Special Properties of Gradient Descent with Large Learning Rates

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Abstract

This article is an overview of the work [MJS23] with some additional experiments. It has been widely observed that usage of larger learning rate in stochastic gradient descent often results into better models. However theoretical reasons for this phenomena are not well understood yet. Previous studies linked it to stochastic noise in SGD. The work focuses on theoretical proof of escaping local minima for some special class of functions. Also it is shown that for certain starting points and loss functions GD with large learning rate has different trajectory and may lead to convergence to another minima, which is likely to be more robust.

1 Main results

Usage of large learning rate is often explained by intuition of escaping local minima. In this work a class C_l of functions is constructed which have at least two minima ($x^\dagger$ and x_*) and with a large learning rate GD with random initialization converges to x_* almost surely, but with smaller learning rate there is strictly positive probability of converging to $x^\dagger$.

2 Theoretical Analysis

For analysis optimization problem using full-batch gradient descent with random initialization was taken:

$$f_* := \min_{x \in \mathbb{R}^d} f(x).$$

f is supposed to be L-smooth over regions of the landscape so that the gradient does not change too sharply. Also we would require sharpness of some regions of f around local minima using μ-one-point-strongly-convexity (OPSC) with respect to x_* over M.

Definition 2.1 (L-smoothness)**.** A function $f : \mathbb{R}^d \to \mathbb{R}$ is L-smooth if f is differentiable and exists L : $\|\nabla f(x) - \nabla f(y)\| \leq L\|x - y\|$, $\forall x, y \in \mathbb{R}^d$

Definition 2.2 (μ-one-point-strongly-convex (OPSC) with respect to x_* over M)**.** A function $f : \mathbb{R}^d \to \mathbb{R}$ is μ-one-point-strongly-convex (OPSC) with respect to x_* over M if it is differentiable and

$$\exists \mu > 0 : \langle \nabla f(x), x - x_* \rangle \geq \mu \|x - x_*\|^2, \ \forall x \in M.$$

Lemma 2.1. *Let f be a function that is L_{global} -smooth with a global minimum x_*. Assume there exists a local minimum $x^\dagger$ around which*

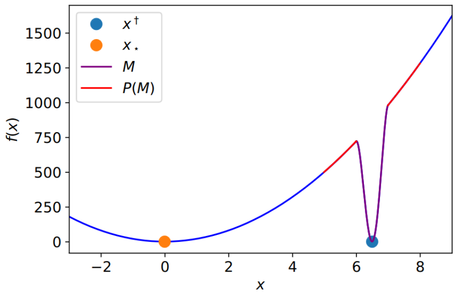
- *f is $\mu^\dagger$-OPSC woth respect to $x^\dagger$ over a set M that contains $x^\dagger$ with diameter r.*
- *Let $P(M)$ be a ball around $x^\dagger$ with radius r_P excluding points M. f is $L < L_{\text{global}}$ -smooth in $P(M)$ and μ_*-OPSC with respect to x_*, such as $\mu^\dagger > \frac{2L^2}{\mu_*}$. r_P depends on $r, \gamma, L_{\text{global}}$.*
- *$\|x_* - x^\dagger\| > \tau$, where τ depends on μ_*, r, γ.*

  Then using learning rate $\frac{2}{\mu^\dagger} < \gamma < \frac{\mu_*}{L^2}$ GD escape M and reach a point closer to x_* than $\|x^\dagger - x_*\| - r$ almost surely.

Proof. □

Theorem 2.2. *Let C_l be the set of functions sudh as f is L-smooth and μ_*-OPSC with respect to the global minima x_* except n a region M that contains local minima $x^\dagger$ and satisfies lemma 2.1.*

Figure 1: Illustation of regions from lemma 2.1



- Gradient descent initialized randomly inside M with learning rate $\gamma < \frac{\mu^\dagger}{L^2_{\text{global}}}$ converges to $x^\dagger$ almost surely.
- Gradient descent initialized randomly in arbitrary set $W : \mathcal{L}(W) > 0$ with learning rate $\frac{2}{\mu^\dagger} < gamma \leq \frac{\mu_*}{L^2}$ converges to x_* almost surely.

Proof. □

Lemma 2.3. Take gradient descent initialized randomly in set W with learning rate $\gamma \leq \frac{1}{2L}$. Let $X \subset \mathbb{R}^d$ arbitrary set of points in the landscape, f is L-smooth over $\mathbb{R}^d \setminus X$. Probabilty of encountering any point of X in first T steps of gradient descent is at most $2^{(T+1)d}\frac{\mathcal{L}(X)}{\mathcal{L}(W)}$.

