Optimization for Machine Learning

Lecture 20: Optimization for Neural networks — II

6.881: MIT

Suvrit Sra
Massachusetts Institute of Technology

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Some Aspects of NN Optimization

- Backprop ➠ SGD
- Mini-batches
- Initialization
- Batchnorm
- Gradient clipping
- Adaptive methods
- Momentum
- Layerwise params
- …and more!

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All while keeping validation / test error performance in mind

Clipping, Adaptivity, Momentum Saddle Points, etc.,...

Gradient Clipping

("hack" for dealing with gradient explosion)

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- Clipped GD can converge arbitrarily faster than fixed-step GD (for differentiable but non C_L^1 functions)

Clipped GD and Normalized GD

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Exercise: Show that clipped GD ~ NGD up to a const factor in step size

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WHY GRADIENT CLIPPING ACCELERATES TRAINING: A THEORETICAL JUSTIFICATION FOR ADAPTIVITY

Jingzhao Zhang, Tianxing He, Suvrit Sra & Ali Jadbabaie
Massachusetts Institute of Technology

Clipped GD

L-smoothness $\|\nabla^2 f(x)\| \le L$

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(L,M)-smoothness $$\|\nabla^2 f(x)\| \leq L_0 + L_1 \|\nabla f(x)\|$$

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Relaxed to once differentiable

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Theorem (informal). GD can be arbitrarily slow to converge to a stationary point for functions satisfying $(L_0, L_1)-$smoothness, whereas Clipped GD converges as $O(1/\epsilon^2)$

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Exercise: Analyze convergence of all other methods under (L_0, L_1)-smoothness for which we previously assumed L-smoothness.

Clipped GD

Clipped GD converges at "usual" speed

Theorem 3. *Let $\mathcal{F}$ denote the class of functions that satisfy Assumptions 1, 2, and 3 in set $\mathcal{S}$ defined in (3). Recall f^* is a global lower bound for function value. With $\eta_c = \frac{1}{10L_0}, \gamma = \min\{\frac{1}{\eta_c}, \frac{1}{10L_1\eta_c}\}$, we can prove that the iteration complexity of clipped GD (Algorithm 5) is upper bounded by*

$$\frac{20L_0(f(x_0) - f^*)}{\epsilon^2} + \frac{20\max\{1, L_1^2\}(f(x_0) - f^*)}{L_0}.$$

GD can be arbitrarily slower

Theorem 4. *Let $\mathcal{F}$ be the class of objectives satisfying Assumptions 1, 2, 3, and 4 with fixed constants $L_0 \geq 1$, $L_1 \geq 1$, $M > 1$. The iteration complexity for the fixed-step gradient descent algorithms parameterized by step size h is at least*

$$\frac{L_1 M(f(x_0) - f^* - 5\epsilon/8)}{8\epsilon^2(\log M + 1)}.$$

Explore: Lower bound for SGD (afaik unknown in this setting)

Momentum, Adaptivity

(Adam, Adam-like methods)

Momentum

Gradient Descent with Momentum

$$m_t = \beta m_{t-1} + \nabla f(\theta_t)$$
$$\theta_{t+1} = \theta_t - \eta m_t$$

https://distill.pub/2017/momentum/

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- accelerated convg. (eg, convex quadratics)
- works well in practice
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Idea: Exponential moving averages $\beta \in (0,1)$

$$G_t = (1-\beta) \sum_{i=1}^{t} \beta^{t-i} g_i g_i^T$$

(analogous to what momentum is doing for gradients…)

ADAM

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bias-correction

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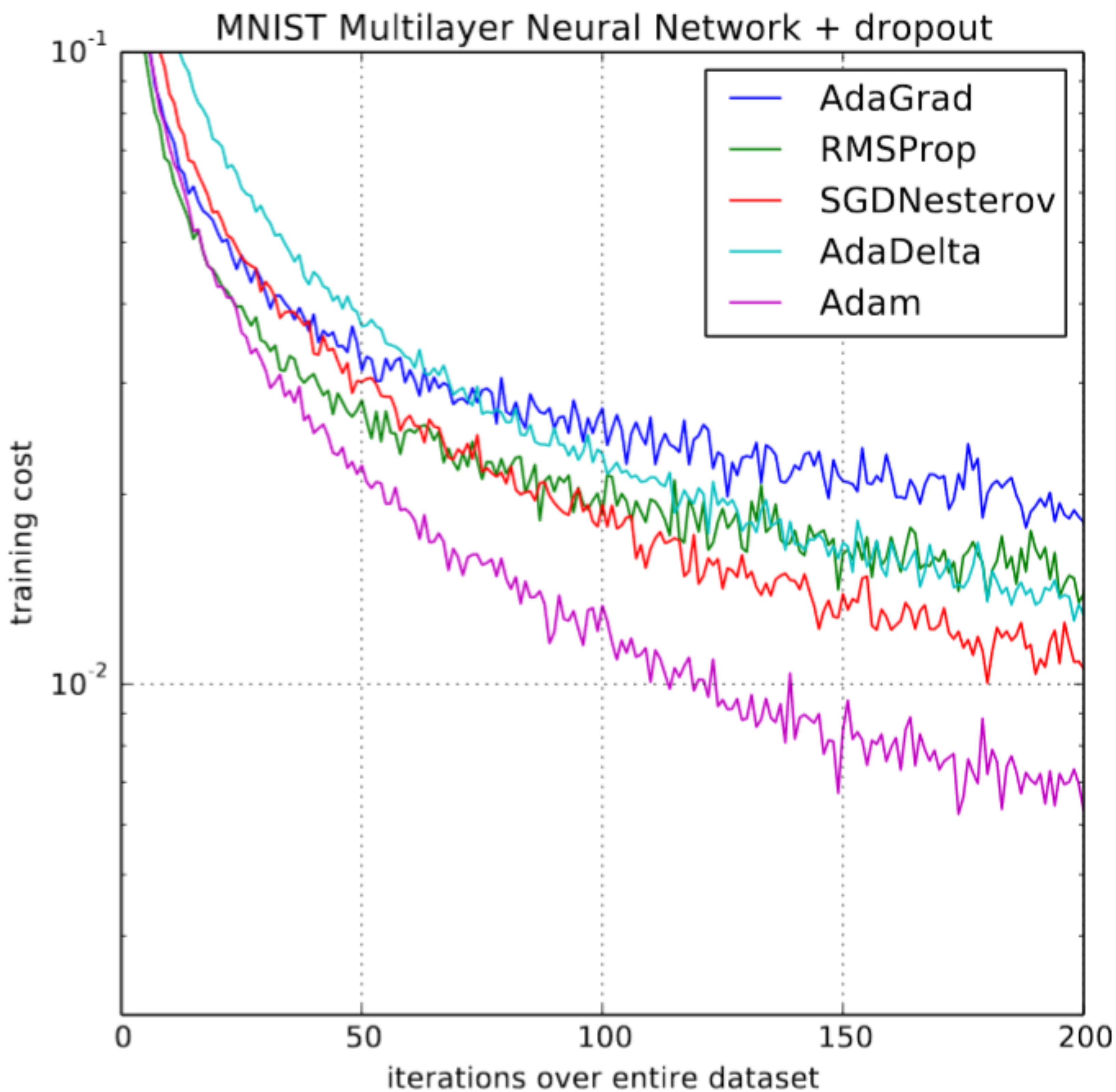

From the ADAM paper: https://arxiv.org/abs/1412.6980

Algorithm 2 LAMB https://arxiv.org/abs/1904.00962

Input: $x_1 \in \mathbb{R}^d$, learning rate $\{\eta_t\}_{t=1}^T$, parameters $0 < \beta_1, \beta_2 < 1$, scaling function ϕ, $\epsilon > 0$

Set $m_0 = 0$, $v_0 = 0$

for $t = 1$ **to** T **do**

  Draw b samples S_t from $\mathbb{P}$.

