

# SDS 385: Stat Models for Big Data

## Lecture 4: GD with momentum.

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# Polyak's heavy ball method

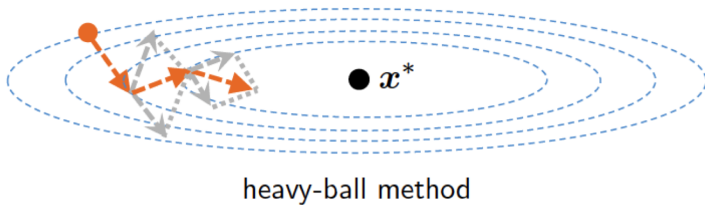
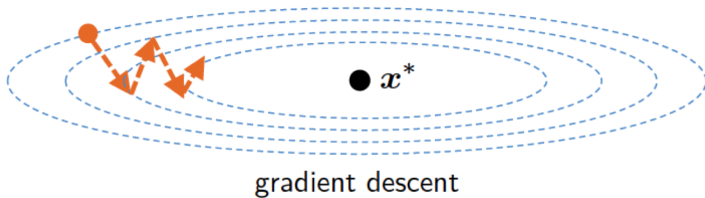
Figure 1: B. Polyak



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$$\beta_{t+1} = \beta_t - \alpha \nabla f(\beta_t) + \underbrace{\theta(\beta_t - \beta_{t-1})}_{\text{momentum term}}$$

# Momentum



## Recall GD?

- For a  $L$  smooth and  $\mu$  convex optimization problem, i.e.  
 $\mu I \preceq \|H\| \preceq LI$ ,

$$\|\beta_t - \beta^*\| \leq \left( \frac{\kappa - 1}{\kappa + 1} \right)^t \|\beta_0 - \beta^*\|$$

where  $\kappa = L/\mu$  i.e. the condition number of the Hessian.

- For the same problem, using Polyak's method we can show that,

$$\left\| \begin{bmatrix} \beta_{t+1} - \beta^* \\ \beta_t - \beta^* \end{bmatrix} \right\| \leq \left( \frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1} \right)^t \left\| \begin{bmatrix} \beta_1 - \beta^* \\ \beta_0 - \beta^* \end{bmatrix} \right\|$$

# Momentum method

- Recall we have:

$$\begin{aligned}\beta_{t+1} - \beta^* &= (1 + \theta)(\beta_t - \beta^*) - \alpha \nabla f(\beta_t) - \theta(\beta_{t-1} - \beta^*) \\ &= ((1 + \theta)I - \alpha \nabla^2 f(z_t))(\beta_t - \beta^*) - \theta(\beta_{t-1} - \beta^*)\end{aligned}$$

- This gives the dynamic system:

$$\begin{bmatrix} \beta_{t+1} - \beta^* \\ \beta_t - \beta^* \end{bmatrix} \leq \begin{bmatrix} (1 + \theta)I - \alpha \nabla^2 f(z_t) & -\theta I \\ I & 0 \end{bmatrix} \begin{bmatrix} \beta_t - \beta^* \\ \beta_{t-1} - \beta^* \end{bmatrix}$$

# Momentum method

- We need to upper bound the norm of

$$M := \begin{bmatrix} (1 + \theta)I - \alpha \nabla^2 f(z_t) & -\theta I \\ I & 0 \end{bmatrix}$$

- It can be shown that:

$$\begin{aligned} \|M\| &= \left\| \begin{bmatrix} (1 + \theta) - \alpha \Lambda & -\theta \\ I & 0 \end{bmatrix} \right\| \\ &= \max_i \left\| \begin{bmatrix} (1 + \theta) - \alpha \lambda_i & -\theta \\ 1 & 0 \end{bmatrix} \right\| \end{aligned}$$

- Eigenvalues of the  $2 \times 2$  matrix can be written as a solution of the following quadratic:

$$\sigma^2 - \sigma((1 + \theta) - \alpha \lambda_i) + \theta = 0$$

# Momentum method

- If  $((1 + \theta) - \alpha\lambda_i)^2 \leq 4\theta$ , the roots are imaginary and the magnitude is  $\sqrt{\theta}$
- This is satisfied if

$$\theta \in [(1 - \sqrt{\alpha\lambda_i})^2, (1 + \sqrt{\alpha\lambda_i})^2]$$

- But recall that  $\lambda_i \in [\mu, L]$ .
- If we set  $1 - \sqrt{\alpha L} = -(1 - \sqrt{\alpha\mu})$ , then we have

$$\alpha = \left( \frac{2}{\sqrt{L} + \sqrt{\mu}} \right)^2 \quad \theta = \left( \frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1} \right)^2$$

