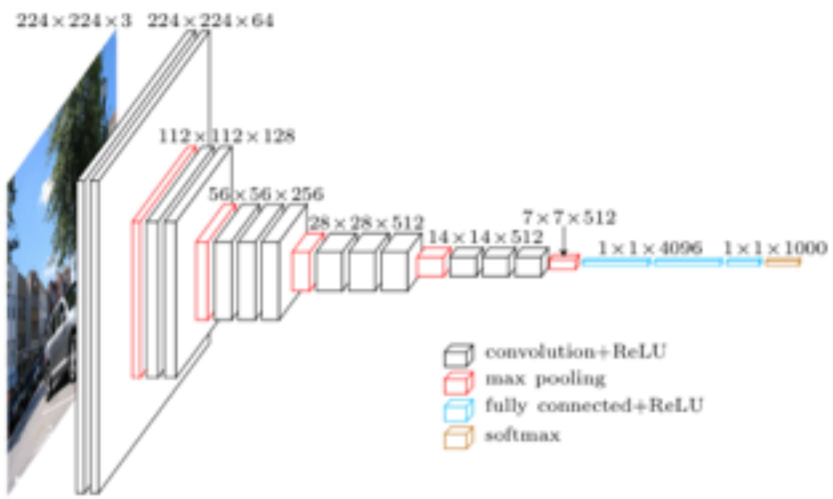
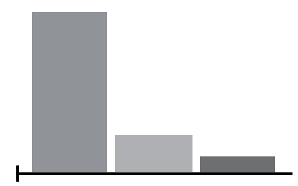
Unraveling the mysteries of stochastic gradient descent on deep neural networks

