Course Notes for EE227C (Spring 2018): Convex Optimization and Approximation

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18 Escaping saddle points

This lecture formalizes and shows the following intuitive statement for nonconvex optimization:

Gradient descent almost never converges to (strict) saddle points.

The result was shown in [LSJR16]. Let's start with some definitions.

Definition 18.1 (Stationary point)**.** We call x^* a stationary point if the gradient vanishes at x^*, i.e., $\nabla f(x^*) = 0$.

We can further classify stationary points into different categories. One important category are saddle points.

Definition 18.2 (Saddle point)**.** A stationary point x^* is a *saddle point* if for all $\epsilon > 0$, there are points $x, y \in B(x^*; \epsilon)$ s.t. $f(x) \leqslant f(x^*) \leqslant f(y)$.

Definition 18.3 (Strict saddle point)**.** For a twice continuously differentiable function $f \in C^2$, a saddle point x^* is a *strict saddle point* if the Hessian at that point is not positive semidefinite, i.e. $\lambda_{\min}(\nabla^2 f(x^*)) < 0$, where $\lambda_{\min}$ denotes the smallest eigenvalue.

18.1 Dynamical systems perspective

It'll be helpful to think of the trajectory defined by gradient descent as a dynamical system. To do so, we view each gradient descent update as a operator. For a fixed step size η, let

$$g(x) = x - \eta \nabla f(x)$$

so the notation for the result of iteration t from our previous discussion of gradient descent carries over as $x_t = g^t(x_0) = g(g(...g(x_0)))$, where g is applied t times on the initial point x_0. We call g the gradient map. Note that x^* is stationary iff. it is a fixed point of the gradient map i.e. $g(x^*) = x^*$. Also note that $Dg(x) = I - \eta \nabla^2 f(x)$ (Jacobian of g) , a fact that will become important later. Now we formalize a notion of the set of "attractors" of x^*.

Definition 18.4. The global stable set of x^*, is defined as

$$W^S(x^*) = \{x \in \mathbb{R}^n : \lim_t g^t(x) = x^*\}$$

In words, this is the set of points that will eventually converge to x^*.

With this definition out of the way, we can state the main claim formally as follows.

Theorem 18.5. *Assume $f \in C^2$ and is β-smooth. Also assume that the step size $\eta < 1/\beta$. Then for all strict saddle points x^*, its set of attractors $W^S(x^*)$ has Lebesgue measure 0.*

Remark 18.6. *In fact, it could be proven with additional technicalities that the Lebesgue measure of $\bigcup_{\text{strict saddle points } x^*} W^S(x^*)$ is also 0. This is just another way to say that gradient descent almost surely converges to local minima.*

Remark 18.7. *By definition, this also holds true to any probability measure absolutely continuous w.r.t. the Lebesgue measure (e.g. any continuous probability distribution). That is,*

$$\mathbb{P}(\lim_t x_t = x^*) = 0$$

However, the theorem above is only an asymptotic statement. Non-asymptotically, even with fairly natural random initialization schemes and non-pathological functions, gradient descent can be significantly slowed down by saddle points. The most recent result [DJL+17] is that gradient descent takes exponential time to escape saddle points (even though the theorem above says that they do escape eventually). We won't prove this result in this lecture.

18.2 The case of quadratics

Before the proof, let's go over two examples that will make the proof more intuitive:

Example 18.8. $f(x) = \frac{1}{2}x^T Hx$ where H is an n-by-n matrix, symmetric but not positive semidefinite. For convenience, assume 0 is not an eigenvalue of H. So 0 is the only stationary point and the only strict saddle point for this problem.

We can calculate $g(x) = x - \eta Hx = (I - \eta H)x$ and $g^t(x) = (I - \eta H)^t x$. And we know that $\lambda_i(I - \eta H) = 1 - \eta\lambda_i(H)$, where λ_i for $i = 1...n$ could denote any one of the eigenvalues. So in order for $\lim_t g^t(x) = \lim_t(1 - \eta\lambda_i(H))^t x$ to converge to 0, we just need $\lim_t(1 - \eta\lambda_i(H))^t$ to converge to 0, that is, $|1 - \eta\lambda_i(H)| < 1$. This implies that

$$W^S(0) = \text{span}\left\{u|Hu = \lambda u, 0 < \lambda < \frac{\eta}{2}\right\}$$

i.e. the set of eigenvectors for the positive eigenvalues smaller than $\frac{\eta}{2}$. Since η can be arbitrarily large, we just consider the larger set of eigenvectors for the positive eigenvalues. By our assumption on H, this set has dimension lower than n, thus has measure 0.