  Compute $g_t = \frac{1}{|\mathcal{S}_t|} \sum_{s_t \in \mathcal{S}_t} \nabla \ell(x_t, s_t)$.

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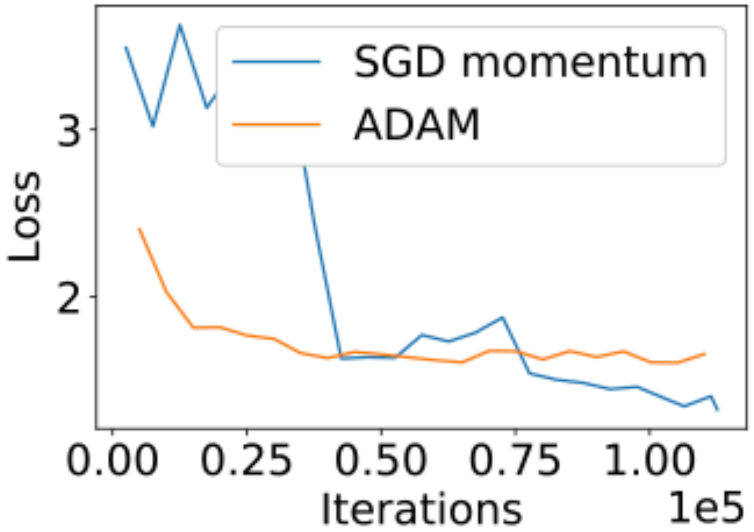
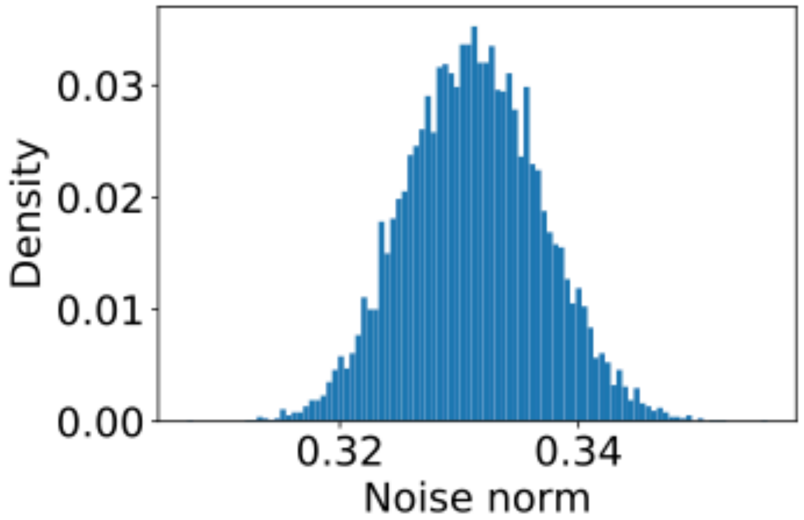
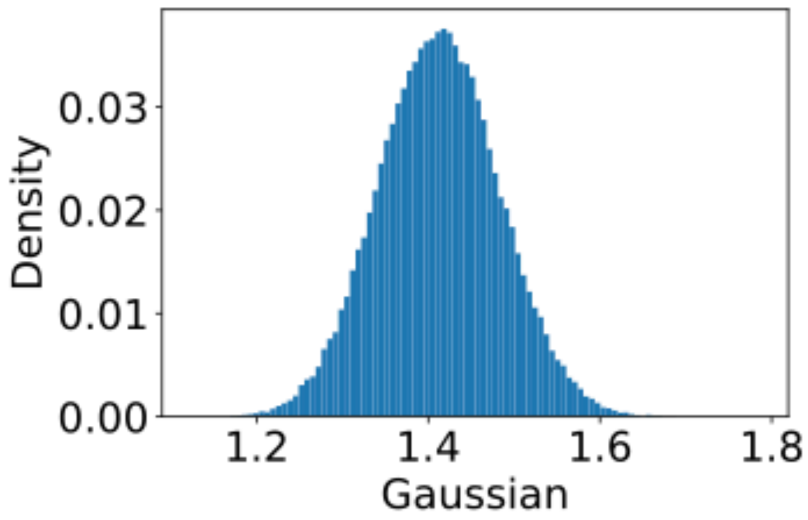
Resnet50 on Imagenet







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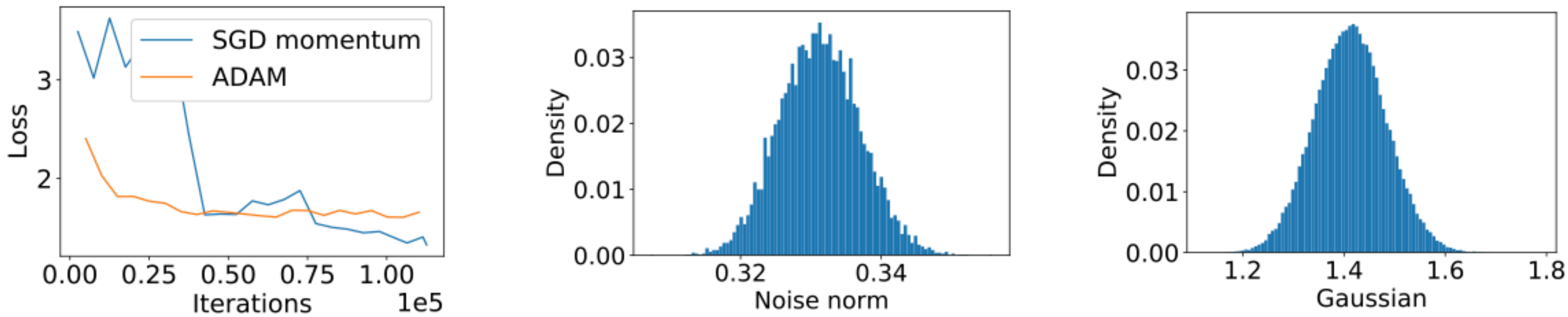
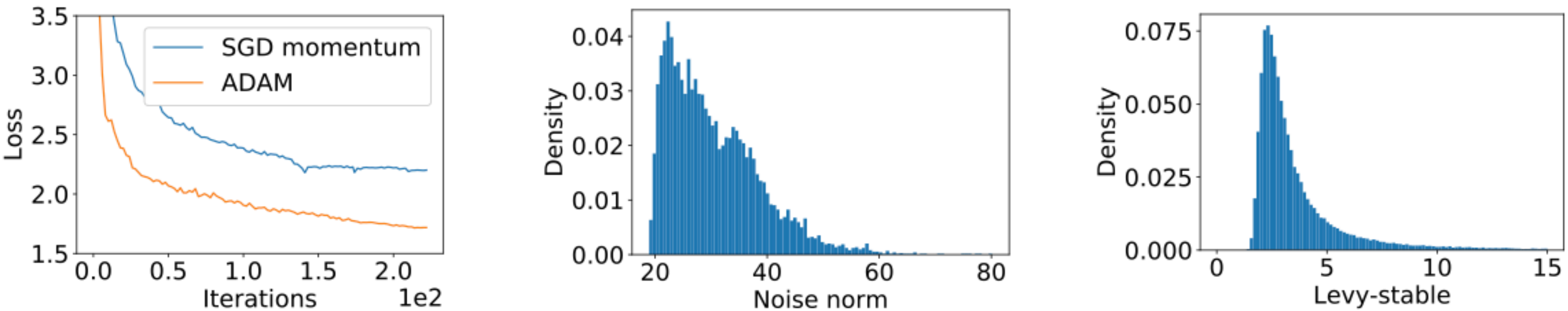