Pratik Chaudhari

UCLA VISION LAB

The question





measures disagreement of predictions with ground truth

$$x^* = \underset{x}{\operatorname{argmin}} f(x)$$

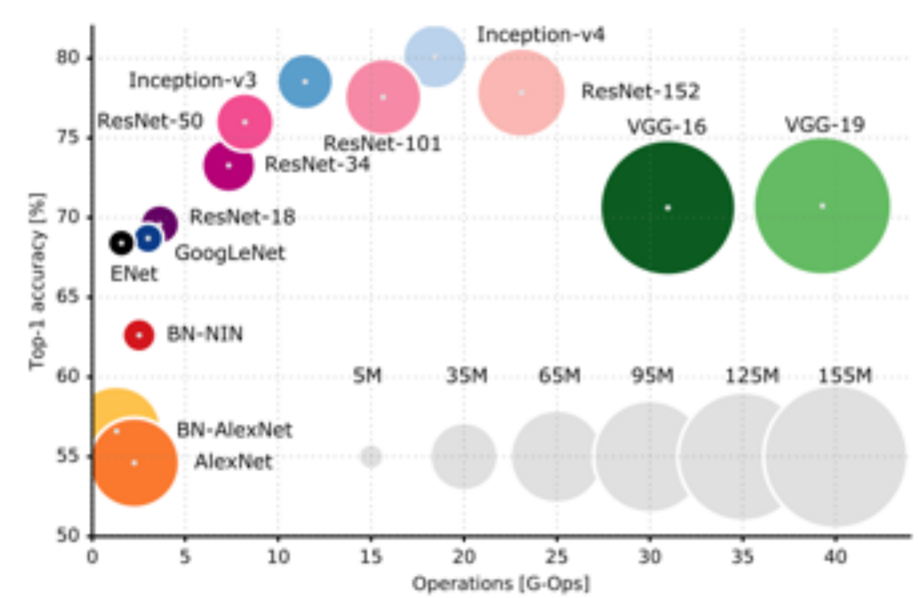
weights aka parameters

Stochastic gradient descent

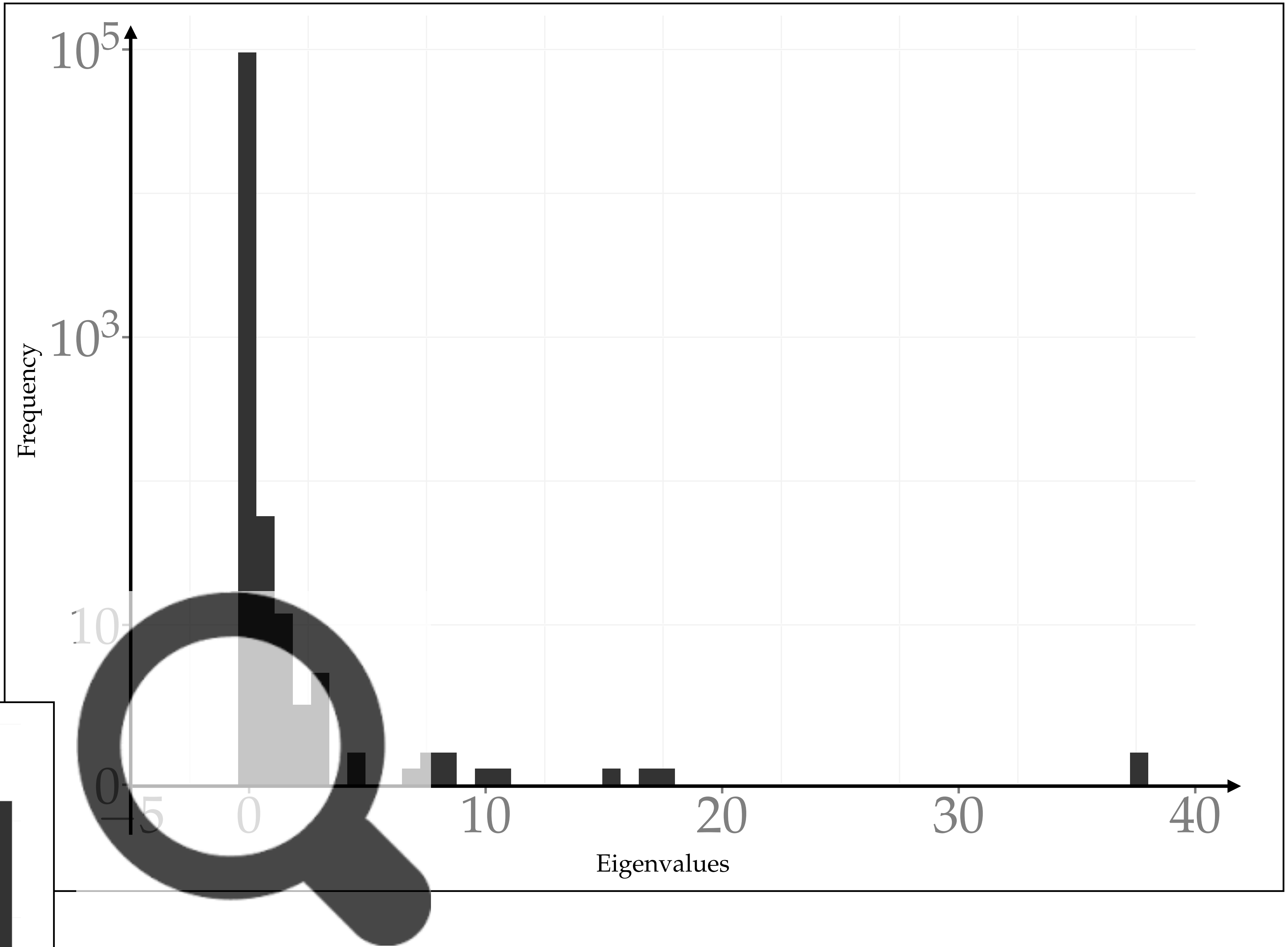
$$x_{k+1} = x_k - \eta \nabla f_{\mathcal{B}}(x_k)$$

