Statistical Models & Computing Methods

Lecture 2: Gradient Methods

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- We now focus on numerical solutions for unconstrained optimization problems

$$\text{minimize} \quad f(x)$$

where $f : \mathbb{R}^n \to \mathbb{R}$ is twice differentiable

- Descent method. We can set up a sequence

$$x^{(k+1)} = x^{(k)} + t^{(k)} \Delta x^{(k)}, \quad t^{(k)} > 0$$

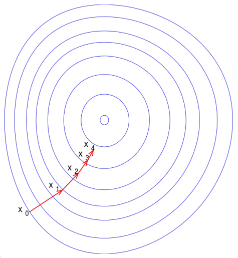
such that $f(x^{(k+1)}) < f(x^{(k)}), \quad k = 0, 1, \dots,$

- $\Delta x^{(k)}$ is called the search direction; $t^{(k)}$ is called the step size or learning rate in machine learning.

A reasonable choice for the search direction is the negative gradient, which leads to gradient descent methods

$$x^{(k+1)} = x^{(k)} - t^{(k)}\nabla f(x^{(k)}), \quad k = 0, 1, \dots$$

- step size $t^{(k)}$ can be constant or determined by line search
- every iteration is cheap, does not require second derivatives



- First-order Taylor expansion

$$f(x+v) \approx f(x) + \nabla f(x)^T v$$

- v is a descent direction iff $\nabla f(x)^T v < 0$
- Negative gradient is the steepest descent direction with respect to the Euclidean norm.

$$\frac{-\nabla f(x)}{\|\nabla f(x)\|_2} = \arg\min_v \{\nabla f(x)^T v \mid \|v\|_2 = 1\}$$

- Consider the second-order Taylor expansion of f at x,

$$\begin{aligned} f(x+v) &\approx f(x) + \nabla f(x)^T v + \frac{1}{2} v^T \nabla^2 f(x) v \\ &\triangleq \tilde{f}(x) \end{aligned}$$

- We find the optimal direction v by minimizing $\tilde{f}(x)$ with respect to v

$$v = -[\nabla^2 f(x)]^{-1} \nabla f(x)$$

- If $\nabla^2 f(x) \succeq 0$ (e.g., convex functions)

$$\nabla f(x)^T v = -\nabla f(x)^T [\nabla^2 f(x)]^{-1} \nabla f(x) < 0$$

when $\nabla f(x) \neq 0$

- The search direction in Newton's method can also be viewed as a steepest descent direction, but with a different metric
- In general, given a positive definite matrix P, we can define a quadratic norm

$$\|v\|_P = (v^T P v)^{1/2}$$

- Similarly, we can show that $-P^{-1}\nabla f(x)$ is the steepest descent direction w.r.t. the quadratic norm $\|\cdot\|_P$

$$\text{minimize } \nabla f(x)^T v, \quad \text{subject to } \|v\|_P = 1$$

- When P is the Hessian $\nabla^2 f(x)$, we get Newton's method

- Computing the Hessian and its inverse could be expensive, we can approximate it with another positive definite matrix $M \succ 0$ which is easier to use
- Update $M^{(k)}$ to learn about the curvature of f in the search direction and maintain a secant condition

$$\nabla f(x^{(k+1)}) - \nabla f(x^{(k)}) = M^{(k+1)}(x^{(k+1)} - x^{(k)})$$

- Rank-one update

$$\begin{aligned}
\Delta x^{(k)} &= x^{(k+1)} - x^{(k)} \\
y^{(k)} &= \nabla f(x^{(k+1)}) - \nabla f(x^{(k)}) \\
v^{(k)} &= y^{(k)} - M^{(k)}\Delta x^{(k)} \\
M^{(k+1)} &= M^{(k)} + \frac{v^{(k)}(v^{(k)})^T}{(v^{(k)})^T \Delta x^{(k)}}
\end{aligned}$$

- Easy to compute the inverse of matrices for low rank updates by **Sherman-Morrison-Woodbury formula**

$$(A + UCV)^{-1} = A^{-1} - A^{-1}U(C^{-1} + VA^{-1}U)^{-1}VA^{-1}$$

  where $A \in \mathbb{R}^{n\times n}, U \in \mathbb{R}^{n\times d}, C \in \mathbb{R}^{d\times d}, V \in \mathbb{R}^{d\times n}$

- Another popular rank-two update method: the BFGS (Broyden-Fletcher-Goldfarb-Shanno) method

$$M^{(k+1)} = M^{(k)} + \frac{y^{(k)}(y^{(k)})^T}{(y^{(k)})^T\Delta x^{(k)}} - \frac{M^{(k)}\Delta x^{(k)}(M^{(k)}\Delta x^{(k)})^T}{(\Delta x^{(k)})^T M^{(k)}\Delta x^{(k)}}$$

