Lecture: The choice of metric in subgradient methods

http://bicmr.pku.edu.cn/~wenzw/opt-2016-fall.html

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Introduction

- Mirror descent methods
- Convergence analysis
- Mirror descent example
- Variable metric subgradient methods
- AdaGrad
- Example

Mirror descent methods

subgradient method without using Euclidean steps

- let h be a differentiable convex function, then associated Bregman divergence is

$$D_h(y,x) = h(y) - h(x) - \nabla h(x)^T(y-x)$$

- mirror (or non-linear) subgradient method

1. get subgradient $g^{(k)} \in \partial f(x^{(k)})$
2. update

$$x^{(k+1)} = \underset{x \in C}{\operatorname{argmin}} \left\{ g^{(k)T}x + \frac{1}{\alpha_k} D_h(x, x^{(k)}) \right\}$$

generalizes projected subgradient decent (take $h(x) = \frac{1}{2}||x||_2^2$)

Convergence analysis

properties of h required: *strong convexity* with respect to norm $||\cdot||$

$$h(y) \geq h(x) + \nabla h(x)^T(y-x) + \frac{1}{2}||x-y||^2$$

For any $x^* \in C$,

$$\begin{aligned} f(x^{(k)}) - f(x^*) &\leq (g^{(k)})^T(x^{(k)} - x^*) \\ &= (g^{(k)})^T(x^{(k+1)} - x^*) + (g^{(k)})^T(x^{(k)} - x^{(k+1)}) \end{aligned}$$

Use optimality conditions for $x^{(k+1)}$:

$$(\alpha_k g^{(k)} + \nabla h(x^{(k+1)}) - \nabla h(x^{(k)}))^T(y - x^{(k+1)}) \geq 0, \forall y \in C$$

so (take $y = x^*$)

$$g^{(k)T}(x^{(k+1)} - x^*) \leq \frac{1}{\alpha_k}(\nabla h(x^{(k+1)}) - \nabla h(x^{(k)}))^T(x^* - x^{(k+1)})$$

Convergence analysis continued

identity for divergences

$$(\nabla h(x^{(k+1)}) - \nabla h(x^{(k)}))^T (x^* - x^{(k+1)})$$
$$= D_h(x^*, x^{(k)}) - D_h(x^*, x^{(k+1)}) - D_h(x^{(k)}, x^{(k+1)})$$

for any $x^* \in C$,

$$f(x^{(k)}) - f(x^*) \leq g^{(k)T}(x^{(k+1)} - x^*) + g^{(k)T}(x^{(k)} - x^{(k+1)})$$
$$\leq \frac{1}{\alpha_k}\left[D_h(x^*, x^{(k)}) - D_h(x^*, x^{(k+1)})\right] - \frac{1}{\alpha_k} D_h(x^{(k)}, x^{(k+1)})$$
$$+ g^{(k)T}(x^{(k)} - x^{(k+1)})$$

apply Fenchel-Young inequality ($x^T y \leq \frac{1}{2\alpha}||x||^2 + \frac{\alpha}{2}||y||_*^2$)

$$\leq \frac{1}{\alpha_k}\left[D_h(x^*, x^{(k)}) - D_h(x^*, x^{(k+1)})\right] - \frac{1}{\alpha_k} D_h(x^{(k)}, x^{(k+1)})$$
$$+ \frac{\alpha_k}{2}||g^{(k)}||_*^2 + \frac{1}{2\alpha_k}||x^{(k)} - x^{(k+1)}||^2$$
$$\leq \frac{1}{\alpha_k}\left[D_h(x^*, x^{(k)}) - D_h(x^*, x^{(k+1)})\right] + \frac{\alpha_k}{2}||g^{(k)}||_*^2$$

Convergence guarantees

with fixed stepsize $\alpha_k = \alpha$,

$$\frac{1}{k}\sum_{i=1}^{k} f(x^{(i)}) - f(x^*) \le \frac{1}{\alpha k} D_h(x^*, x^{(1)}) + \frac{\alpha}{2k} \max_i ||g^{(i)}||_*^2$$

in general, converges if

- $D_h(x^*, x^{(1)}) < \infty$
- $\sum_k \alpha_k = \infty$ and $\alpha_k \to 0$
- for all $g \in \partial f(x)$ and $x \in C$, $||g||_* \le G$ for some $G < \infty$