BERT pretraining (Wikipedia+Books data)



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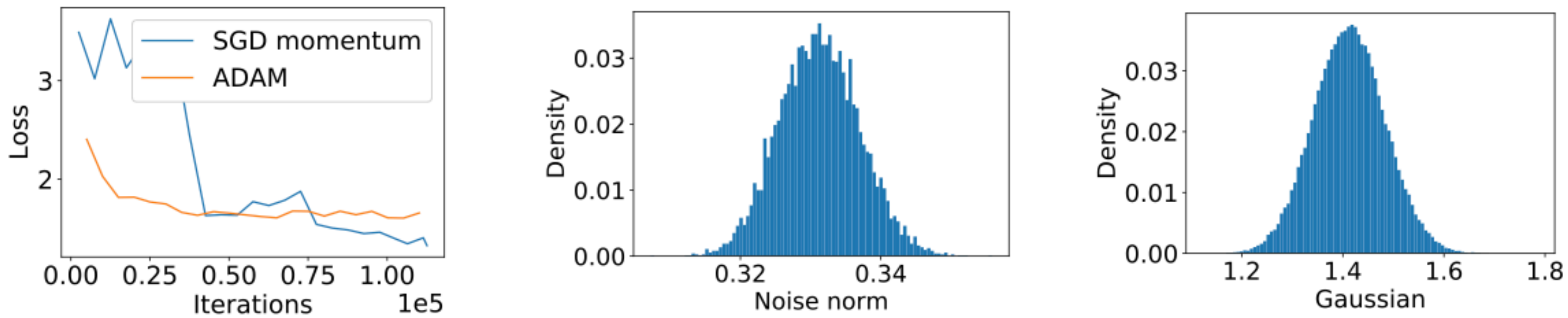

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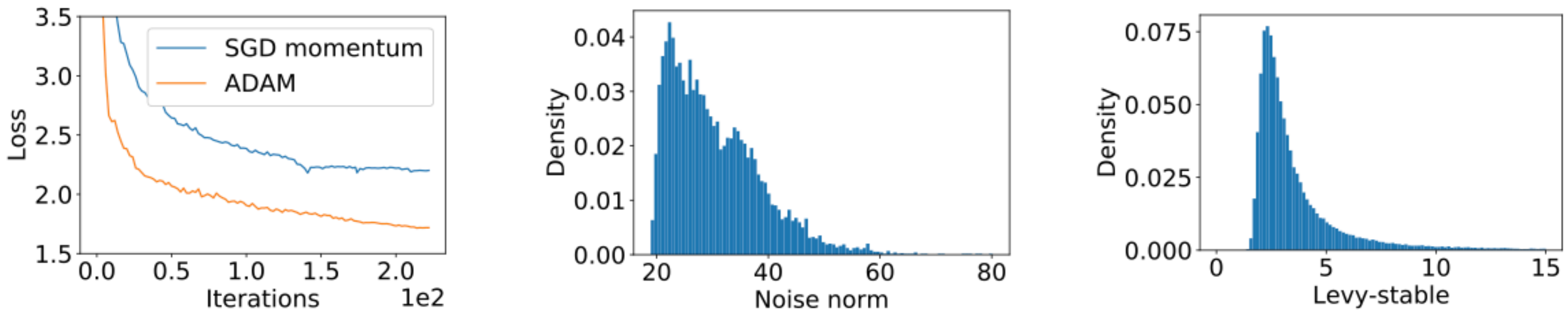

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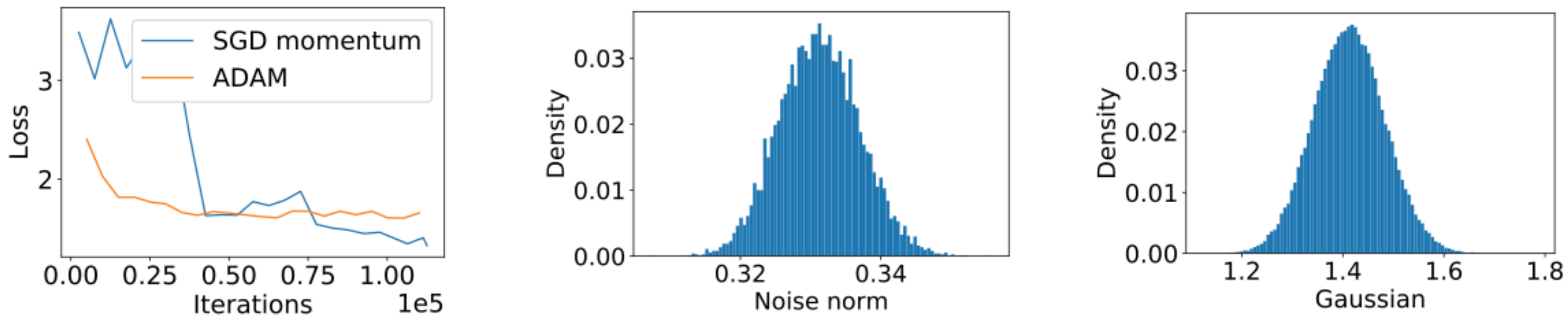

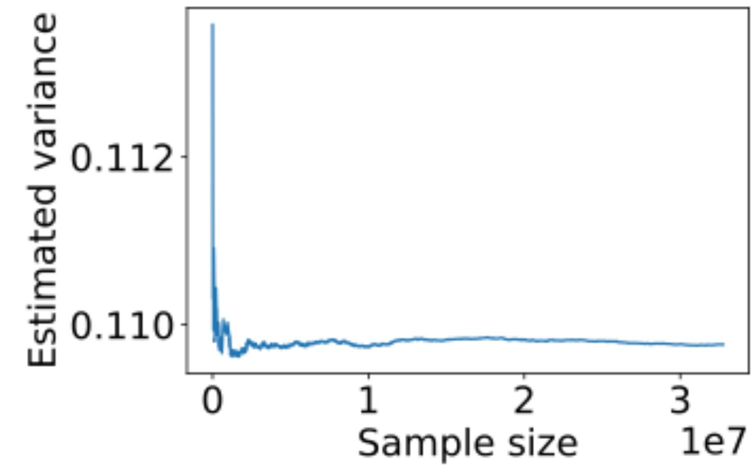

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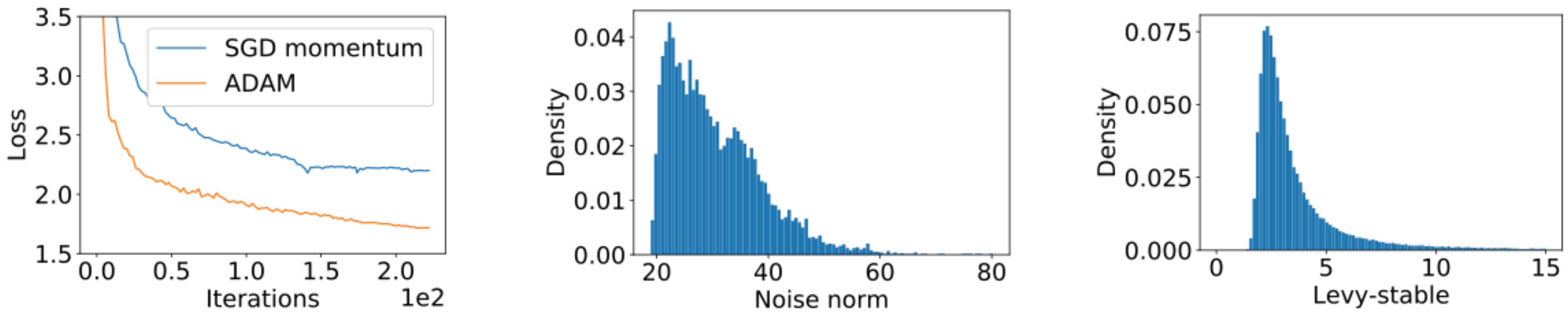