- In the frequentist framework, we typically perform statistical inference by maximizing the log-likelihood $L(\theta)$, or equivalently minimizing negative log-likelihood, which is also known as the energy function
- Some notations we introduced before
  - Score function: $s(\theta) = \nabla_\theta L(\theta)$
  - Observed Fisher information: $J(\theta) = -\nabla_\theta^2 L(\theta)$
  - Fisher information: $\mathcal{I}(\theta) = \mathbb{E}(-\nabla_\theta^2 L(\theta))$
- Newton's method for MLE:

$$\theta^{(k+1)} = \theta^{(k)} + (J(\theta^{(k)}))^{-1} s(\theta^{(k)})$$

Fisher Scoring Algorithm

- If we use the Fisher information instead of the observed information, the resulting method is called the *Fisher scoring* algorithm

$$\theta^{(k+1)} = \theta^{(k)} + (\mathcal{I}(\theta^{(k)}))^{-1} s(\theta^{(k)})$$

- It seems that the Fisher scoring algorithm is less sensitive to the initial guess. On the other hand, the Newton's method tends to converge faster
- For exponential family models with natural parameters and generalized linear models (GLMs) with canonical links, the two methods are identical

- A generalized linear model (GLM) assumes a set of independent random variables $Y_1, \ldots, Y_n$ that follow exponential family distributions of the same form

$$p(y_i|\theta_i) = \exp\left(y_i b(\theta_i) + c(\theta_i) + d(y_i)\right)$$

- The parameters θ_i are typically not of direct interest. Instead, we usually assume that the expectation of Y_i can be related to a vector of parameters β via a transformation (link function)

$$E(Y_i) = \mu_i, \quad g(\mu_i) = x_i^T \beta$$

where x_i is the observed covariates for y_i.

- Using the link function, we can now write the score function in terms of β
- Let $g(\mu_i) = \eta_i$, we can show that for jth parameter

$$s(\beta_j) = \sum_{i=1}^{n} \frac{(y_i - \mu_i)x_{ij}}{\mathbb{V}\mathrm{ar}(Y_i)} \frac{\partial \mu_i}{\partial \eta_i}$$

  where $\partial \mu_i / \partial \eta_i$ depends on the link function we choose
- It is also easy to show that the Fisher information matrix is

$$\begin{aligned}\mathcal{I}(\beta_j, \beta_k) &= \mathbb{E}(s(\beta_j)s(\beta_k)) \\ &= \sum_{i=1}^{n} \frac{x_{ij}x_{ik}}{\mathbb{V}\mathrm{ar}(Y_i)} \left(\frac{\partial \mu_i}{\partial \eta_i}\right)^2\end{aligned}$$

- Note that the Fisher information matrix can be written as

$$\mathcal{I}(\beta) = X^T W X$$

where W is the $n \times n$ diagonal matrix with elements

$$w_{ii} = \frac{1}{\mathbb{V}\mathrm{ar}(Y_i)} \left(\frac{\partial \mu_i}{\partial \eta_i} \right)^2$$

- Rewriting Fisher scoring algorithm for updating β as

$$\mathcal{I}(\beta^{(k)})\beta^{(k+1)} = \mathcal{I}(\beta^{(k)})\beta^{(k)} + s(\beta^{(k)})$$

- After few simple steps, we have

$$X^T W^{(k)} X \beta^{(k+1)} = X^T W^{(k)} Z^{(k)}$$

where

$$z_i^{(k)} = \eta_i^{(k)} + (y_i - \mu_i^{(k)}) \frac{\partial \eta_i^{(k)}}{\partial \mu_i^{(k)}}$$

- Therefore, we can find the next estimate as follows

$$\beta^{(k+1)} = (X^T W^{(k)} X)^{-1} X^T W^{(k)} Z^{(k)}$$

- The above estimate is similar to the weighted least square estimate, except that the weights W and the response variable Z change from one iteration to another
- We iteratively estimate β until the algorithm converges

- Recall that the Log-likelihood for logistic regression is

$$L(Y|p) = \sum_{i=1}^{n} y_i \log \frac{p_i}{1-p_i} + \log(1-p_i)$$

- The natural parameters are $\theta_i = \log \frac{p_i}{1-p_i}$. We use $g(x) = \log \frac{x}{1-x}$ as the link function, $\theta_i = g(p_i) = x_i^T \beta$
- We now write the log-likelihood as follows

$$L(\beta) = Y^T X\beta - \sum_{i=1}^{n} \log(1 + \exp(x_i^T \beta))$$

- The score function is

$$s(\beta) = X^T(Y-p), \quad p = \frac{1}{1+\exp(-X\beta)}$$

Example: Logistic Regression

- The observed Fisher information matrix is

$$J(\beta) = X^T W X$$

where W is a diagonal matrix with elements

$$w_{ii} = p_i(1 - p_i)$$

- Note that $J(\beta)$ does not depend on Y, meaning that it is also the Fisher information matrix $\mathcal{I}(\beta) = J(\beta)$
- Newton's update

$$\beta^{(k+1)} = \beta^{(k)} + \left(X^T W^{(k)} X\right)^{-1} \left(X^T (Y - p^{(k)})\right)$$