Mirror descent examples

- Usual (projected) subgradient descent: $h(x) = \frac{1}{2}||x||_2^2$
- With constrains of simplex, $C = \{x \in R_+^n | \mathbf{1}^T x = 1\}$,use negative entropy

$$h(x) = \sum_{i=1}^{n} x_i \log x_i$$

1. Strongly convex with respect to l_1-norm
2. With $x^{(1)} = 1/n$, have $D_h(x^*, x^{(1)}) \leq \log n$ for $x^* \in C$
3. If $G_\infty \geq ||g||_\infty$ for $g \in \partial f(x)$ for $x \in C$,

$$f_{best}^{(k)} - f^* \leq \frac{\log n}{\alpha k} + \frac{\alpha}{2k} G_\infty$$

4. Can be much better than regular subgradient decent...

Example

Robust regression problem (an LP):

$$\text{minimize } f(x) = ||Ax - b||_1 = \sum_{i=1}^{m} |a_i^T x - b_i|$$

$$\text{subject to } x \in C = \{x \in R_+^n | 1^T x = 1\}$$

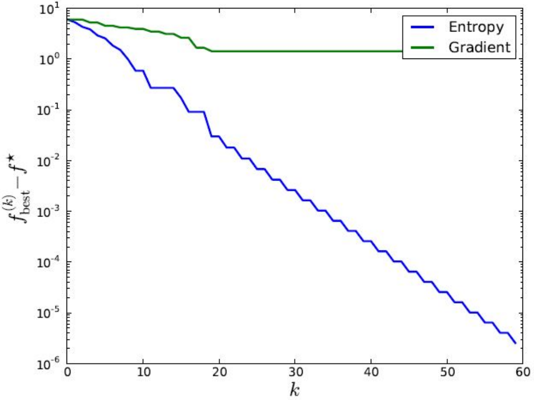
subgradient of objective is $g = \sum_{i=1}^{m} sign(a_i^T x - b_i)a_i$

- Projected subgradient update $(h(x) = (1/2)||x||_2^2)$:
- Mirror descent update $(h(x) = \sum_{i=1}^{n} x_i \log x_i)$:

$$x_i^{(k+1)} = \frac{x_i(k) \exp(-\alpha g_i^{(k)})}{\sum_{j=1}^{n} x_j^{(k)} \exp(-\alpha g_j^{(k)})}$$

Example

Robust regression problem with $a_i \sim N(0, I_{n\times n})$ and $b_i = (a_{i,1} + a_{i,2})/2 + \varepsilon_i$ where $\varepsilon_i \sim N(0, 10^{-2}), m = 20, n = 3000$



stepsizes chosen according to best bounds (but still sensitive to stepsize choice)

Variable metric subgradient methods

subgradient method with variable metric $H_k \succ 0$:

1. get subgradient $g^{(k)} \in \partial f(x^{(k)})$
2. update (diagonal) metric H_k
3. update $x^{(k+1)} = x^{(k)} - H_k^{-1} g^{(k)}$

- matrix H_k generalizes step-length α_k

there are many such methods (Ellipsoid method, AdaGrad,...)

Variable metric projected subgradient method

same, with projection carried out in the H_k metric:

1. get subgradient $g^{(k)} \in \partial f(x^{(k)})$
2. update (diagonal) metric H_k
3. update $x^{(k+1)} = P_{\chi}^{H_k}(x^{(k)} - H_k^{-1} g^{(k)})$

where

$$\Pi_{\chi}^{H}(y) = \underset{x \in \chi}{\operatorname{argmin}} \, ||x - y||_H^2$$

and $||x||_H = \sqrt{x^T H x}$.

