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

50.579 Optimization for Machine Learning
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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.
Theorem (GD avoids strict saddles). Let $f : \mathbb{R}^n \rightarrow \mathbb{R}$ 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.

- This is only true in the unconstrained case!
Recap

**Theorem** (GD avoids strict saddles). Let \( f : \mathbb{R}^n \rightarrow \mathbb{R} \) 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.

- This is only true in the **unconstrained** case!

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

\[
\min_{x,y} -xye^{-x^2-y^2} + \frac{1}{2}y^2 \quad s.t \; x + y \leq 0.
\]

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

**Theorem** (GD avoids strict saddles). Let $f : \mathbb{R}^n \rightarrow \mathbb{R}$ 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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- $\nabla f(0, 0) = 0$.

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

**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 $\epsilon_t$ 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 $f(x) = \frac{1}{2}x^TAx$. GD boils down to:

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

Therefore $x_{t+1} = \prod_{z=t}^0 (I - \epsilon_zA)x_0$
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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 $\epsilon_t$ 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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Therefore

$$x_{t+1} = \prod_{z=t}^{0} (I - \epsilon_z A) x_0$$

Since $A$ is symmetric, $A = P^T \Delta P$ with $\Delta$ diagonal matrix, $P^T P = I$.

Therefore

$$x_{t+1} = P^T \prod_{z=t}^{0} (I - \epsilon_z \Delta) P x_0$$
Vanishing step-sizes

Therefore \( x_{t+1} = P^\top \prod_{z=t}^0 (I - \epsilon_z \Delta) P x_0 \)

Observe that \( \prod_{z=t}^0 (I - \epsilon_z \Delta) = \Delta' \), where \( \Delta' \) is diagonal with entry \((i, i)\)

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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 \( P x_0 \perp e_i \).
Definitions

**Assumption (Hessian Lipschitz).** We assume that the twice differentiable functions we are dealing with have Hessian $\rho$-Lipschitz, that is

$$\|\nabla^2 f(x) - \nabla^2 f(y)\|_2 \leq \rho \|x - y\|_2.$$

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

- A point $x^*$ is an $\epsilon$—first order stationary point (or critical point) of $f$ if $\|\nabla f(x^*)\|_2 \leq \epsilon$.

- A point $x^*$ of $f$ is an $\epsilon$—strict saddle point if it is an $\epsilon$-first order stationary point and $\lambda_{\min}(\nabla^2 f(x^*)) < -\sqrt{\rho \epsilon}$.

- The $\epsilon$-first order points that are not $\epsilon$-strict saddles are called $\epsilon$-second order stationary points.
Convergence to first order stationarity

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

**Proof.** Recall

$$f(x - \frac{1}{L} \nabla f(x)) - f(x) \leq -\frac{1}{2L} \|\nabla f(x)\|_2^2.$$
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Assume that $\|\nabla f(x_t)\|_2 > \epsilon$ for $t = 1, \ldots, T$. We get that

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

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

Therefore $f(x^*) - f(x_0) \leq f(x_T) - f(x_0) < -\frac{\varepsilon^2 T}{2L} = f(x^*) - f(x_0)$. 

Optimization for Machine Learning
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Therefore $f(x^*) - f(x_0) \leq f(x_T) - f(x_0) < -\frac{\epsilon^2 T}{2L} = f(x^*) - f(x_0)$.

**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 $\eta$, perturbation radius $r$.
2. **For** $t=1 \ldots T$ **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 $\rho$-Lipschitz. For any $\epsilon, \delta > 0$, set $\eta = \Theta\left(\frac{1}{L}\right)$, $r = \Theta\left(\frac{\epsilon}{\log^4 d/(\delta \epsilon)}\right)$. PGD will visit an $\epsilon$-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.
Analysis of Perturbed Gradient Descent

• High level proof strategy:

1) When the current iterate is not an $\epsilon$-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.
Analysis of Perturbed Gradient Descent

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

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

**Proof.**

\[
f(x_{t+1}) - f(x_t) \leq \nabla f(x_t)^	op (x_{t+1} - x_t) + \frac{L}{2} \|x_{t+1} - x_t\|_2^2 \text{ L-smooth,}
\]
Analysis of Perturbed Gradient Descent

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

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

**Proof.**

$$f(x_{t+1}) - f(x_t) \leq \nabla f(x_t)^\top (x_{t+1} - x_t) + \frac{L}{2} \|x_{t+1} - x_t\|^2 \quad \text{L-smooth,}$$

$$= -\frac{1}{L} \nabla f(x_t)^\top \nabla f(x_t) - \frac{1}{L} \xi_t^\top \nabla f(x_t) + \frac{L}{2} \frac{1}{L^2} \|\nabla f(x) + \xi_t\|^2,$$
Analysis of Perturbed Gradient Descent

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

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

**Proof.**

$$f(x_{t+1}) - f(x_t) \leq \nabla f(x_t)^\top (x_{t+1} - x_t) + \frac{L}{2} \|x_{t+1} - x_t\|^2 \text{ L-smooth,}$$

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

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

This is of order \( \Theta(\epsilon^2) \) if we are in case (a).
Analysis of Perturbed Gradient Descent

Lemma (Escaping saddle points). Assume $f$ is twice differentiable $L$-smooth and has hessian $\rho$-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

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

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

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

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).