- While gradient descent is simple and intuitive, it has many problems as well.
  - Saddle-point problem
  - Not applicable to non-differential objectives
  - Could be slow
  - How to scale to big data problems
- In what follows, we will discuss some advanced techniques that can alleviate these problems

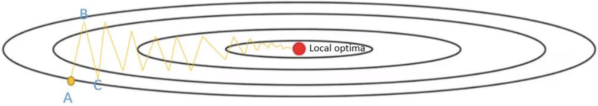
- Introduced in 1964 by Polyak, momentum method is a technique that can accelerate gradient descent by taking accounts of previous gradients in the update rule at each iteration.

$$
\begin{aligned}
m^{(k)} &= \mu m^{(k-1)} + (1-\mu)\nabla f(x^{(k)}) \\
x^{(k+1)} &= x^{(k)} - \alpha m^{(k)}
\end{aligned}
$$

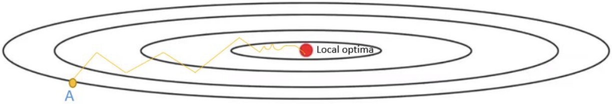
  where $0 \leq \mu < 1$
- When $\mu = 0$, gradient descent is recovered.

How Does Momentum Work?

- The vanilla gradient descent may suffer from oscillations when the magnitudes of gradient varies a lot across different directions.



- Using the exponential weighted gradient (momentum), those oscillations are more likely to be damped out, resulting in faster rate of convergence.



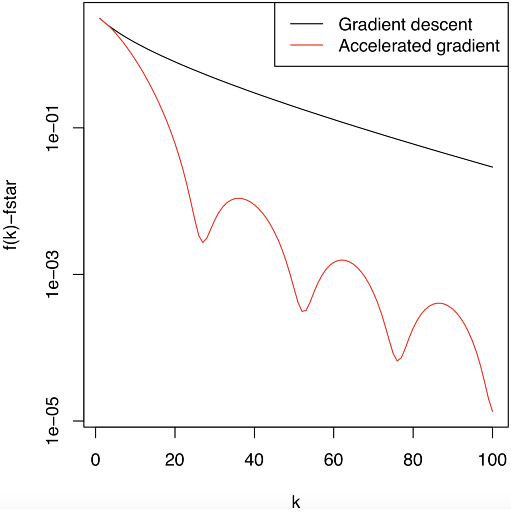
- Choose any initial $x^{(0)} = x^{(-1)}$, $\forall\, k = 1, 2, 3, \ldots$

$$y = x^{(k-1)} + \frac{k-2}{k+1}(x^{(k-1)} - x^{(k-2)})$$
$$x^{(k)} = y - t_k \nabla f(y)$$

- The first two steps are the usually gradient updates
- After that, $y = x^{(k-1)} + \frac{k-2}{k+1}(x^{(k-1)} - x^{(k-2)})$ carries some "momentum" from previous iterations, and $x^{(k)} = y - t_k \nabla f(y)$ uses *lookahead* gradient at y.

Example

Logistic regression



Assumptions

- f is convex and continuously differentiable on $\mathbb{R}^n$
- $\nabla f(x)$ is L-Lipschitz continuous w.r.t Euclidean norm: for any $x, y \in \mathbb{R}^n$

$$\|\nabla f(x) - \nabla f(y)\| \leq L\|x - y\|$$

- optimal value $f^* = \inf_x f(x)$ is finite and attained at x^*.

Theorem: Gradient descent with $0 < t \leq 1/L$ satisfies

$$f(x^{(k)}) - f^* \leq \frac{1}{2kt}\|x^{(0)} - x^*\|^2$$

Some Useful Lemma and Strong Convexity

- If f is L-Lipschitz, then for any $x, y \in \mathbb{R}^n$

$$f(y) \leq f(x) + \nabla f(x)^T(y-x) + \frac{L}{2}\|y-x\|^2$$

- If f is differentiable and m-strongly convex, then

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

  If $m = 0$, we cover the standard(weak) convexity
- In other words, f is *sandwiched* between two quadratic functions

Proof

- If $x^+ = x - t\nabla f(x)$ and $0 < t \leq 1/L$

$$\begin{aligned} f(x^+) &\leq f(x) - t\|\nabla f(x)\|^2 + \frac{t^2 L}{2}\|\nabla f(x)\|^2 \\ &\leq f(x) - \frac{t}{2}\|\nabla f(x)\|^2 \end{aligned}$$