Convergence analysis

since $\Pi_{\chi}^{H_k}$ is non-expansive in the $||\cdot||_{H_k}$ norm, we get

$$\begin{aligned} ||x^{(k+1)} - x^*||_{H^{(k)}}^2 &= ||P_{\chi}^{H_k}(x^{(k)} - H_k^{-1} g^{(k)}) - P_{\chi}^{H_k}(x^*)||_{H_k}^2 \\ &\leq ||x^{(k)} - H_k^{-1} g^{(k)} - x^*||_{H_k}^2 \\ &= ||x^{(k)} - x^*||_{H_k}^2 - 2(g^{(k)})^T(x^{(k)} - x^*) + ||g^{(k)}||_{H_k^{-1}}^2 \\ &\leq ||x^{(k)} - x^*||_{H_k}^2 - 2(f(x^{(k)}) - f^*) + ||g^{(k)}||_{H_k^{-1}}^2. \end{aligned}$$

using $f^* = f(x^*) \geq f(x^{(k)}) + g^{(k)T}(x^* - x^{(k)})$

apply recursively, use

$$\sum_{i=1}^{k} (f(x^{(i)}) - f^*) \geq k(f_{best}^{(k)} - f^*)$$

and rearrange to get

$$f_{best}^{(k)} - f^* \leq \frac{||x^{(1)} - x^*||_{H_1}^2 + \sum_{i=1}^{k} ||g^{(i)}||_{H_i^{-1}}^2}{2k} + \frac{\sum_{i=2}^{k} \left(||x^{(i)} - x^*||_{H_i}^2 - ||x^{(i)} - x^*||_{H_{i-1}}^2 \right)}{2k}$$

numeration of additional term can be bounded to get estimates

- for general $H_k = \mathrm{diag}(h_k)$

$$f_{best}^{(k)} - f^* \leq \frac{R_\infty^2 ||H_1||_1 + \sum_{i=1}^k ||g^{(i)}||_{H_i^{-1}}^2}{2k} + \frac{R_\infty^2 \sum_{i=2}^k ||H_i - H_{i-1}||_1}{2k}$$

- $H_k = \mathrm{diag}(h_k)$ with $h_i \geq h_{i-1}$ for all i

$$f_{best}^{(k)} - f^* \leq \frac{\sum_{i=1}^k ||g^{(i)}||_{H_i^{-1}}^2}{2k} + \frac{R_\infty^2 ||h_k||_1}{2k}$$

where $\max_{1 \leq i \leq k} ||x^{(i)} - x^*||_\infty \leq R_\infty$

converges if

- $R_\infty < \infty$ (e.g. if χ is compact)
- $\sum_{i=1}^{k} ||g^{(i)}||^2_{H_i^{-1}}$ grows slower than k
- $\sum_{i=2}^{k} ||H_i - H_{i-1}||_1$ grows slower than k **or**
  $h_i \geq h_{i-1}$ for all i and $||h_k||_1$ grows slower than k

AdaGrad

AdaGrad-adaptive subgradient method

1. get subgradient $g^{(k)} \in \partial f(x^{(k)})$
2. choose metric H_k :
   - set $S_k = \sum_{i=1}^{k} \operatorname{diag}(g^{(i)})^2$
   - set $H_k = \frac{1}{\alpha} S_k^{\frac{1}{2}}$
3. update $x^{(k+1)} = P_{\mathcal{X}}^{H_k}(x^{(k)} - H_k^{-1} g^{(k)})$

where $\alpha > 0$ is step-size

AdaGrad-motivation

- for fixed $H_k = H$ we have estimate:

$$f_{best}^{(k)} - f^* \leq \frac{1}{2k}(x^{(1)} - x^*)^T H(x^{(1)} - x^*) + \frac{1}{2k}\sum_{i=1}^{k} ||g^{(i)}||_{H^{-1}}^2$$

- **idea**: Choose *diagonal* $H_k \succ 0$ that minimizes this estimate in hindsight:

$$H_k = \underset{h}{\operatorname{argmin}} \max_{x,y \in C}(x-y)^T \operatorname{diag}(h)(x-y) + \sum_{i=1}^{k} ||g^{(i)}||_{\operatorname{diag}(h)^{-1}}^2$$

- optimal $H_k = \frac{1}{R_\infty}\operatorname{diag}\left(\sqrt{\sum_{i=1}^{k}(g_1^{(i)})^2}, \ldots, \sqrt{\sum_{i=1}^{k}(g_n^{(i)})^2}\right)$
- **intuition**: adapt step-length based on historical step lengths