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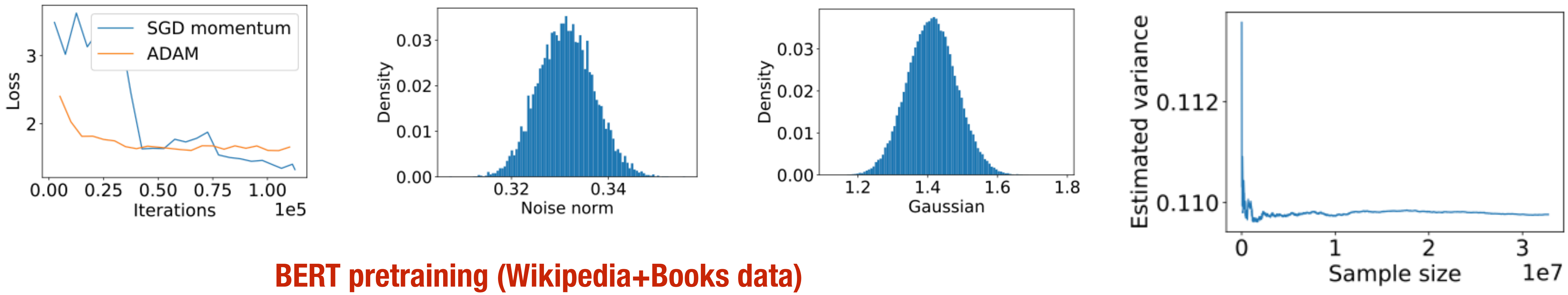

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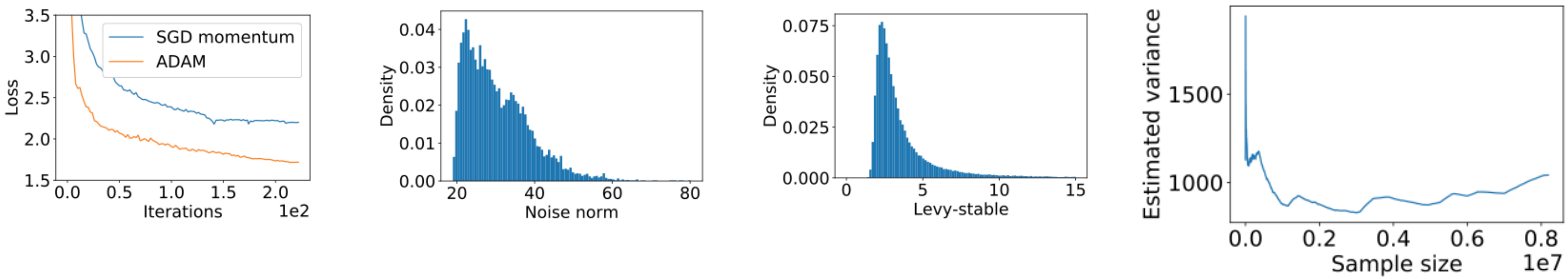

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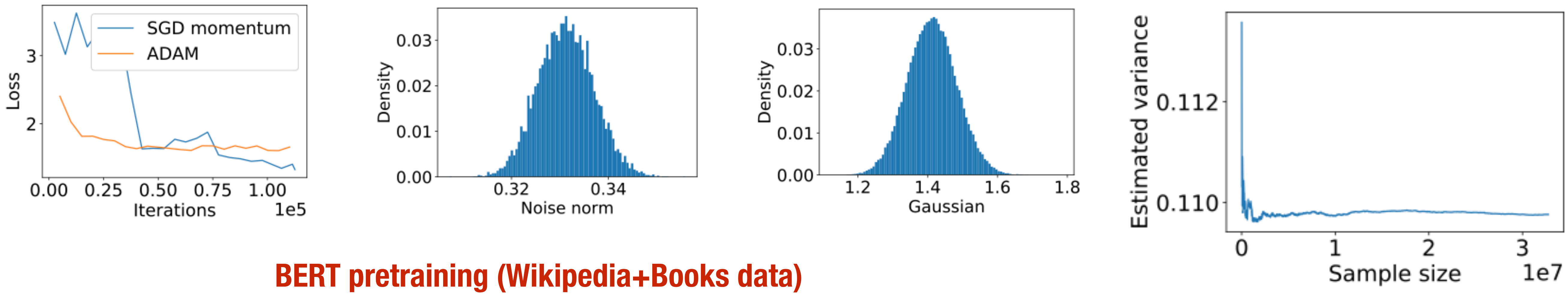

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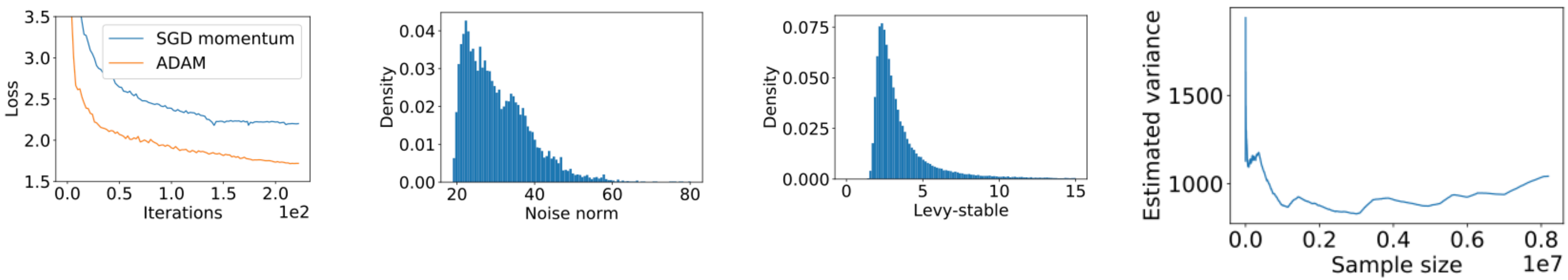

The heavy-tailed noise could explain why ADAM works better than SGD?

Convergence rates under heavy-tailed noise

	Strongly Convex Function		Non-Convex Function	
	Heavy-tailed noise ($\alpha \in (1,2)$)	Standard noise ($\alpha \geq 2$)	Heavy-tailed noise ($\alpha \in (1,2)$)	Standard noise ($\alpha \geq 2$)
SGD	N/A	$\mathcal{O}\left(k^{-1}\right)$	N/A	$\mathcal{O}\left(k^{-\frac{1}{4}}\right)$
GClip	$\mathcal{O}\left(k^{\frac{-(\alpha-1)}{\alpha}}\right)$	$\mathcal{O}\left(k^{-1}\right)$	$\mathcal{O}\left(k^{\frac{-(\alpha-1)}{3\alpha-2}}\right)$	$\mathcal{O}\left(k^{-\frac{1}{4}}\right)$
LowerBound	$\Omega\left(k^{\frac{-(\alpha-1)}{\alpha}}\right)$	$\Omega\left(k^{-1}\right)$	$\Omega\left(k^{\frac{-(\alpha-1)}{3\alpha-2}}\right)$	$\Omega\left(k^{-\frac{1}{4}}\right)$

Error bounds (f-f^* for cvx; $\|\nabla f\|$ for noncvx).