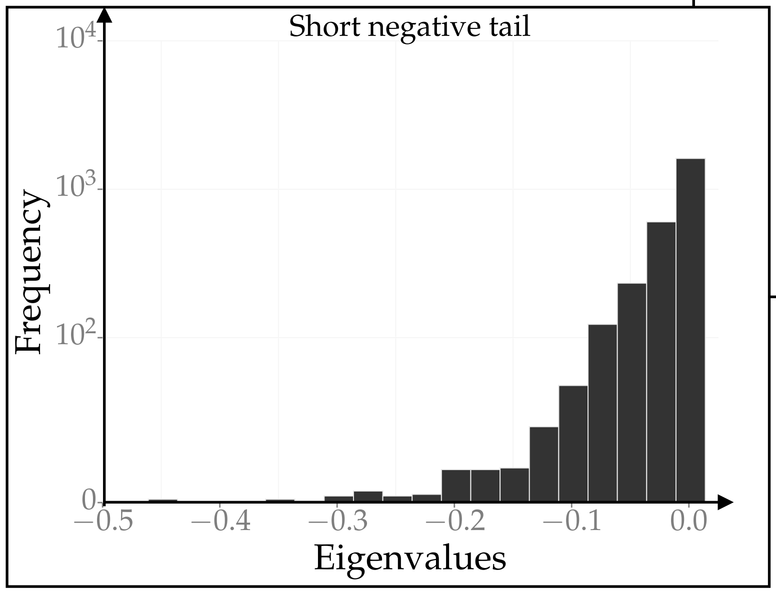
Many, many variants:
AdaGrad, rmsprop, Adam, SAG, SVRG, Catalyst, APPA, Natasha, Katyusha…

Why is SGD so special?



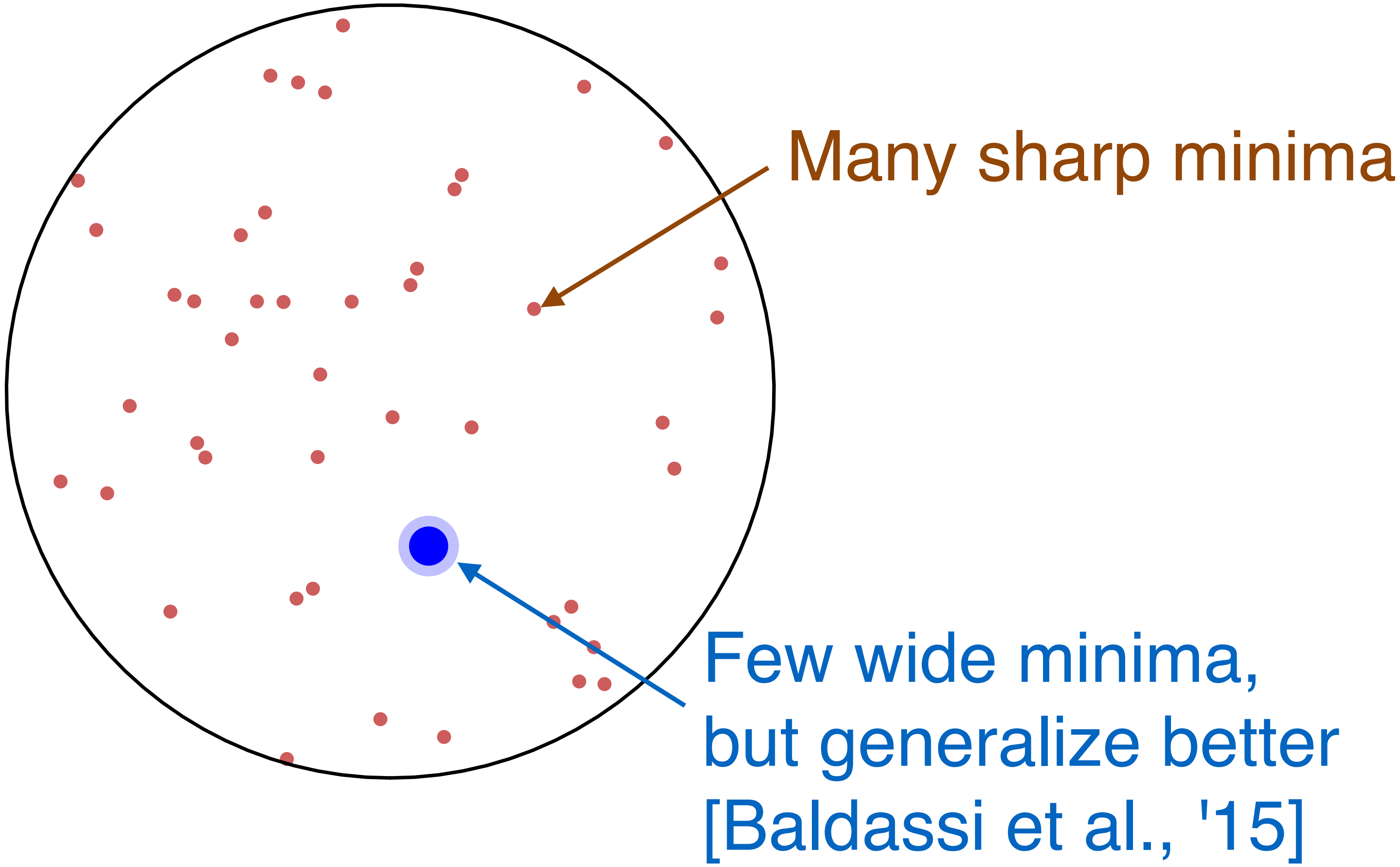
Empirical evidence: wide "minima"





