L05 Non-convex Optimization: GD + noise converges to second order stationarity

50.579 Optimization for Machine Learning Ioannis Panageas ISTD, SUTD

Theorem (GD avoids strict saddles). Let $f : \mathbb{R}^n \to \mathbb{R}$ be a twice differentiable function, L-smooth and x^* be a strict saddle point and $\epsilon < 1/L$. For any continuous distribution D, if we sample initialization x_0 from D, GD converges to x^* with probability zero.

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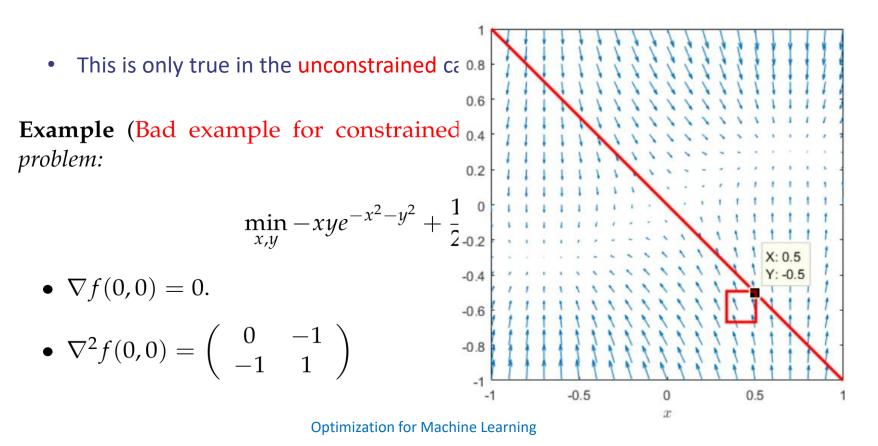
Example (Bad example for constrained). *Consider the following optimization problem:*

$$\min_{x,y} - xye^{-x^2 - y^2} + \frac{1}{2}y^2 \ s.t \ x + y \le 0.$$

•
$$\nabla f(0,0) = 0.$$

•
$$\nabla^2 f(0,0) = \begin{pmatrix} 0 & -1 \\ -1 & 1 \end{pmatrix}$$

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Theorem (GD avoids strict saddles with vanishing stepsize). Let $f : \mathbb{R}^n \to \mathbb{R}$ be a twice differentiable function, L-smooth and x^* be a strict saddle point and ϵ_t is of order $\Omega(\frac{1}{t})$ (vanishing). For any continuous distribution D, if we sample initialization x_0 from D, GD converges to x^* with probability zero.

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Fact (GD for Quadratic). Let $f(x) = \frac{1}{2}x^T A x$. GD boils down to:

$$x_{t+1} = x_t - \epsilon_t A x_t = (I - \epsilon_t A) x_t.$$

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Since A is symmetric, $A = P^{\top} \Delta P$ with Δ diagonal matrix, $P^{\top} P = I$.

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$$\prod_{z} (1 - \epsilon_z \lambda_i).$$

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Hence the eigenvalues are $e^{\sum \ln(1-\epsilon_z\lambda_i)} \approx e^{-\lambda_i \sum \epsilon_z}$

Assume that $\lambda_i < 0$ As long as $\sum_{z=0}^{\infty} \epsilon_z = \infty$ then for GD to converge to zero, we must have that $Px_0 \perp e_i$.

Definitions

Assumption (Hessian Lipschitz). We assume that the twice differentiable functions we are deadling with have Hessian ρ -Lipschitz, that is

$$\left\| \nabla^2 f(x) - \nabla^2 f(y) \right\|_2 \le \rho \, \|x - y\|_2.$$

Definition (Approximate first/second order stationary point). *We provide the following definitions:*

- A point x^* is an ϵ -first order stationary point (or critical point) of f if $\|\nabla f(x^*)\|_2 \leq \epsilon$.
- A point x^* of f is an ϵ -strict saddle point if it is an ϵ -first order stationary point and $\lambda_{\min}(\nabla^2 f(x^*)) < -\sqrt{\rho\epsilon}$
- The ϵ -first order points that are not ϵ -strict saddles are called ϵ -second order stationary points.

Theorem (GD converges to first-order stationarity). For any $\epsilon > 0$, assume the differentiable function is L-smooth and let $\alpha = \frac{1}{L}$. Moreover, let $f(x^*)$ be the global minimum of f. Then, the gradient descent algorithm in

$$x_{t+1} = x_t - \alpha \nabla f(x_t)$$

will visit an ϵ *-stationary point at least once in at most* $T := \frac{2L(f(x_0) - f(x^*))}{\epsilon^2}$ *iterations.*

Proof. Recall

$$f(x - \frac{1}{L}\nabla f(x)) - f(x) \le -\frac{1}{2L} \|\nabla f(x)\|_{2}^{2}$$

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Assume that $\|\nabla f(x_t)\|_2 > \epsilon$ for t = 1, ..., T. We get that

$$f(x_T) - f(x_{T-1}) + f(x_{T-1}) - f(x_{T-2}) + \dots + f(x_1) - f(x_0) < -\frac{\epsilon^2 T}{2L}.$$

Optimization for Machine Learning

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Contradiction!