AdaGrad- convergence

by construction, $H_i = \frac{1}{\alpha}\mathrm{diag}(h_i)$ and $h_i \geq h_{i-1}$, so

$$\begin{aligned} f_{best}^{(k)} - f^* &\leq \frac{1}{2k}\sum_{i=1}^{k} ||g^{(i)}||^2_{H_i^{-1}} + \frac{1}{2k\alpha} R_\infty^2 ||h_k||_1 \\ &\leq \frac{\alpha}{k}||h_k||_1 + \frac{1}{2k\alpha} R_\infty^2 ||h_k||_1 \end{aligned}$$

(second line is a theorem)
also have (with $\alpha = R_\infty^2$) and for compact sets C

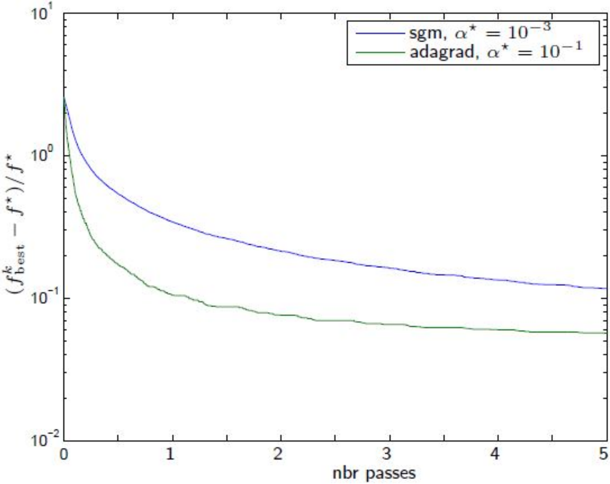
$$f_{best}^{(k)} - f^* \leq \frac{2}{k} \inf_{h \geq 0} \left\{ \sup_{x,y \in C} (x-y)^T \mathrm{diag}(h)(x-y) + \sum_{i=1}^{k} ||g^{(i)}||^2_{\mathrm{diag}(h)^{-1}} \right\}$$

Example

Classification problem:

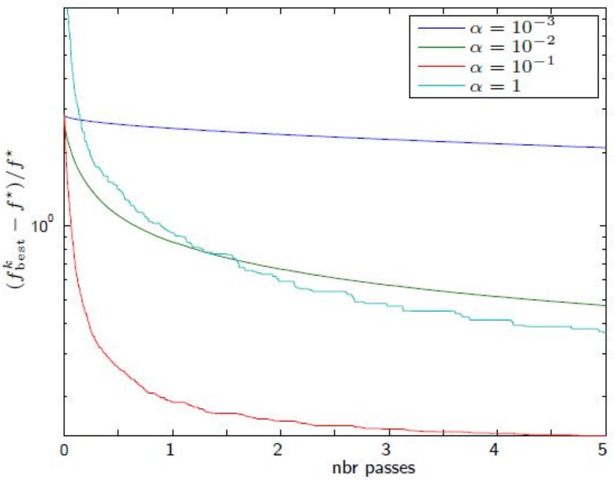
- **Data**: $\{a_i, b_i\}, i = 1, ..., 50000$
  - $a_i \in \mathbf{R}^{1000}$
  - $b \in \{-1, 1\}$
  - Data created with 5% mis-classifications w.r.t $\omega = 1, \nu = 0$
- **Objective**: find classifiers $\omega \in \mathbf{R}^{1000}$ and $\nu \in \mathbf{R}$ such that
  - $a_i^T \omega + \nu > 1$ if $b = 1$
  - $a_i^T \omega + \nu < 1$ if $b = -1$
- **Optimization method**:
  - Minimize hinge-loss: $\sum_i \max(0, 1 - b_i(a_i^T \omega + \nu))$
  - Choose example uniformly at random, take sub-gradient step w.r.t that example

Best subgradient method vs best AdaGrad



Often best AdaGrad performs better than best subgradient method

AdaGrad with different step-sizes α:



Sensitive to step-size selection (like standard subgradient method)