Proof. □

Theorem 2.4. Let X be an arbitrary set of points, f is μ_*-OPSC with respect to a minima $x_* \notin X$ over $\mathbb{R}^d \setminus X$. Let $c_X := \inf\{\|x - x_*\| \mid x \in X\}$ and $r_W := \sup\{\|x - x_*\| \mid x \in W\}$. The probability of not encountering ant points of X during gradient descent with learning rate $\gamma \leq \frac{\mu_*}{L^2}$ is at least $1 - \frac{r_W}{c_X}^{\frac{-d}{\log_2(1-\gamma\mu_*)}}\frac{\mathcal{L}(X)}{\mathcal{L}(W)}2^d$ if $c_X \leq r_W$ and 1 otherwise.

Proof. □

Proposition

Take the case of SGD

$$x_{t+1} := x_t - \gamma\left(\nabla f(x_t) + \xi_t\right),$$

where ξ_t considered to be Uniform$(-\sigma, \sigma)$.

Proposition 2.5. Consider SGD on the function from figure 1, starting close to $x^\dagger$. If the learning rate is sufficiently small the iterations will never converge to x_* nor to a small region around it, regardless of the magnitude of the noise. If the learning rate is large enough and stochastic noise satisfies certain bounds, SGD will converge to x_* from any starting point.

Proof. □

3 Experiments

1D Example

Study different GD behaviour depending on starting point and learning rate on the function f.

$$f(x) := \begin{cases} -1600(x-2.5)^5 - 2000(x-2.5)^4 + 800(x-2.5)^3 + 1020(x-2.5)^2 & 2 \le x \le 3 \\ 1411.2 \times \big(1 - 10^4(x-8.4)\big) & 8.4 \le x \le 8.40001 \\ 0 & 8.40001 \le x \le 8.59999, \\ 1479.2 \times \big(10^4(x-8.6)+1\big) & 8.59999 \le x \le 8.6, \\ 20x^2 & \textit{otherwise} \end{cases}$$

Figure 2: Visual comparison of GD with different learning rates.

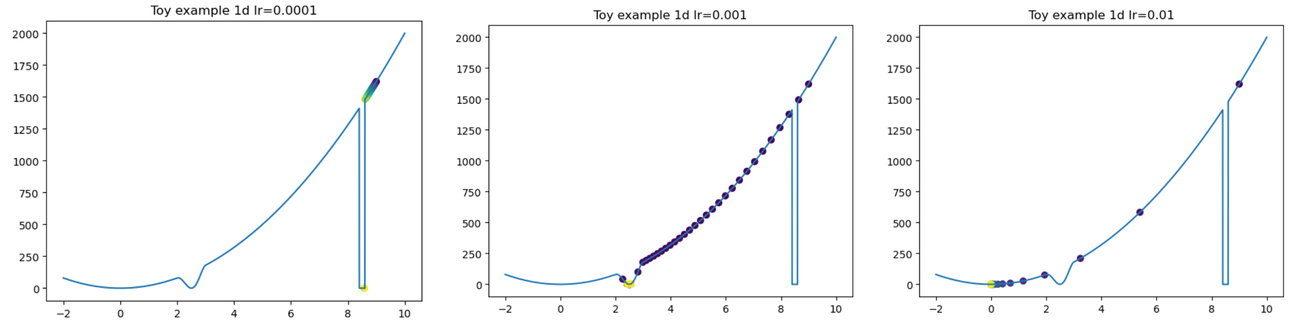
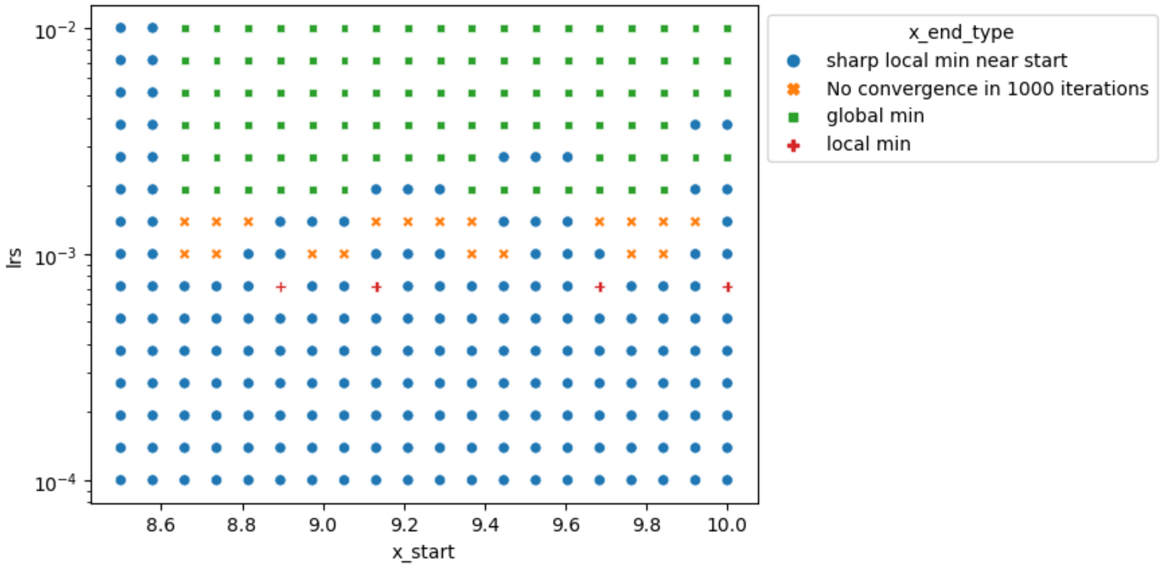


Figure 3: GD converged to local minima close to start.