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LowerBound	$\Omega\big(k^{\frac{-(\alpha-1)}{\alpha}}\big)$	$\Omega\big(k^{-1}\big)$	$\Omega\big(k^{\frac{-(\alpha-1)}{3\alpha-2}}\big)$	$\Omega\big(k^{-\frac{1}{4}}\big)$

Error bounds (f-f^* for cvx; $\|\nabla f\|$ for noncvx).

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Convergence rates under heavy-tailed noise

	Strongly Convex Function		Non-Convex Function	
	Heavy-tailed noise ($\alpha \in (1,2)$)	Standard noise ($\alpha \geq 2$)	Heavy-tailed noise ($\alpha \in (1,2)$)	Standard noise ($\alpha \geq 2$)
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Check out the details and experiments in

Why are Adaptive Methods Good for Attention Models?

Jingzhao Zhang, Sai Praneeth Karimireddy, Andreas Veit, Seungyeon Kim, Sashank J Reddi, Sanjiv Kumar, Suvrit Sra

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Algorithm 1 ACClip

$x, m_k \leftarrow x_0, 0$
for $k = 1, \cdot, T$ **do**
$\quad m_k \leftarrow \beta_1 m_{k-1} + (1 - \beta_1) g_k$
$\quad \tau_k^\alpha \leftarrow \beta_2 \tau_{k-1}^\alpha + (1 - \beta_2)|g_k|^\alpha$
$\quad \hat{g}_k \leftarrow \min\{\frac{\tau_k}{|m_k|+\epsilon}, 1\} m_k$
$\quad x_k \leftarrow x_{k-1} - \eta_k \hat{g}_k$
end forreturn x_K, where random

$x_{k+1} = x_k - \eta_k \min\{$ ... $\frac{\tau_k}{|g_k|}, 1\} g_k \,, \; \tau_k \in \mathbb{R}^d_{\geq 0}$

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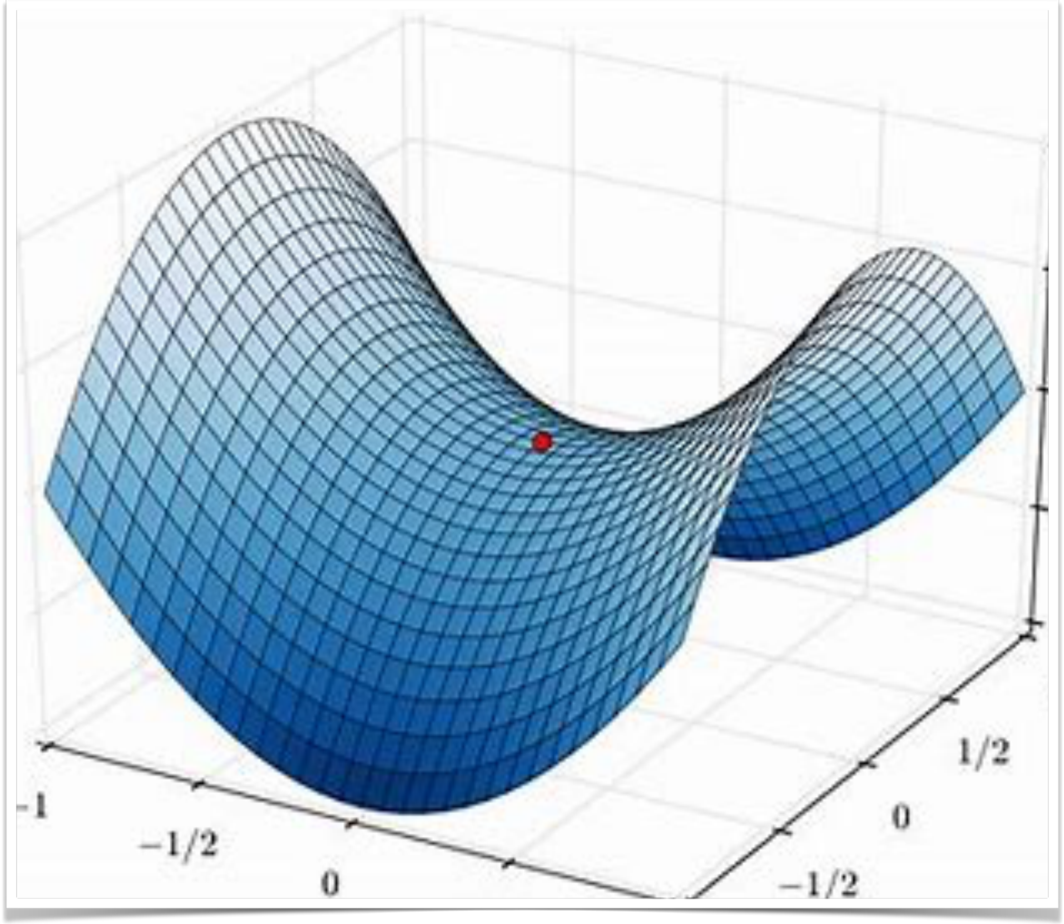
Escaping Saddle Points

Background

Background



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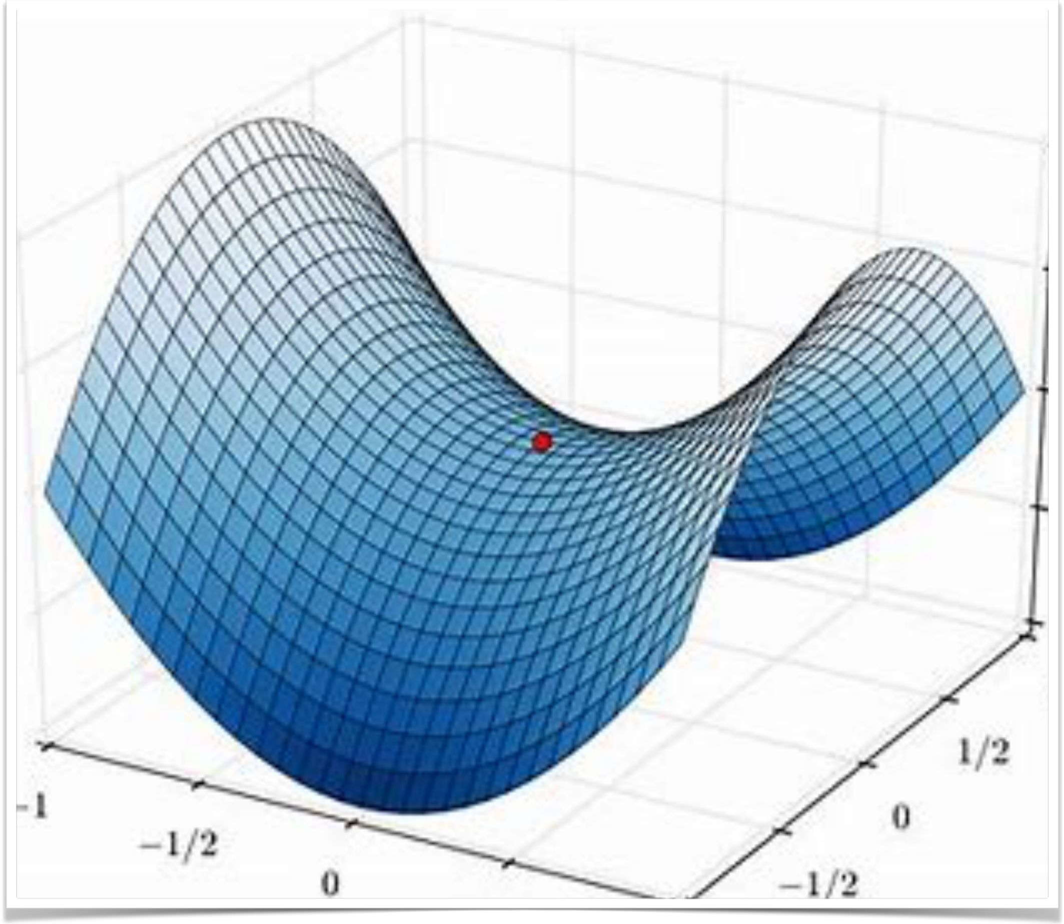
At a stationary point $\nabla f(x) = 0$