- So the new contraction factor becomes  $\frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1}$

# Nesterov's Accelerated Gradient

- If we only assume that  $\|\nabla^2 f(x)\| \leq L$  and not strong convexity, then in your homework you will prove that

$$f(\beta_t) - f(\beta^*) \leq c_L \frac{\|\beta_0 - \beta^*\|^2}{t}$$

- Note that this is much weaker than the linear convergence we saw before.
- Question is can we do better?



# Nesterov's Accelerated Gradient

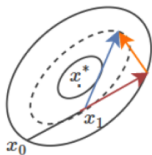
Figure 2: Y. Nesterov



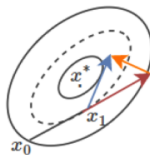
- Keep track of two vectors  $x_t$  and  $y_t$
- $x_{t+1} = y_t - \alpha_t \nabla f(y_t)$
- $y_{t+1} = x_{t+1} + \underbrace{\frac{t}{t+3}}_{\mu_{t+1}} (x_{t+1} - x_t)$

# Nesterov's Accelerated Gradient

*Polyak's Momentum*



*Nesterov Momentum*



- Can be re-written as:

$$x_{t+1} = x_t + \mu(x_t - x_{t-1}) - \alpha_t \nabla f(x_t + \mu_t(x_t - x_{t-1}))$$

- Very much like the momentum method, but computes the derivative at a future step.

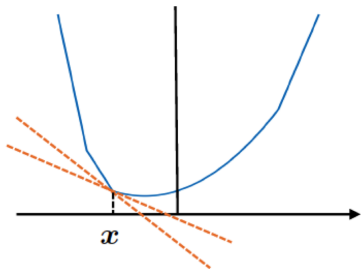
# Nesterov's Accelerated Gradient

- Not a descent method.
- If  $f$  is convex and  $L$  smooth and the learning rate is  $1/L$ , this obtains the optimal  $O(1/t^2)$  error after  $t$  steps.
- Proof is complicated, but can be simplified using intuitions from differential equations.

# Subgradient methods

- So far we have assumed differentiable  $f$ .
- What if  $f$  is not differentiable?
- Instead of a gradient we will define a subgradient.

# Subgradient methods



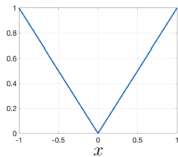
- We will say that  $g$  is a subgradient of  $f$  at point  $x$  if

$$f(z) \geq f(x) + g^T(z - x), \quad \forall z$$

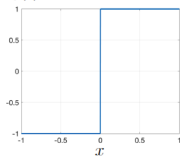
- Set of all gradients is called the sub-differential of  $f$  at point  $x$  and is denoted by  $\partial f(x)$

# Example

$$f(x) = |x|$$

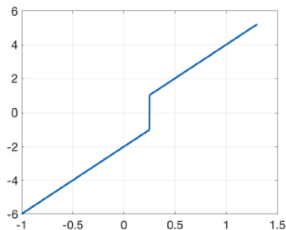
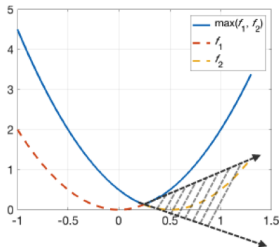


$$\partial f(x)$$



$$f(x) = |x| \quad \partial f(x) = \begin{cases} \{-1\} & \text{if } x < 0 \\ [-1, 1] & \text{if } x = 0 \\ \{1\} & \text{if } x > 0 \end{cases}$$

## Example



$f(x) = \max\{f_1(x), f_2(x)\}$  where  $f_1$  and  $f_2$  are differentiable

$$\partial f(x) = \begin{cases} \{f'_1(x)\}, & \text{if } f_1(x) > f_2(x) \\ [f'_1(x), f'_2(x)], & \text{if } f_1(x) = f_2(x) \end{cases}$$