- From convexity

$$f(x) \leq f^* + \nabla f(x)^T(x - x^*) - \frac{m}{2}\|x - x^*\|^2$$

- Add the above two inequalities

$$f(x^+) - f^* \leq \nabla f(x)^T(x - x^*) - \frac{t}{2}\|\nabla f(x)\|^2 - \frac{m}{2}\|x - x^*\|^2$$

Proof

- Continue ...

$$
\begin{aligned}
&\le \frac{1}{2t}(\|x - x^*\|^2 - \|x^+ - x^*\|^2) - \frac{m}{2}\|x - x^*\|^2 \\
&= \frac{1}{2t}\left((1 - mt)\|x - x^*\|^2 - \|x^+ - x^*\|^2\right) \qquad (1) \\
&\le \frac{1}{2t}(\|x - x^*\|^2 - \|x^+ - x^*\|^2) \qquad (2)
\end{aligned}
$$

- For gradient descent updates

$$
\begin{aligned}
\sum_{i=1}^{k}(f(x^{(i)}) - f^*) &\le \frac{1}{2t}\sum_{i=1}^{k}(\|x^{(i-1)} - x^*\|^2 - \|x^{(i)} - x^*\|^2) \\
&= \frac{1}{2t}(\|x^{(0)} - x^*\|^2 - \|x^{(k)} - x^*\|^2)
\end{aligned}
$$

Proof

- Since $f(x^{(i)})$ is non-increasing

$$f(x^{(k)}) - f^* \le \frac{1}{2kt}\|x^{(0)} - x^*\|^2$$

- If f is m-strongly convex, and $m > 0$, from (1)

$$\|x^{(i)} - x^*\|^2 \le (1 - mt)\|x^{(i-1)} - x^*\|^2, \quad \forall i = 1, 2, \ldots$$

- Therefore

$$\|x^{(k)} - x^*\|^2 \le (1 - mt)^k\|x^{(0)} - x^*\|^2$$

$i.e.$, linear convergence if f is strongly convex ($m > 0$)

- First order method: any iterative algorithm that selects $x^{(k+1)}$ in the set

$$x^{(0)} + \operatorname{span}\{\nabla f(x^{(0)}), \nabla f(x^{(1)}), \ldots, \nabla f(x^{(k)})\}$$

- **Theorem** (Nesterov): for every integer $k \leq (n-1)/2$ and every $x^{(0)}$, there exist functions that satisfy the assumptions such that for any first-order method

$$f(x^{(k)}) - f^* \geq \frac{3}{32} \frac{L\|x_0 - x^*\|^2}{(k+1)^2}$$

- Therefore, $1/k^2$ is the best convergence rate for all first-order methods.

- Accelerated gradient descent with fixed step size $t \leq 1/L$ satisfies
$$f(x^{(k)}) - f^* \leq \frac{2\|x^{(0)} - x^*\|^2}{t(k+1)^2}$$
- Nesterov's accelerated gradient (**NAG**) descent achieve the oracle convergence rate of first-order methods!

Reformulation of NAG

- Initialize $x^{(0)} = u^{(0)}$, and for $k = 1, 2, \dots$

$$
\begin{aligned}
y &= (1-\theta_k)x^{(k-1)} + \theta_k u^{(k-1)} \\
x^{(k)} &= y - t_k \nabla f(y) \\
u^{(k)} &= x^{(k-1)} + \frac{1}{\theta_k}(x^{(k)} - x^{(k-1)})
\end{aligned}
$$

  with $\theta_k = 2/(k+1)$.

- This is equivalent to the formulation of NAG presented earlier (slide 5), and makes convergence analysis easier

Proof

- If $y = (1-\theta)x + \theta u$, $x^+ = y - t\nabla f(y)$, and $0 < t \leq 1/L$

$$f(x^+) \leq f(y) + \nabla f(y)^T(x^+ - y) + \frac{1}{2t}\|x^+ - y\|^2$$

- From convexity, $\forall z \in \mathbb{R}^n$

$$f(y) \leq f(z) + \nabla f(y)^T(y - z)$$

- Add these together

$$f(x^+) \leq f(z) + \frac{1}{t}(x^+ - y)(z - x^+) + \frac{1}{2t}\|x^+ - y\|^2 \qquad (3)$$

Proof

- Let $u^+ = x + \frac{1}{\theta}(x^+ - x)$, using bound (3) at $z = x$ and $z = x^*$

$$
\begin{aligned}
f(x^+) &- f^* - (1-\theta)(f(x) - f^*) \\
&\leq \frac{1}{t}(x^+ - y)^T(\theta x^* + (1-\theta)x - x^+) + \frac{1}{2t}\|x^+ - y\|^2 \\
&= \frac{\theta^2}{2t}\left(\|u - x^*\|^2 - \|u^+ - x^*\|^2\right)
\end{aligned}
$$