Perturbed Gradient Descent

Definition (Perturbed Gradient Descent). Let $f : \mathbb{R}^d \to \mathbb{R}$ be a differentiable function. The Perturbed Gradient Descent is defined as follows:

1. Initialization x^0 , stepsize η , perturbation radius r.

2. For t=1 ... T do

3.
$$x_{t+1} = x_t - \eta(\nabla f(x_t) + \xi_t)$$
 with $\xi_t \sim \mathcal{N}(0, (r^2/d)I)$

4. End For

Theorem (PGD converges to second-order stationarity). Let f be a twice differentiable L-smooth function with Hessian ρ -Lipschitz. For any $\epsilon, \delta > 0$, set $\eta = \Theta(\frac{1}{L}), r = \Theta\left(\frac{\epsilon}{\log^4 d/(\delta\epsilon)}\right)$. PGD will visit an ϵ -second-order stationary point at least once with probability at least $1 - \delta$ in at most $T = O\left(\frac{L(f(x_0) - f(x^*))}{\epsilon^2}\log^4 \frac{d}{\rho\epsilon\delta}\right)$ iterations.

• High level proof strategy:

1) When the current iterate is not an ϵ -second order stationary point, it must either (a) have a large gradient or (b) have a strictly negative eigenvalue the Hessian.

2) We can show in both cases that yield a significant decrease in function value in a controlled number of iterations.

3) Since the decrease cannot be more that $f(x_0) - f(x^*)$ (global minimum is bounded) we can reach contradiction.

Lemma (Descent Lemma). Assume f is twice differentiable L-smooth and $\eta = \frac{1}{L}$. Then it holds with probability $1 - \delta$

$$f(x_{t+1}) - f(x_t) \le -\frac{\|\nabla f(x_t)\|^2}{2L} + O\left(r^4/d^2\log\frac{1}{\delta}\right).$$

Proof.

$$f(x_{t+1}) - f(x_t) \le \nabla f(x_t)^\top (x_{t+1} - x_t) + \frac{L}{2} ||x_{t+1} - x_t||_2^2$$
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Lemma (Descent Lemma). *Assume* f *is twice differentiable* L-smooth and $\eta = \frac{1}{L}$. *Then it holds with probability* $1 - \delta$

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= $-\frac{1}{L} \nabla f(x_t)^\top \nabla f(x_t) - \frac{1}{L} \xi_t^\top \nabla f(x_t) + \frac{L}{2} \frac{1}{L^2} ||\nabla f(x) + \xi_t||_2^2,$

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$$\leq -\frac{1}{2L} ||\nabla f(x)||_2^2 + \frac{1}{2L} ||\xi_t||_2^2.$$

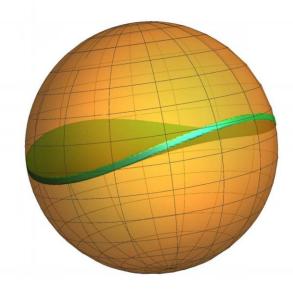
This is of order $\Theta(\epsilon^2)$ if we are in case (a).

Optimization for Machine Learning

Lemma (Escaping saddle points). Assume f is twice differentiable L-smooth and has hessian ρ -Lipschitz. Moreover assume that $\|\nabla f(x_0)\|_2 \leq \epsilon$ and also $\lambda_{min}(\nabla^2 f(x_0)) \leq -\sqrt{\rho\epsilon}$. Assume we run PGD from x_0 , then

$$\Pr[f(x_t) - f(x_0) \le -\frac{t'}{2}] \ge 1 - \frac{L\sqrt{d}}{\sqrt{\rho\epsilon}} e^{-\Theta(\log^4 \frac{d}{\rho\epsilon})},$$

for
$$t = \frac{L}{\sqrt{\rho\epsilon}} \Theta(\log^4 \frac{d}{\rho\epsilon})$$
 and $t' = \frac{\epsilon^2}{\sqrt{\rho\epsilon}} \Theta(\log^4 \frac{d}{\rho\epsilon})$.

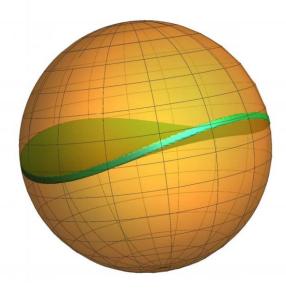


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Since $f(x^*) - f(x_0)$ is bounded and t is $\Theta(t'\epsilon^2)$, after $\Theta(\frac{f(x^*) - f(x_0)}{\epsilon^2})$ we reach a second order stationary point (contradiction otherwise).



Conclusion

- Introduction to Non-convex Optimization.
 - Perturbed Gradient Descent avoids strict saddles!
 - Same is true for Perturbed SGD.
- Next lecture we will talk about more about accelerated methods.
- Week 8 we are going to talk about min-max optimization (GANs).