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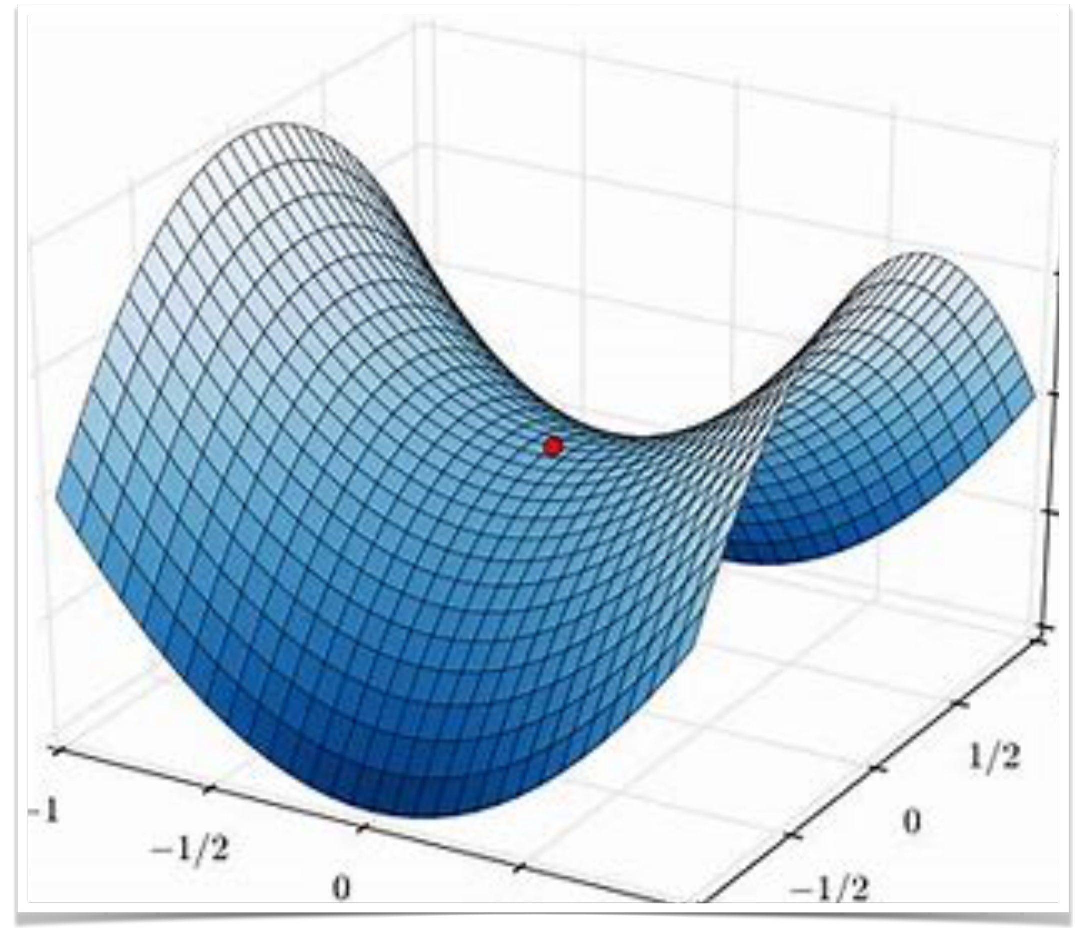

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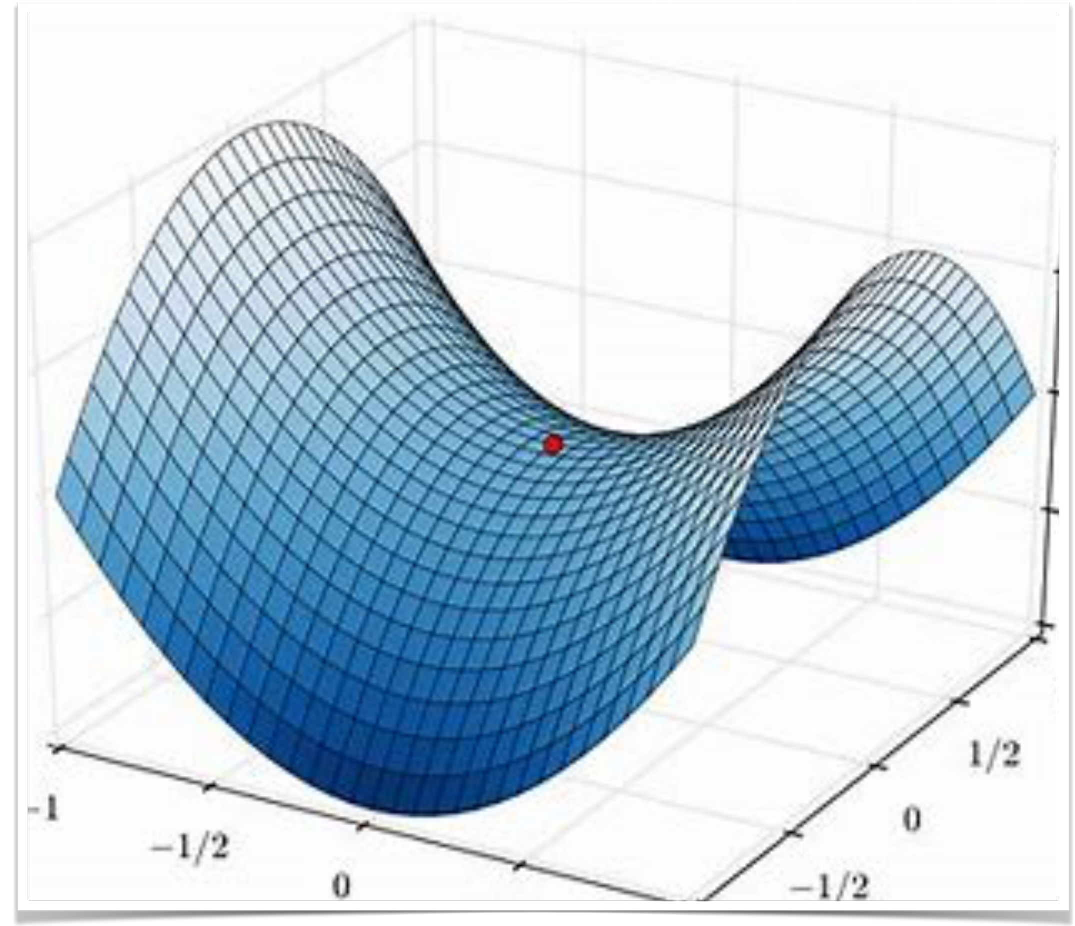