- *i.e.*, at iteration k

$$
\begin{aligned}
&\frac{t}{\theta_k^2}(f(x^{(k)}) - f^*) + \frac{1}{2}\|u^{(k)} - x^*\|^2 \\
&\quad \leq \frac{(1-\theta_k)t}{\theta_k^2}(f(x^{(k-1)}) - f^*) + \frac{1}{2}\|u^{(k-1)} - x^*\|^2
\end{aligned}
$$

Proof

- Using $(1-\theta_i)/\theta_i^2 \le 1/\theta_{i-1}^2$, and iterating this inequlity

$$\begin{aligned}
&\frac{t}{\theta_k^2}(f(x^{(k)}) - f^*) + \frac{1}{2}\|u^{(k)} - x^*\|^2 \\
&\quad \le \frac{(1-\theta_1)t}{\theta_1^2}(f(x^{(0)}) - f^*) + \frac{1}{2}\|u^{(0)} - x^*\|^2 \\
&\quad = \frac{1}{2}\|x^{(0)} - x^*\|^2
\end{aligned}$$

- Therefore

$$f(x^{(k)}) - f^* \le \frac{\theta_k^2}{2t}\|x^{(0)} - x^*\|^2 = \frac{2}{t(k+1)^2}\|x^{(0)} - x^*\|^2$$

- Although the algebraic manipulations of the proof is beautiful, the acceleration effect in NAG has been mysterious and hard to understand
- Recent works reinterpreted the NAG algorithm from different point of views, including Zhu et al (2017) and Su et al (2014)
- Here we introduce the ODE explanation from Su et al (2014)

- Su et al (2014) proposed an ODE based explanation where NAG can be viewed as a discretization of the following ordinary differential equation

$$\ddot{X} + \frac{3}{t}\dot{X} + \nabla f(X) = 0, \quad t > 0 \tag{4}$$

with initial conditions $X(0) = x^{(0)}, \dot{X}(0) = 0$.

- **Theorem** (Su et al): For any $f \in \mathcal{F}_\infty \triangleq \cap_{L>0}\mathcal{F}_L$ and any $x^{(0)} \in \mathbb{R}^n$, the ODE (4) with initial conditions $X(0) = x^{(0)}, \dot{X}(0) = 0$ has a unique global solution $X \in C^2((0,\infty);\mathbb{R}^n) \cap C^1([0,\infty);\mathbb{R}^n)$.

- **Theorem** (Su et al): For any $f \in \mathcal{F}_\infty$, let $X(t)$ be the unique global solution to (4) with initial conditions $X(0) = x^{(0)}, \dot{X}(0) = 0$. For any $t > 0$,

$$f(X(t)) - f^* \leq \frac{2\|x^{(0)} - x^*\|^2}{t^2}$$

- Consider the energy functional defined as

$$\mathcal{E}(t) \triangleq t^2(f(X(t)) - f^*) + 2\|X + \frac{t}{2}\dot{X} - x^*\|^2$$

- The derivative of the energy function is

$$\dot{\mathcal{E}} = 2t(f(X) - f^*) + t^2\langle \nabla f, \dot{X}\rangle + 4\langle X + \frac{t}{2}\dot{X} - x^*, \frac{3}{2}\dot{X} + \frac{t}{2}\ddot{X}\rangle$$

- Substituting $3\dot{X}/2 + t\ddot{X}/2$ with $-t\nabla f(X)/2$

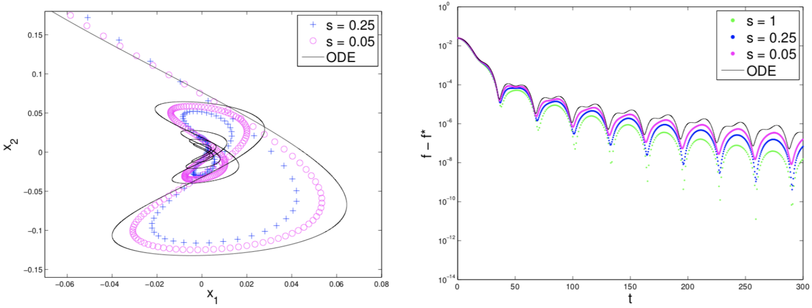
$$\begin{aligned}\dot{\mathcal{E}} &= 2t(f(X) - f^*) + 4\langle X - x^*, -\frac{t}{2}\nabla f(X)\rangle \\ &= 2t(f(X) - f^*) - 2t\langle X - x^*, \nabla f(X)\rangle \\ &\leq 0\end{aligned}$$

  where the last inequality follows from the convexity of f.
- Therefore,

$$f(X(t) - f^*) \leq \mathcal{E}(t)/t^2 \leq \mathcal{E}(0)/t^2 = \frac{2\|x^{(0)} - x^*\|^2}{t^2}$$