- $\partial(\alpha f) = \alpha \partial f$
- $\partial(f + g) = \partial f + \partial g$



$$f(\mathbf{x}) = \|\mathbf{x}\|_1 = \sum_{i=1}^n \underbrace{|x_i|}_{:=f_i(\mathbf{x})}$$

since

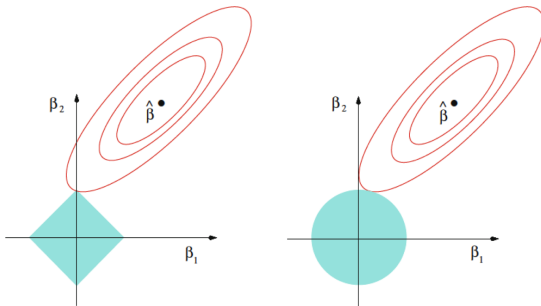
$$\partial f_i(\mathbf{x}) = \begin{cases} \operatorname{sgn}(x_i) \mathbf{e}_i, & \text{if } x_i \neq 0 \\ [-1, 1] \cdot \mathbf{e}_i, & \text{if } x_i = 0 \end{cases}$$

we have

$$\sum_{i: x_i \neq 0} \operatorname{sgn}(x_i) \mathbf{e}_i \in \partial f(\mathbf{x})$$

# Lets talk about Lasso

$$\hat{\beta}_{LASSO} = \min_{\beta} (\mathbf{y} - \mathbf{x}\beta)^{\top} (\mathbf{y} - \mathbf{x}\beta) + \lambda \sum_{j=1}^p |\beta_j| \quad (1)$$



**FIGURE 3.11.** Estimation picture for the lasso (left) and ridge regression (right). Shown are contours of the error and constraint functions. The solid blue areas are the constraint regions  $|\beta_1| + |\beta_2| \leq t$  and  $\beta_1^2 + \beta_2^2 \leq t^2$ , respectively, while the red ellipses are the contours of the least squares error function.

## Alternative formulation

$$\hat{\beta}_{ridge} = \min_{\beta} (\mathbf{y} - \mathbf{x}\beta)^{\top} (\mathbf{y} - \mathbf{x}\beta) \quad \text{Subject to } \beta^{\top} \beta \leq \tau^2 \quad (2)$$

$$\hat{\beta}_{lasso} = \min_{\beta} (\mathbf{y} - \mathbf{x}\beta)^{\top} (\mathbf{y} - \mathbf{x}\beta) \quad \text{Subject to } \|\beta\|_1 \leq \tau \quad (3)$$

# Optimality condition

- For differentiable  $f$

$$f(x^*) = \min_x f(x) \leftrightarrow \nabla f(x^*) = 0$$

- For convex  $f$  that may not be differentiable,

$$f(x^*) = \min_x f(x) \leftrightarrow 0 \in \delta f'(x^*)$$

- Just plug into the definition of a subgradient!

$$f(y) \geq f(x^*) + 0^T(y - x^*) = f(x^*)$$

# Soft thresholding

- Consider the easier problem

$$x = \arg \min \frac{1}{2} \|y - x\|^2 + \lambda \|x\|_1$$

- Show that the soft thresholding operator  $x^* = S_\lambda(y)$  is the solution to this.

$$S_\lambda(y) = \begin{cases} y_i - \lambda & \text{if } y_i > \lambda \\ 0 & \text{if } y_i \in [-\lambda, \lambda] \\ y_i + \lambda & \text{if } y_i < -\lambda \end{cases}$$

# Sub-gradient method

- $\beta_{k+1} = \beta_k - \alpha_k g_{k-1}$
- Here  $g_{k-1}$  is any subgradient at the  $\beta_{k-1}$
- Note that subgradient direction is not always a direction of descent
- So we do

$$f(\beta_k^{best}) = \min_{i=1,\dots,k} f(\beta_i)$$

- We did not cover backtracking line search, but since this is not a descent method we cannot choose the step size adaptively.
- We can choose it as
  - Fixed, i.e.  $t_k = \alpha$
  - Or diminishing such that  $\sum_k t_k^2 < \infty, \sum_k t_k = \infty$



# Acknowledgment

Y. Chen's large scale Optimization class at Princeton and Hastie and Tibshirani's book