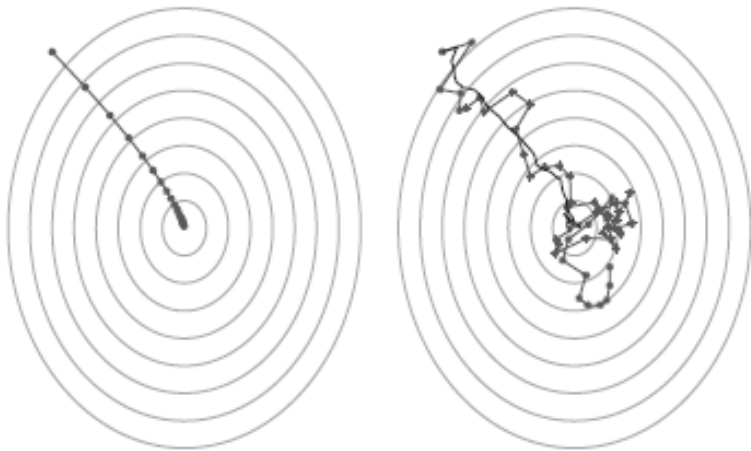
# So what to do?

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

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

- Does this also converge?

# Convergence



**Figure 1:** Gradient descent vs Stochastic gradient descent

# Convergence

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

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

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

- 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,

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

- It takes  $2/\alpha\mu \log M$  steps to achieve  $C$  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  $\alpha$  we converge to a larger noise ball.
- But convergence time is  $2/\alpha\mu \log M$ , i.e. inversely proportional to step size  $\alpha$ .
- So there is a tradeoff.

## 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

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

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

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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