THE UNIVERSITY OF TEXAS AT AUSTIN
Department of Statistics and Data Sciences
College of Natural Sciences

SDS 385: Stat Models for Big Data

Lecture 4: GD with momentum.

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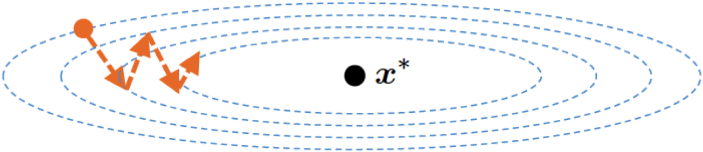
Polyak's heavy ball method

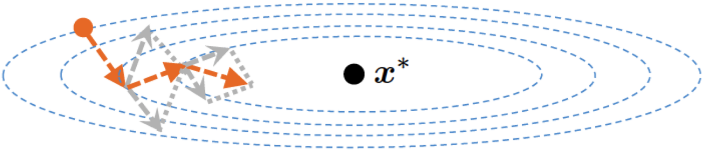
Figure 1: B. Polyak

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

Momentum



gradient descent



heavy-ball method

Recall GD?

- For a L smooth and μ 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:

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

- Eigenvalues of the 2×2 matrix can be written as a solution of the following quadratic:

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

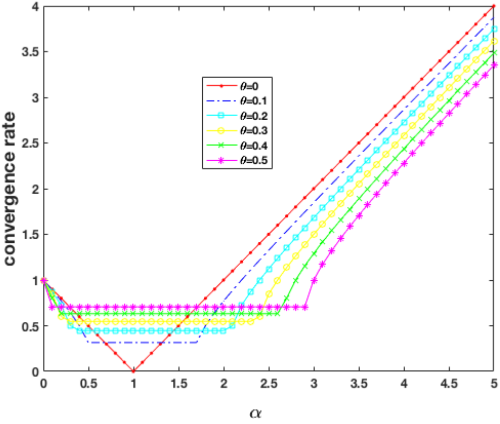
Momentum method - simple example

- Take $f(x) = \frac{h}{2}x^2$.
- Now $M := \begin{bmatrix} 1+\theta-\alpha h & -\theta \\ 1 & 0 \end{bmatrix}$
- The two eigenvalues of this matrix are:

$$\sigma_1 = \frac{1}{2}\left(1 - \alpha h + \theta + \sqrt{(1+\theta-\alpha h)^2 - 4\theta}\right)$$
$$\sigma_2 = \frac{1}{2}\left(1 - \alpha h + \theta - \sqrt{(1+\theta-\alpha h)^2 - 4\theta}\right)$$

- When $(1+\theta-\alpha h)^2 < 4\theta$, then the roots are complex conjugates, and each have the same absolute value $\sqrt{\theta}$

Momentum method - simple example



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

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

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

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

- 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

- 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.

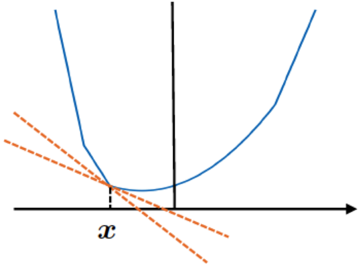
Nesterov's Accelerated Gradient

- 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

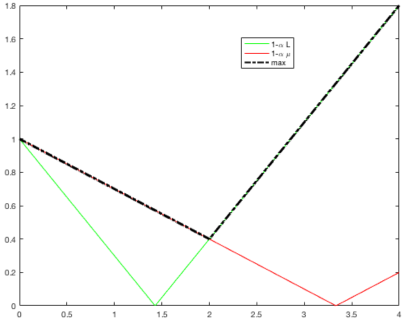


- We will say that g is a subgradient of f at point x if

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

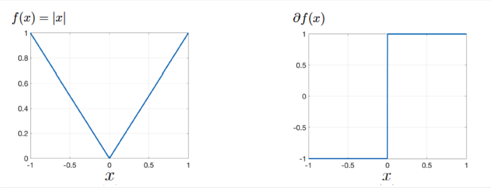
- Set of all gradients is called the sub-differential of f at point x and is denoted by $\partial f(x)$

Example



$$f(x) = \max(g(x), h(x)) \qquad \delta f(x) = \begin{cases} \{g'(x)\} & \text{If } g(x) > h(x) \\ \in [g'(x), h'(x)] & \text{If } g(x) = h(x) \\ \{h'(x)\} & \text{If } g(x) < h(x) \end{cases}$$

Example



$$f(x) = |x| \qquad \delta f(x) = \begin{cases} \{-1\} & \text{If } x < 0 \\ [-1, 1] & \text{If } x = 0 \\ \{1\} & \text{If } x > 0 \end{cases}$$

Subgradients

Behaves very much like a gradient;