Example

$$f(x) = 0.02x_1^2 + 0.005x_2^2, \quad x^{(0)} = (1,1)$$



The objective in many unconstrained optimization problems can be split in two components

$$\text{minimize } f(x) = g(x) + h(x)$$

- g is convex and differentiable on $\mathbb{R}^n$
- h is convex and simple, but may be non-differentiable

Examples

- Indicator function of closed convex set C

$$h(x) = \mathbf{1}_C(x) = \begin{cases} 0, & x \in C \\ +\infty, & x \notin C \end{cases}$$

- L_1 regularization (LASSO): $h(x) = \|x\|_1$

The **proximal mapping** (or **proximal-operator**) of a convex function h is defined as

$$\mathrm{prox}_h(x) = \arg\min_u \left(h(u) + \frac{1}{2}\|u - x\|_2^2 \right)$$

Examples

- $h(x) = 0$: $\mathrm{prox}_h(x) = x$
- $h(x) = \mathbf{1}_C(x)$: prox_h is projection on C

$$\mathrm{prox}_h(x) = \arg\min_{u \in C} \|u - x\|_2^2 = P_C(x)$$

- $h(x) = \|x\|_1$: prox_h is the "soft-threshold" (shrinkage) operation

$$\mathrm{prox}_h(x)_i = \begin{cases} x_i - 1 & x_i \geq 1 \\ 0 & |x_i| \leq 1 \\ x_i + 1 & x_i \leq -1 \end{cases}$$

- **Proximal gradient algorithm**

$$x^{(k+1)} = \mathrm{prox}_{t_k h}(x^{(k)} - t_k \nabla g(x^{(k)})), \quad k = 0, 1, \ldots$$

- Interpretation. If $x^+ = \mathrm{prox}_{th}(x - t\nabla g(x))$, from the definition of proximal mapping

$$\begin{aligned} x^+ &= \arg\min_u \left(h(u) + \frac{1}{2t}\|u - x + t\nabla g(x)\|_2^2 \right) \\ &= \arg\min_u \left(h(u) + g(x) + \nabla g(x)^T (u - x) + \frac{1}{2t}\|u - x\|_2^2 \right) \end{aligned}$$

- x^+ minimizes $h(u)$ plus a simple quadratic local approximation of $g(u)$ around x

- **Gradient Descent**: special case with $h(x) = 0$

$$x^+ = x - t\nabla g(x)$$

- **Projected Gradient Descent**: special case with $h(x) = \mathbf{1}_C(x)$

$$x^+ = P_C(x - t\nabla g(x))$$

- **ISTA** (Iterative Shrinkage-Thresholding Algorithm): special case with $h(x) = \|x\|_1$

$$x^+ = \mathcal{S}_t(x - t\nabla g(x))$$

where

$$\mathcal{S}_t(u) = (|u| - t)_+ \mathrm{sign}(u)$$

- If h is convex and closed,

$$\mathrm{prox}_h(x) = \arg\min_u \left(h(u) + \frac{1}{2}\|u - x\|_2^2 \right)$$

exists and is unique for all x. Moreover, it has the following useful properties

$$\begin{aligned} u = \mathrm{prox}_h(x) &\iff x - u \in \partial h(u) \\ &\iff h(z) \geq h(u) + (x-u)^T(z-u),\ \forall z \end{aligned}$$

- Proximal gradient descent has the same convergence rate as gradient descent when $0 < t \leq 1/L$

$$f(x^{(k)}) - f^* \leq \frac{1}{2kt}\|x^{(0)} - x^*\|_2^2$$

- Similarly, we can apply Nesterov's acceleration for proximal gradient descent. Choose any initial $x^{(0)} = x^{(-1)}$, $\forall\ k = 1, \ldots$

$$y = x^{(k-1)} + \frac{k-2}{k+1}(x^{(k-1)} - x^{(k-2)})$$
$$x^{(k)} = \mathrm{prox}_{t_k h}(y - t_k \nabla g(y))$$