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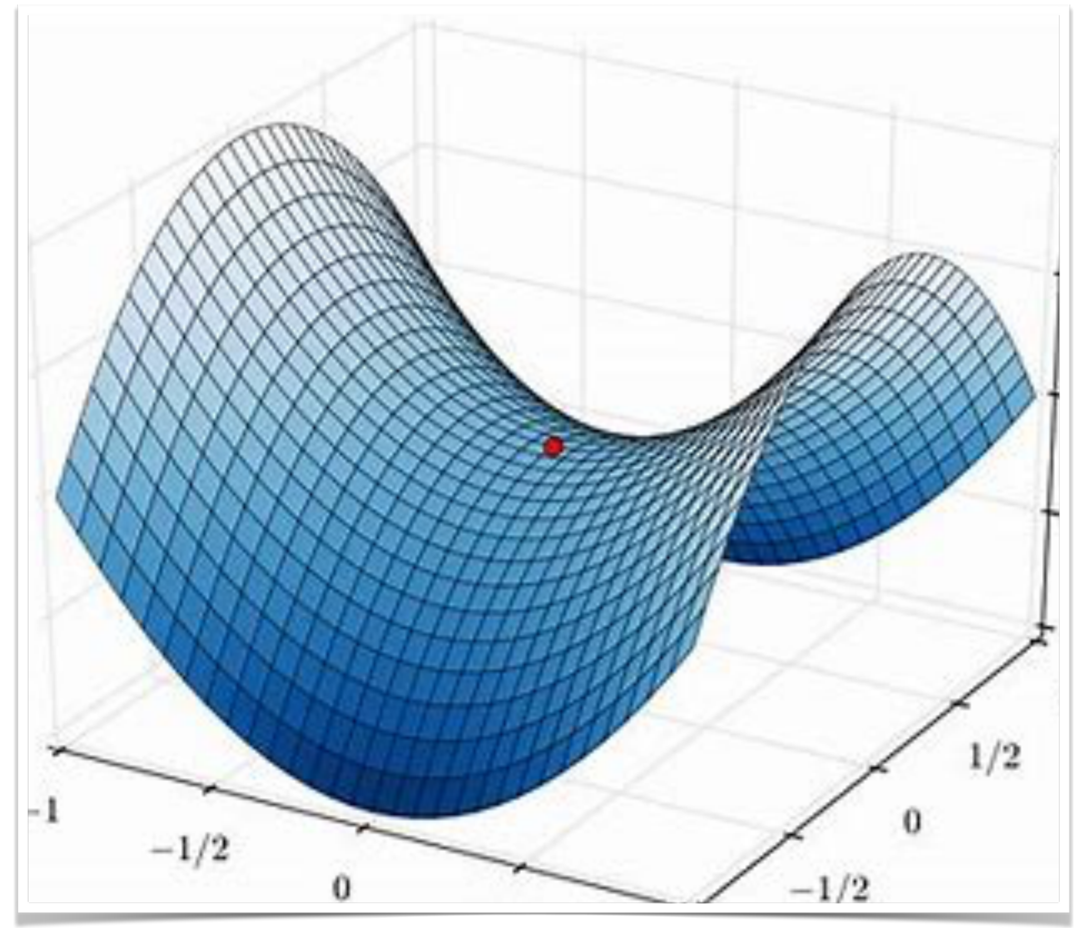
Almost always stationary point can have an *indefinite* Hessian



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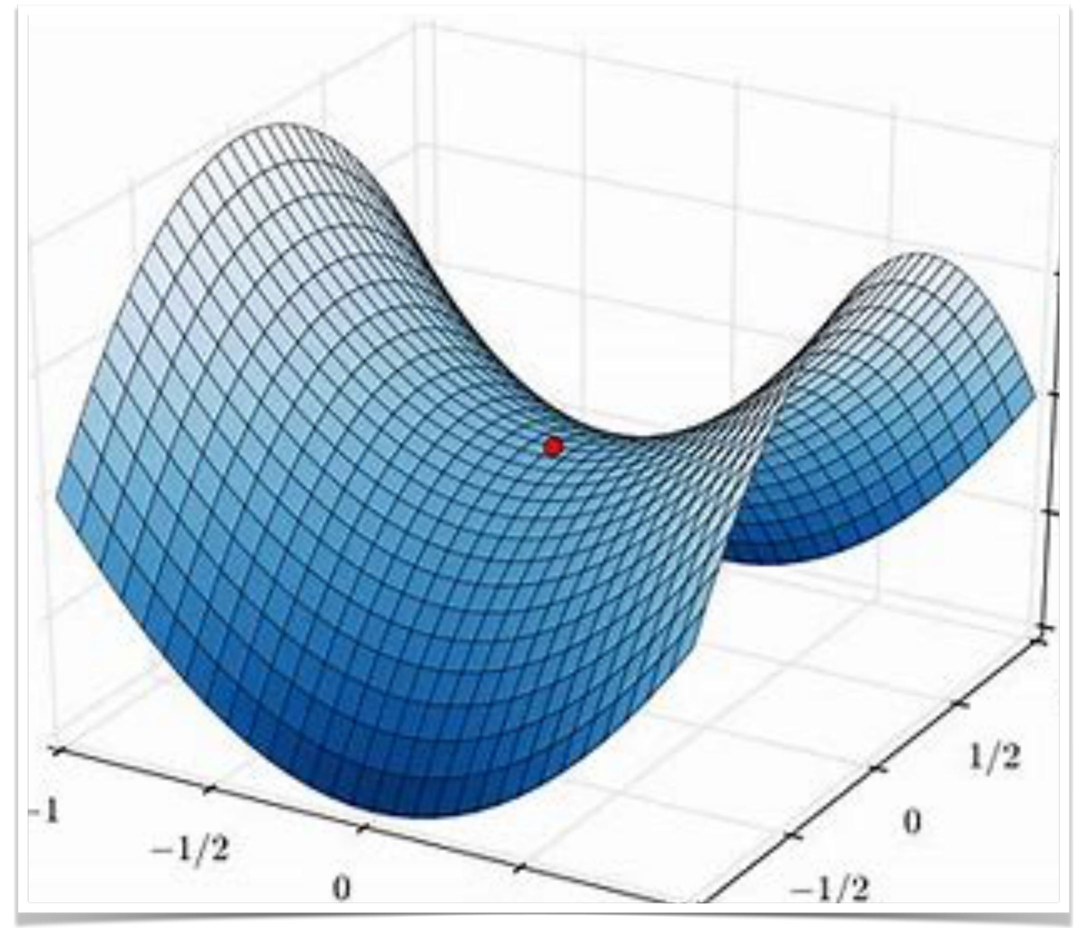