A bit of statistical physics

- Energy landscape of a binary perceptron



- Wide minima are a large deviations phenomenon

Tilting the Gibbs measure

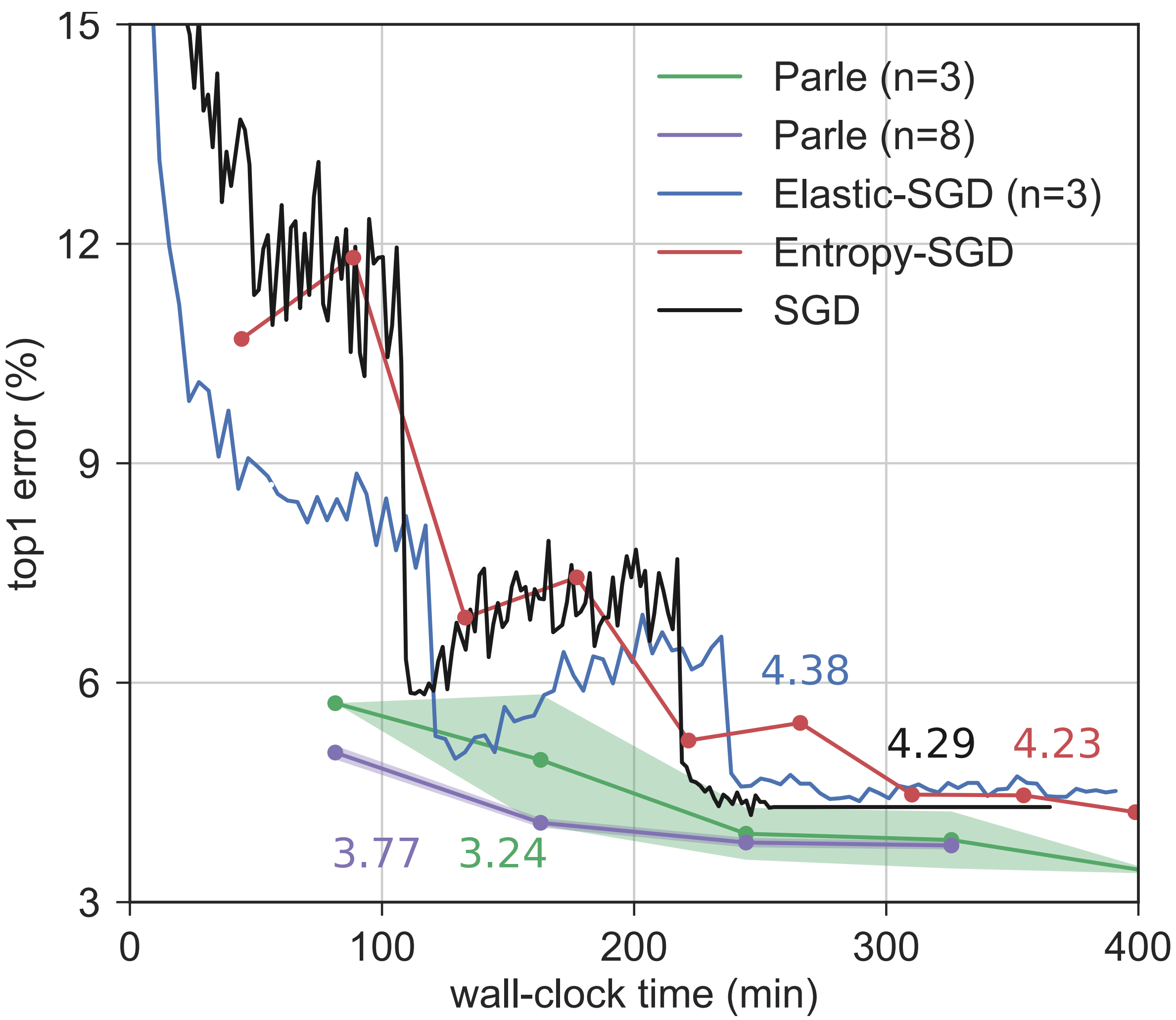
- Local Entropy [Chaudhari et al., ICLR '17]