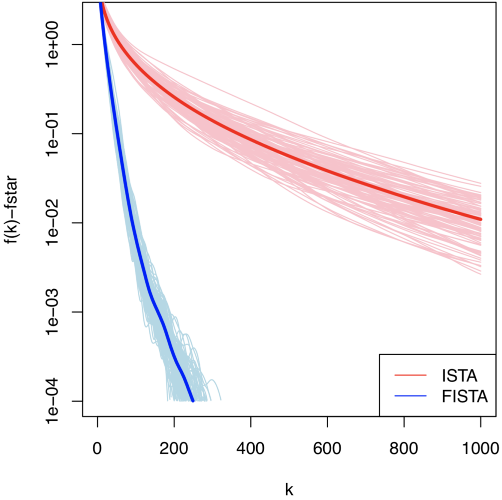
- Convergence rate is the same with NAG if $0 < t \leq 1/L$

$$f(x^{(k)}) - f^* \leq \frac{2\|x^{(0)} - x^*\|^2}{t(k+1)^2}$$

- When applied to LASSO, this is called **FISTA** (Fast Iterative Shrinkage-Thresholding Algorithm)

Example: ISTA vs FISTA

LASSO Logistic regression: 100 instances



Consider the following stochastic optimization problem

$$\min_x \; f(x) = \mathbb{E}_\xi(F(x,\xi)) = \int F(x,\xi)p(\xi)d\xi$$

- ξ is a random variable
- The challenge: evaluation of the expectation/integration

Example

- Supervised Learning

$$\min_w f(w) = \mathbb{E}_{(x,y)\sim D(x,y)}(\ell(h_w(x),y))$$

where $D(x,y)$ is the data distribution, $\ell(\cdot,\cdot)$ is certain loss, w is the model parameter

- Gradient descent with stochastic approximation (SA)

$$x^{(k+1)} = x^{(k)} - t_k g(x^{(k)})$$

where $\mathbb{E}(g(x)) = \nabla f(x),\ \forall x$

- Example. Consider supervised learning with observations $\mathcal{D} = \{x_i, y_i\}_{i=1}^N$

$$\min_w f(w) = \frac{1}{N} \sum_{i=1}^{N} \ell(h_w(x^{(i)}, y^{(i)}))$$

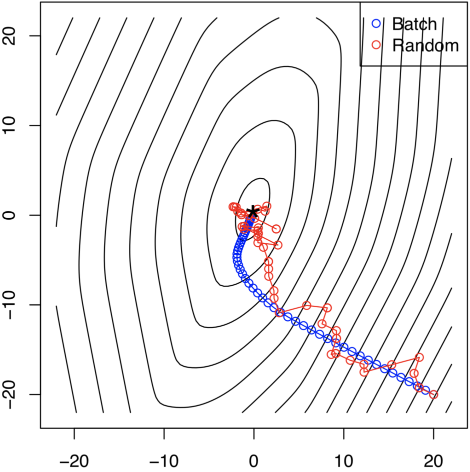
SGD

$$w^{(k+1)} = w^{(k)} - t_k \nabla \ell(h_w(x^{(i_k)}, y^{(i_k)}))$$

where $i_k \in \{1, \ldots, m\}$ is some chosen index at iteration k.

Example

Stochastic logistic regression



- Assume that $\mathbb{E}(\|g(x)\|^2) \le M^2$ and $f(x)$ is convex

$$\mathbb{E}f(\tilde{x}^{[0:k]}) - f^* \le \frac{\|x^{(0)} - x^*\|_2^2 + M^2 \sum_{j=0}^{k} t_j^2}{2\sum_{j=0}^{k} t_k}$$

where $\tilde{x}^{[0:k]} = \sum_{j=1}^{k} t_j x^{(j)} / \sum_{j=1}^{k} t_j$

- Fix the number of iterations K and constant step sizes $t_j = \frac{\|x^{(0)} - x^*\|}{M\sqrt{K}}$, $j = 0, 1, \ldots, K$, we have

$$\mathbb{E}(f(\bar{x}^K)) - f^* \le \frac{\|x^{(0)} - x^*\| M}{\sqrt{K}}$$

where $\bar{x}^K = \frac{1}{K+1} \sum_{j=0}^{K} x^{(j)}$

Proof

By convexity, we have $f(x^{(k)}) - f^* \leq \nabla f(x^{(k)})^T (x^{(k)} - x^*)$

$$
\begin{aligned}
t_k \mathbb{E}(f(x^{(k)})) - t_k f^* &\leq t_k \mathbb{E}(g(x^{(k)})^T (x^{(k)} - x^*)) \\
&= \frac{1}{2}(\mathbb{E}\|x^{(k)} - x^*\|_2^2 - \mathbb{E}\|x^{(k+1)} - x^*\|_2^2) + \frac{1}{2} t_k^2 \mathbb{E}\|g(x^{(k)})\|_2^2 \\
&\leq \frac{1}{2}(\mathbb{E}\|x^{(k)} - x^*\|_2^2 - \mathbb{E}\|x^{(k+1)} - x^*\|_2^2) + \frac{1}{2} t_k^2 M^2
\end{aligned}
$$