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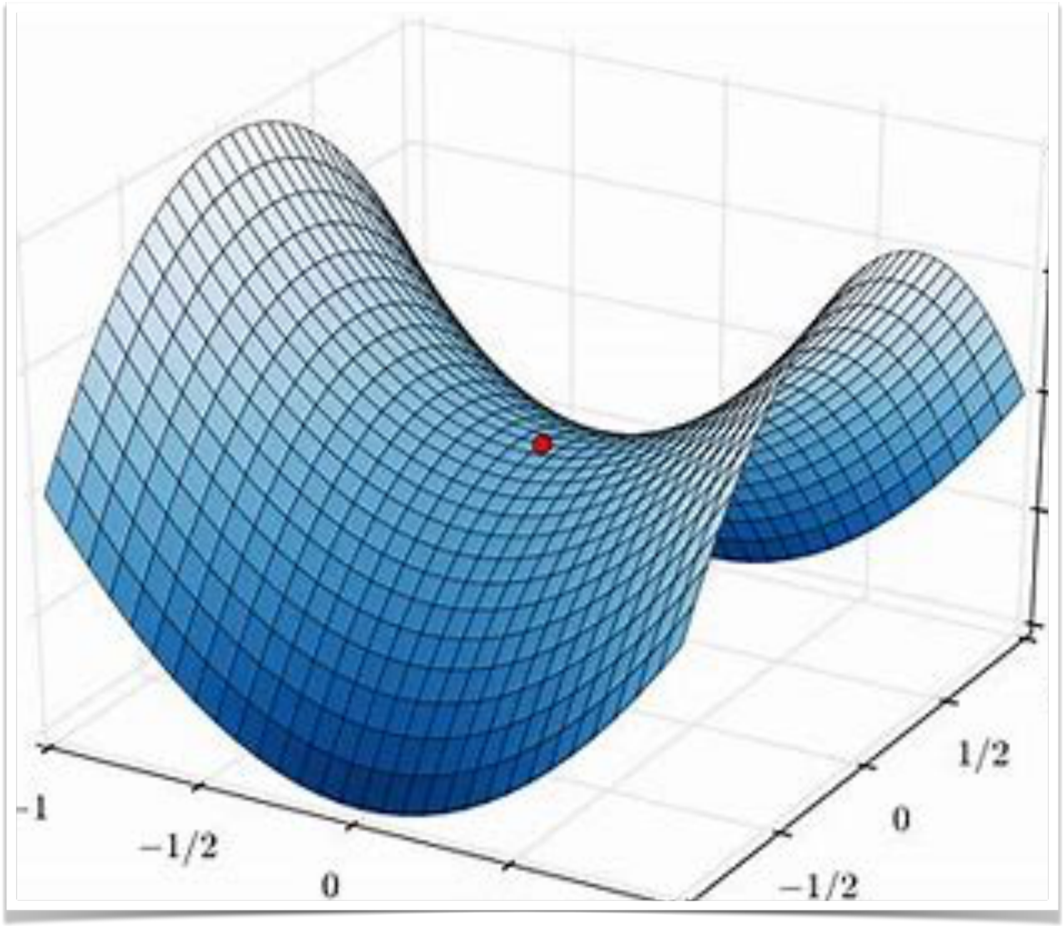

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Explore: Should we worry about saddle points in deep learning? Why?

Gradient descent escapes saddles

First-order methods almost always avoid strict saddle points

Jason D. Lee[1] · Ioannis Panageas[2] · Georgios Piliouras[3] · Max Simchowitz[4] · Michael I. Jordan[4] · Benjamin Recht[4]

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Assumption 1: f is C^2 and L-smooth (i.e., C_L^1)

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Theorem (informal). Let θ_0 be initialized randomly. Then with $\eta < 1/L$, under Assumptions 1, 2, GD avoids converging to saddle points.

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Key idea: show that GD *eventually* escapes any saddle point, by showing that the set of "stable strict saddles" is of measure 0. "Stable" in the sense of: an attracting equilibrium point for a dynamical system.

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What about a non-asymptotic result?

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Gradient Descent Can Take Exponential Time to Escape Saddle Points

Simon S. Du
Carnegie Mellon University
ssdu@cs.cmu.edu

Chi Jin
University of California, Berkeley
chijin@berkeley.edu

Jason D. Lee
University of Southern California
jasonlee@marshall.usc.edu

Michael I. Jordan
University of California, Berkeley
jordan@cs.berkeley.edu

Barnabás Póczos
Carnegie Mellon University
bapoczos@cs.cmu.edu

Aarti Singh
Carnegie Mellon University
aartisingh@cmu.edu

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$$\theta_{t+1} = \theta_t - \eta[\nabla f(\theta_t) + \xi_t], \qquad \xi_t \sim \mathrm{Unif}(\mathbb{B}(r))$$

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Theorem 4.1 (Uniform initialization over a unit cube)**.** *Suppose the initialization point is uniformly sampled from* $[-1,1]^d$. *There exists a function* f *defined on* $\mathbb{R}^d$ *that is* B*-bounded,* ℓ*-gradient Lipschitz and* ρ*-Hessian Lipschitz with parameters* B, ℓ, ρ *at most* $\mathrm{poly}(d)$ *such that:*

1. *with probability one, gradient descent with step size* $\eta \le 1/\ell$ *will be* $\Omega(1)$ *distance away from any local minima for any* $T \le e^{\Omega(d)}$.
2. *for any* $\epsilon > 0$*, with probability* $1 - e^{-d}$*, perturbed gradient descent (Algorithm 1) will find a point* x *such that* $\|x - x^*\|_2 \le \epsilon$ *for some local minimum* x^* *in* $\mathrm{poly}(d, \frac{1}{\epsilon})$ *iterations.*

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Question: Can this be improved?

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where $\tilde{\mathcal{O}}$ and $\tilde{\Theta}$ hide polylogarithmic factors in $d, \ell, \rho, 1/\epsilon, 1/\delta$ and $\Delta_f := f(\mathbf{x}_0) - f^\star$.

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Reference: Jin, Netrapalli, Ge, Kakade, Jordan. *"On Nonconvex Optimization for Machine Learning: Gradients, Stochasticity, and Saddle Points"*. arXiv:1902.04811

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Recommended reading:

On Nonconvex Optimization for Machine Learning: Gradients, Stochasticity, and Saddle Points

Chi Jin
University of California, Berkeley
chijin@cs.berkeley.edu

Praneeth Netrapalli
Microsoft Research, India
praneeth@microsoft.com

Rong Ge
Duke University
rongge@cs.duke.edu

Sham M. Kakade
University of Washington, Seattle
sham@cs.washington.edu

Michael I. Jordan

Other methods

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- SPIDER (variance reduced SGD) yields $O(\epsilon^{-3})$
- SGD with averaging and some tricks $O(\epsilon^{-3.5})$

Other methods

Escaping Saddle Points with Adaptive Gradient Methods

Matthew Staib*
MIT EECS
mstaib@mit.edu

Sashank Reddi
Google Research, New York
sashank@google.com

Satyen Kale
Google Research, New York
satyenkale@google.com

Sanjiv Kumar
Google Research, New York
sanjivk@google.com

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ADAM-like methods can escape saddle points faster than SGD

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Matthew Staib* MIT EECS mstaib@mit.edu

Sashank Reddi Google Research, New York sashank@google.com

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Matthew Staib*
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satyenkale@google.com

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Key question: Can SGD/ADAM escape fast without perturbation?

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Matthew Staib*
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Satyen Kale
Google Research, New York
satyenkale@google.com

Sanjiv Kumar
Google Research, New York
sanjivk@google.com

Suvrit Sra
MIT EECS
suvrit@mit.edu

ADAM-like methods can escape saddle points faster than SGD

However, iteration bound of the type $O(d^4\epsilon^{-5})$ for escaping saddles. SGD has a similar rate, but the "constants" for ADAM-like method can be much better.

Key question: Can SGD/ADAM escape fast without perturbation?

Sharp Analysis for Nonconvex SGD Escaping from Saddle Points

Cong Fang * Zhouchen Lin † Tong Zhang ‡

Other methods

Escaping Saddle Points with Adaptive Gradient Methods

Matthew Staib*
MIT EECS
mstaib@mit.edu

Sashank Reddi
Google Research, New York
sashank@google.com

Satyen Kale
Google Research, New York
satyenkale@google.com

Sanjiv Kumar
Google Research, New York
sanjivk@google.com

Suvrit Sra
MIT EECS
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This paper claims so, but by assuming "dispersive noise" on SGD. Clean results missing!