$$
\begin{aligned}
x^* &= \underset{x}{\operatorname{argmin}} \; f(x) \\
&= \underset{x}{\operatorname{argmax}} \; e^{-f(x)} \\
&\approx \underset{x}{\operatorname{argmin}} \; -\log\left(G_\gamma * e^{-f(x)}\right)
\end{aligned}
$$

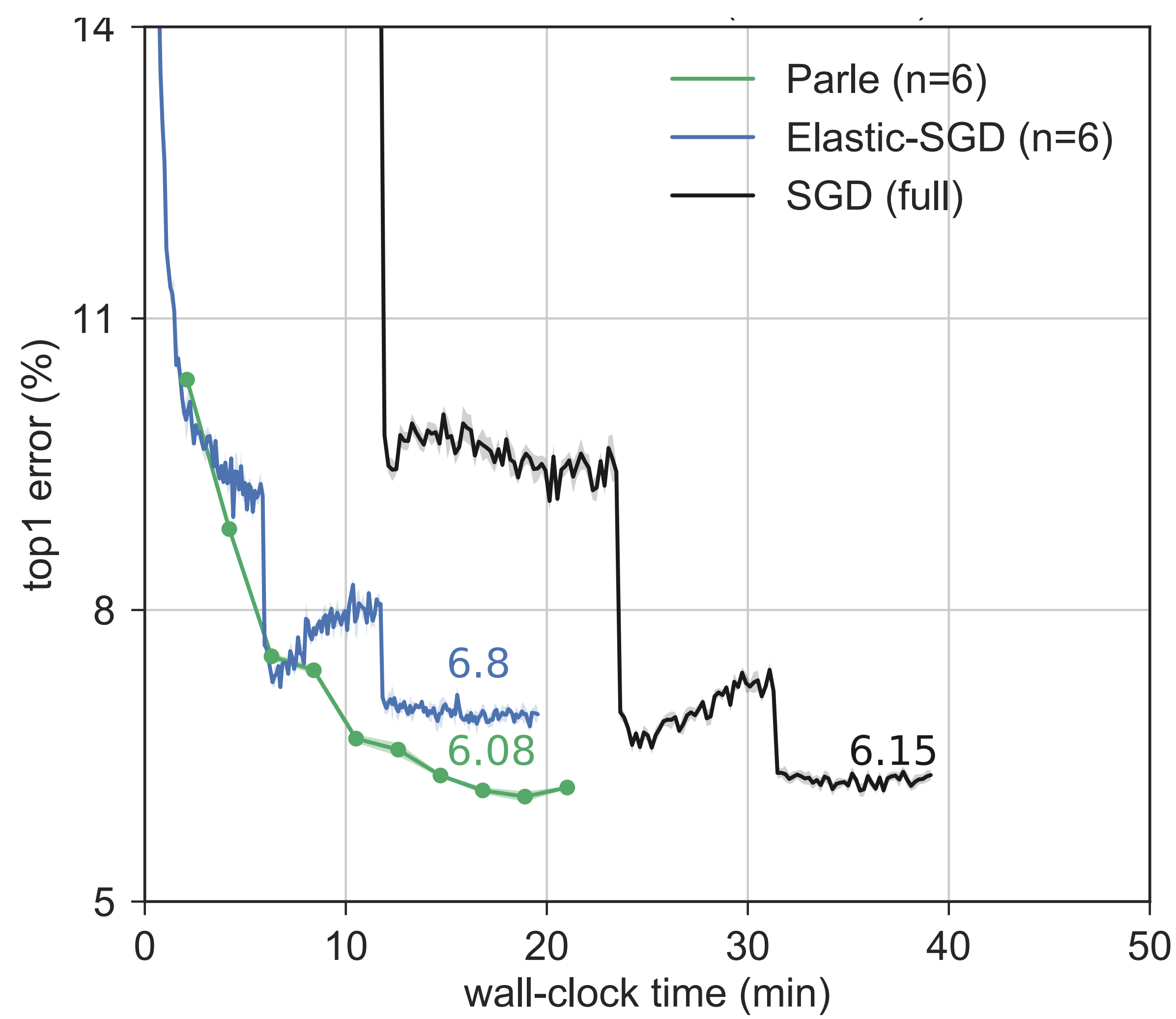
Gaussian kernel
of variance γ

Parle: parallelization of SGD

- State-of-the-art performance [Chaudhari et al., SysML '18]



Wide-ResNet: CIFAR-10



All-CNN: CIFAR-10 (25% data)

The question

Why is SGD so special?

A continuous-time view of SGD

- **Diffusion matrix:** variance of mini-batch gradients

$$\operatorname{var}\big(\nabla f_{\mathcal{b}}(x)\big) = \frac{D(x)}{\mathcal{b}}$$
$$= \frac{1}{\mathcal{b}}\left(\frac{1}{N}\sum_{k=1}^{N} \nabla f_k(x)\, \nabla f_k(x)^\top - \nabla f(x)\, \nabla f(x)^\top\right)$$

- **Temperature:** ratio of learning rate and step-size

$$\beta^{-1} = \frac{\eta}{2\mathcal{b}}$$

A continuous-time view of SGD

- Continuous-time limit of discrete-time updates

$$dx = -\nabla f(x) \underbrace{dt}_{\triangleq \eta} + \sqrt{2\beta^{-1} D(x)}\, dW(t)$$

will assume $x \in \Omega \subset \mathbb{R}^d$

- Fokker-Planck (FP) equation gives the distribution on the weight space induced by SGD