- $\partial(\alpha f) = \alpha \partial f$ for $\alpha \geq 0$
- $\partial(f + g) = \partial f + \partial g$
- For convex f, if $g(x) = f(Ax + b)$, $\partial g(x) = A^T \partial f(Ax + b)$

ℓ_1 norm

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

since

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

we have

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

Lets talk about Lasso

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

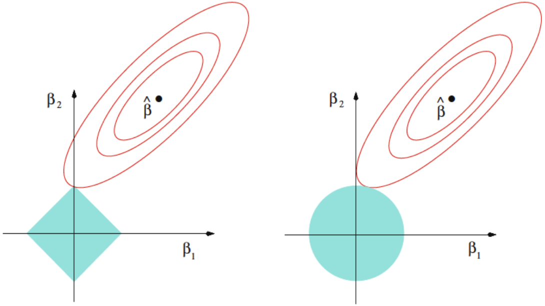


FIGURE 3.11. *Estimation picture for the lasso (left) and ridge regression (right). Shown are contours of the error and constraint functions. The solid blue areas are the constraint regions $|\beta_1| + |\beta_2| \leq t$ and $\beta_1^2 + \beta_2^2 \leq t^2$, respectively, while the red ellipses are the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

Alternative formulation

$$\hat{\boldsymbol{\beta}}_{ridge} = \min_{\boldsymbol{\beta}} (\boldsymbol{y} - \boldsymbol{x}\boldsymbol{\beta})^\top (\boldsymbol{y} - \boldsymbol{x}\boldsymbol{\beta}) \qquad \text{Subject to } \boldsymbol{\beta}^\top \boldsymbol{\beta} \le \tau^2 \tag{2}$$

$$\hat{\boldsymbol{\beta}}_{lasso} = \min_{\boldsymbol{\beta}} (\boldsymbol{y} - \boldsymbol{x}\boldsymbol{\beta})^\top (\boldsymbol{y} - \boldsymbol{x}\boldsymbol{\beta}) \qquad \text{Subject to } \|\boldsymbol{\beta}\|_1 \le \tau \tag{3}$$

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

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

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

- 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 $\sum_k t_k^2 < \infty, \sum_k t_k = \infty$

Convergence

Assume that f convex, $\mathrm{dom}(f) = \mathbb{R}^n$, and also that f is Lipschitz continuous with constant $G > 0$, i.e.,

$$|f(x) - f(y)| \le G\|x - y\|_2 \quad \text{for all } x, y$$

Theorem: For a fixed step size t, subgradient method satisfies

$$\lim_{k\to\infty} f(x_{\text{best}}^{(k)}) \le f^\star + G^2 t/2$$

Theorem: For diminishing step sizes, subgradient method satisfies

$$\lim_{k\to\infty} f(x_{\text{best}}^{(k)}) = f^\star$$

Regularized logistic regression

- Let $\{x_i, y_i\}_{i=1}^n$ with $x_i \in \Re^p$ and $y_i \in \{-1, 1\}$
- The logistic regression loss is:

$$f(\beta) = \sum_i \left(-y_i x_i^T \beta + \log(1 + \exp(x_i^T \beta)) \right)$$

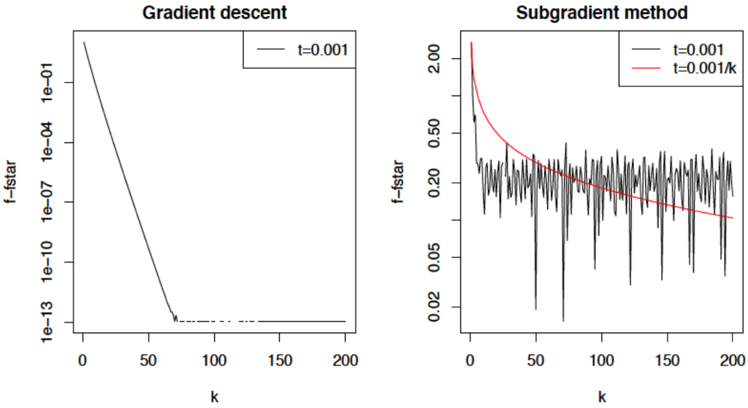
- With lasso regularization we have:

$$\hat{\beta} = \arg\min f(\beta) + \lambda \|\beta\|_1$$

- So, use

$$\Delta_\beta = \underbrace{\sum_i (y_i - p_i(\beta)) x_i}_{gradient} + \underbrace{\partial \|\beta\|_1}_{subgradient}$$

Convergence



Convergence

- Gradient descent takes $1/\epsilon$ time to converge, whereas subgradient descent with variable step-size takes $1/\epsilon^2$ time to converge.

Theorem
For any $k \leq n-1$ and starting point $\beta^{(0)}$, there is a function such that any non-smooth first order method satisfies:

$$f(\beta^{(k)}) - f^* \geq \frac{G\|\beta^{(0)} - \beta^*\|}{2(1+\sqrt{k+1})}$$

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- So it seems like we cant really improve on sub-gradient methods.

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