$\forall k \geq 0$. Therefore

$$
\sum_{j=0}^{k} t_j \mathbb{E}(f(x^{(j)})) - \sum_{j=0}^{k} t_j f^* \leq \frac{1}{2}\|x^{(0)} - x^*\|_2^2 + \frac{M^2}{2} \sum_{j=0}^{k} t_j^2
$$

Dividing both size with $\sum_{j=0}^{k} t_j$ together with convexity complete the proof

Pros and Cons of Vanilla SGD

What We Love About SGD

- Efficient in computation and memory usage, naturally scalable for big data problems
- Less likely to be trapped at local modes

What Needs to Be Improved

- In general, vanilla SGD is slow to converge (only $1/k$ even with strong convexity). Variance reduction seems to be a good remedy, see algorithms like SVRG, SAGA, etc.
- Choosing a proper learning rate can be difficult, require much effort in hyperparameter tuning to get good results
- The same learning rate applies to all parameter updates

Inspiration From Fisher Scoring

- Assume that f can be related to a probabilistic model, *i.e.*

$$f(\theta) = -\mathbb{E}_{y\sim P_{data}} L(y|\theta) = -\mathbb{E}_{y\sim P_{data}} \log p(y|\theta)$$

- Recall that Fisher information is defined as

$$\mathcal{I}(\theta) = \mathbb{E}_{y\sim p(y|\theta)} (\nabla L(y|\theta)(\nabla L(y|\theta))^T) \tag{5}$$

- We can use Fisher information to adapt the learning rate according to the local curvature. (5) inspire us to use some average of $g(\theta^{(t)})(g(\theta^{(t)}))^T$

- Previously, we performed an update for all parameters using the same learning rate
- Duchi et al (2011) proposed an improved version of SGD, AdaGrad, that adapts the learning rate to the parameters, according to the frequencies of their associated features
- Denote the vector of parameters as θ and the gradient at iteration t as g_t. Let η be the usual learning rate for SGD. AdaGrad's update rule:

$$\theta_{t+1} = \theta_t - \frac{\eta}{\sqrt{G_t + \epsilon}} \odot g_t$$

  where G_t is a diagonal matrix where each diagonal element is the sum of the squares of the corresponding gradients up to time step t

RMSprop

- A potential weakness about AdaGrad is its accumulation of the squared gradients in G_t, which in turn cause the learning rate to shrink and eventually become very small
- RMSprop (Geoff Hinton): resolve AdaGrad's diminishing learning rate via the exponentially decaying average

$$\mathbb{E}(g^2)_t = 0.9\mathbb{E}(g^2)_{t-1} + 0.1 g_t^2$$

$$\theta_{t+1} = \theta_t - \frac{\eta}{\sqrt{\mathbb{E}(g^2)_t + \epsilon}} g_t$$

- Presumably the most popular stochastic gradient methods in machine learning, proposed by D.P. Kingma et al (2014).
- In addition to the squared gradients, Adam also keeps an exponentially decaying average of the past gradients

$$m_t = \beta_1 m_{t-1} + (1-\beta_1) g_t, \quad v_t = \beta_2 v_{t-1} + (1-\beta_2) g_t^2$$

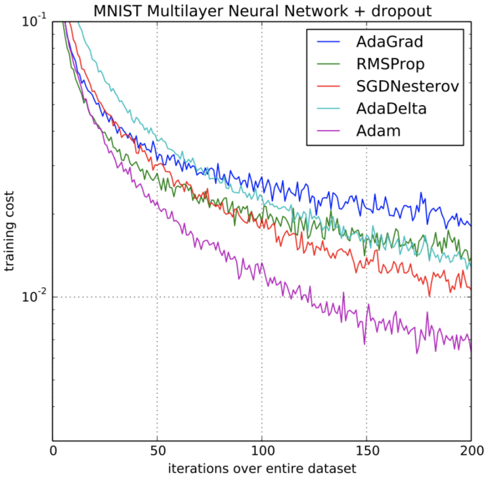
- Bias correction for zero initialization

$$\hat{m}_t = \frac{m_t}{1-\beta_1^t}, \quad \hat{v}_t = \frac{v_t}{1-\beta_2^t}$$

- Adam uses the same update rule

$$\theta_{t+1} = \theta_t - \frac{\eta}{\sqrt{\hat{v}_t + \epsilon}} \hat{m}_t$$

Test on MNIST Images



Pros and Cons for Adaptive Methods

Pros

- Faster training speed and smoother learning curve
- Easier to choose hyperparameters
- Better when data are very sparse

Cons

- Worse performance on unseen data (Wilson et al., 2017)
- Convergence issue: non-decreasing learning rates, extreme learning rates

Some recent proposals for improvement: AMSGrad (Reddi et al., 2018), AdaBound (Luo et al., 2019), etc.

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