$$\rho_t = \text{div}\Big(\underbrace{\nabla f \rho}_{\text{drift}} + \underbrace{\beta^{-1} \text{div}\big(D\, \rho\big)}_{\text{diffusion}} \Big) \qquad \text{where } x(t) \sim \rho(t)$$

Wasserstein gradient flow

- Heat equation $\rho_t = \mathrm{div}\big(I\ \nabla\rho\big)$ performs steepest descent on the Dirichlet energy

$$\frac{1}{2}\int_\Omega \left|\nabla\rho(x)\right|^2\ dx$$

- It is also the steepest descent in the Wasserstein metric for

$$-H(\rho) = \int_\Omega \log\rho\ d\rho$$

$$\rho^\tau_{k+1} \in \operatorname*{argmin}_\rho \left\{-H(\rho) + \frac{\mathbb{W}_2^2(\rho,\rho^\tau_k)}{2\tau}\right\}$$

converges to trajectories of the heat equation

- Negative entropy is a Lyapunov functional for Brownian motion

$$\rho^{ss}_{\text{heat}} = \operatorname*{argmin}_\rho -H(\rho)$$

Wasserstein gradient flow: with drift

- If $D = I$, the Fokker-Planck equation

$$\rho_t = \operatorname{div}\left(\nabla f \rho \; + \beta^{-1} I \; \nabla \rho\right)$$

has the Jordan-Kinderleher-Otto (JKO) functional [Jordan et al., '97]

$$\rho^{\text{ss}}(x) = \underset{\rho}{\operatorname{argmin}} \; \underbrace{\mathbb{E}_{x\sim\rho}\left[f(x)\right]}_{\text{energetic term}} \; - \; \underbrace{\beta^{-1} \; H(\rho)}_{\text{entropic term}}$$

as the Lyapunov functional.