Figure 4: GD converged to local minima.

Figure 5: GD converged to global minima.

Figure 6: Types of convegence of GD depending on startpoint and learning rate.



From the experiments we can see that usage of larger learning rates helps to escape local minima and converge to a flatter one.

3.1 2D Example

Study different GD behaviour depending on learning rate on the function f

$$f(x, y) := x^2 + y^2 - 200\mathrm{ReLU}(|x| - 1)\mathrm{ReLU}(|y| - 1)\mathrm{ReLU}(2 - |x|)\mathrm{ReLU}(2 - |x|)$$

Figure 7: Visual comparison of GD with different learning rates.

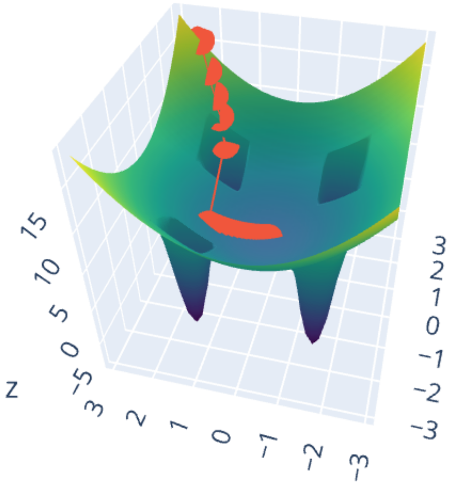


Figure 8: GD converged to flat minima.

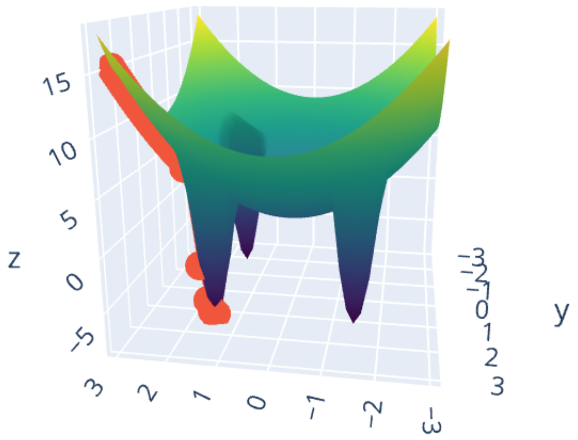
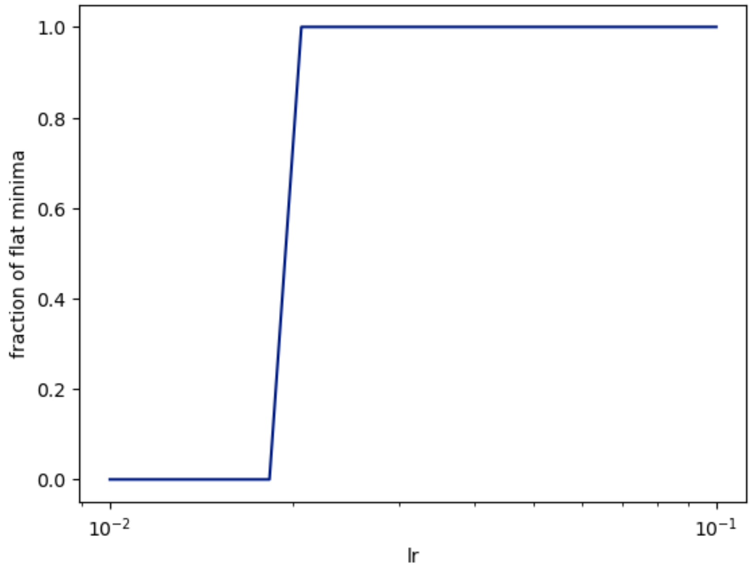


Figure 9: GD converged to sharp minima.

Figure 10: Share of GDs that obtained flat minima if starting point is random $3 \le x, y \le 4$.



3.2 MNIST example

Not yet finished experiments

- Warm up NN using small learning rate. Use large and small learning rate, according to figure 7 from [MJS23] they might have different trajectories and converge to different minima.
- Test hypothesis that minima obtained using larger learning rate is more robust. Train NN using large and small learning rate. Then change the training dataset and continue to train. Compare distance between minima of different datasets obtained small and large learning rate.

References

[MJS23] Amirkeivan Mohtashami, Martin Jaggi, and Sebastian Stich. Special properties of gradient descent with large learning rates, 2023.