Example 18.9. Consider the function $f(x, y) = \frac{1}{2}x^2 + \frac{1}{4}y^4 - \frac{1}{2}y^2$ with corresponding gradient update

$$g(x, y) = \begin{bmatrix} (1-\eta)x \\ (1+\eta)y - \eta y^3 \end{bmatrix},$$

and Hessian

$$\nabla^2 f(x, y) = \begin{bmatrix} 1 & 0 \\ 0 & 3y^2 - 1 \end{bmatrix}.$$

We can see that $(0, -1)$ and $(0, 1)$ are the local minima, and $(0, 0)$ is the only strict saddle point. Similar to in the previous example, $W^S(0)$ is a low-dimensional subspace.

18.3 The general case

We conclude this lecture with a proof of the main theorem.

Proof of Theorem 18.5. First define the local stable set of x^* as

$$W^S_\epsilon(x^*) = \{x \in B(x^*; \epsilon) : g^t(x) \in B(x^*; \epsilon)\ \forall t\}$$

Intuitively, this describes the subset of $B(x^*; \epsilon)$ that stays in $B(x^*; \epsilon)$ under arbitrarily many gradient maps. This establishes a notion of locality that matters for gradient descent convergence, instead of $B(x^*; \epsilon)$ which has positive measure.

Now we state a simplified version of the stable manifold theorem without proof: For a diffeomorphism $g : \mathbb{R}^n \to \mathbb{R}^n$, if x^* is a fixed point of g, then for all ϵ small enough, $W^S_\epsilon(x^*)$ is a submanifold of dimension equal to the number of eigenvalues of the $Dg(x^*)$ that are $\leqslant 1$. A diffeomorphism, roughly speaking, is a differentiable isomorphism. In fact, since differentiability is assumed for g, we will focus on the isomorphism.

Let x^* be a strict saddle point. Once we have proven the fact that g is a diffeomorphism (using the assumption that $\eta < 1/\beta$), we can apply the stable manifold theorem since x^* is a fixed point of g. Because $\nabla^f(x^*)$ must have an eigenvalue < 0, Dg must have an eigenvalue > 1, so the dimension of $W^S_\epsilon(x^*)$ is less than n and $W^S_\epsilon(x^*)$ has measure 0.

If $g^t(x)$ converges x^*, there must $\exists T$ large enough s.t. $g^T(x) \in W^S_\epsilon(x^*)$. So $W^S(x^*) \subseteq \bigcup_{t \geqslant 0} g^{-t}(W^S_\epsilon(x^*))$. For each t, g^t is in particular an isomorphism (as a composition of isomorphisms), and so it g^{-t}. Therefore $g^{-t}(W^S_\epsilon(x^*))$ has the same cardinality as $W^S_\epsilon(x^*)$ and has measure 0. Because the union is over a countable set, the union also has measure 0, thus its subset $W^S(x^*)$ ends up with measure 0 and we have the desired result.

Finally we show that g is bijective to establish the isomorphism (since it is assumed to be smooth). It is injective because, assuming $g(x) = g(y)$, by smoothness,

$$\|x - y\| = \|g(x) + \eta\nabla f(x) - g(y) - \eta\nabla f(x)\| = \eta\|\nabla f(x) - \nabla f(y)\| \leqslant \eta\beta\|x - y\|$$

Because $\eta\beta < 1$, we must have $\|x - y\| = 0$. To prove that g is surjective, we construct an inverse function

$$h(y) = \operatorname*{argmin}_x \frac{1}{2}\|x - y\|^2 - \eta f(x)$$

a.k.a. the proximal update. For $\eta < 1/\beta$, h is strongly convex, and by the KKT condition, $y = h(y) - \nabla f(h(y)) = g(h(y))$. This completes the proof. ■

References

[DJL+17] Simon S Du, Chi Jin, Jason D Lee, Michael I Jordan, Aarti Singh, and Barnabas Poczos. Gradient descent can take exponential time to escape saddle points. In *Advances in Neural Information Processing Systems*, pages 1067–1077, 2017.

[LSJR16] Jason D Lee, Max Simchowitz, Michael I Jordan, and Benjamin Recht. Gradient descent converges to minimizers. *arXiv preprint arXiv:1602.04915*, 2016.