- FP is the steepest descent on JKO in the Wasserstein metric

What happens for non-isotropic noise?

$$\rho_t = \mathrm{div}\Big(\underbrace{\nabla f \rho}_{\text{drift}} + \underbrace{\beta^{-1} \mathrm{div}\big(D\, \rho\big)}_{\text{diffusion}} \Big)$$

- FP monotonically minimizes the free energy

$$\rho^{\mathrm{ss}}(x) = \underset{\rho}{\mathrm{argmin}}\ \mathbb{E}_{x \sim \rho}\Big[\Phi(x)\Big] - \beta^{-1} H(\rho)$$

- Rewrite as

$$F(\rho) = \beta^{-1} \mathrm{KL}\left(\rho \,\|\, \rho^{\mathrm{ss}}\right)$$

compare with |x - x*| for deterministic optimization.

SGD performs variational inference

Theorem [Chaudhari & Soatto, ICLR '18]

The functional

$$F(\rho) = \beta^{-1} \mathrm{KL}\left(\rho \,\|\, \rho^{\mathrm{ss}}\right)$$

is minimized monotonically by trajectories of the Fokker-Planck equation

$$\rho_t = \mathrm{div}\Big(\nabla f \rho + \beta^{-1} \mathrm{div}\left(D \, \rho\right)\Big)$$

with ρ^{ss} as the steady-state distribution. Moreover,

$$\Phi = -\beta^{-1} \log \rho^{\mathrm{ss}}$$

up to a constant.

Some implications

- Learning rate should scale linearly with batch-size

$$\beta^{-1} = \frac{\eta}{2\mathscr{b}} \quad \text{should not be small}$$

- Sampling with replacement regularizes better than without

$$\beta^{-1}_{\text{w/o replacement}} = \frac{\eta}{2\mathscr{b}}\left(1 - \frac{\mathscr{b}}{N}\right)$$

also generalizes better.

Information Bottleneck Principle

- Minimize mutual information of the representation with the training data [Tishby '99, Achille & Soatto '17]

$$\mathrm{IB}_\beta(\theta) = \mathbb{E}_{x\sim\rho_\theta}\left[f(x)\right] - \beta^{-1}\,\mathrm{KL}\left(\rho_\theta \,\|\, \text{prior}\right)$$

- Minimizing these functionals is hard, SGD does it naturally

Potential Phi vs. original loss f

- The solution of the variational problem is

$$\rho^{ss}(x) = \frac{1}{Z_\beta} e^{-\beta\,\Phi(x)}$$

- Key point

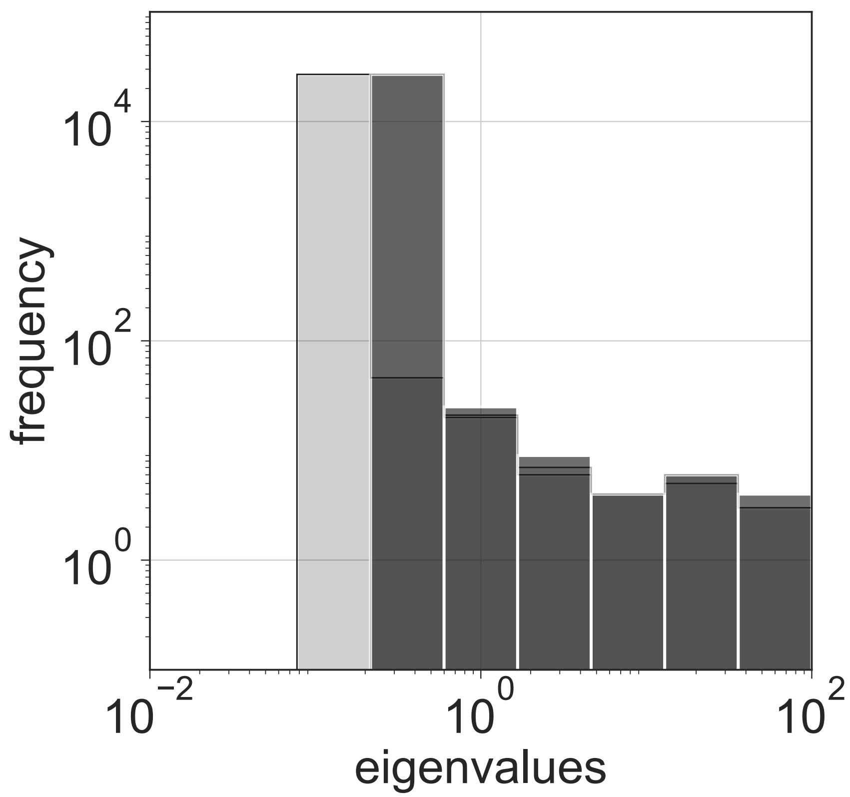
$$\rho^{ss}(x) \neq \frac{1}{Z'_\beta} e^{-\beta\,f(x)}$$

Most likely locations of SGD are not the critical points of the original loss

- The two losses are equal if and only if noise is isotropic

$$D(x) = I \quad \Leftrightarrow \quad \Phi(x) = f(x)$$

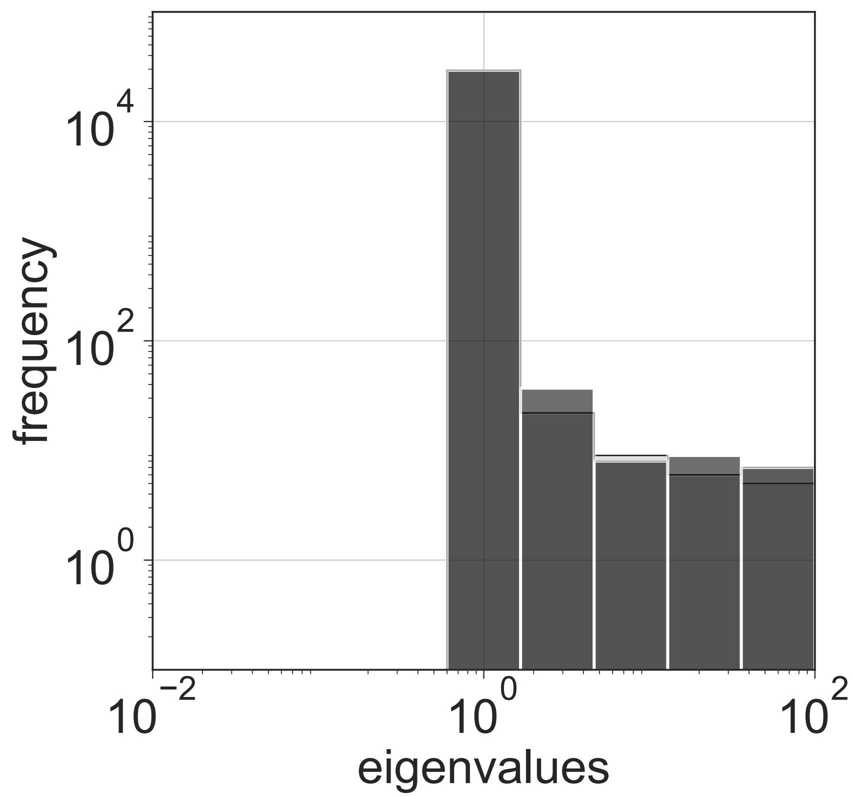
Deep networks have highly non-isotropic noise



CIFAR-10

$\lambda(D) = 0.27 \pm 0.84$

$\text{rank}(D) = 0.34\%$



CIFAR-100

$\lambda(D) = 0.98 \pm 2.16$

$\text{rank}(D) = 0.47\%$

- Evaluate neural architectures using the diffusion matrix

How different are cats and dogs, really?

SGD converges to limit cycles

Theorem [Chaudhari & Soatto, ICLR '18]

The most likely trajectories of SGD are

$$\dot{x} = j(x),$$

where the "leftover" vector field

$$j(x) = -\nabla f(x) + D(x)\,\nabla\Phi(x) - \beta^{-1}\,\mathrm{div}\,D(x)$$

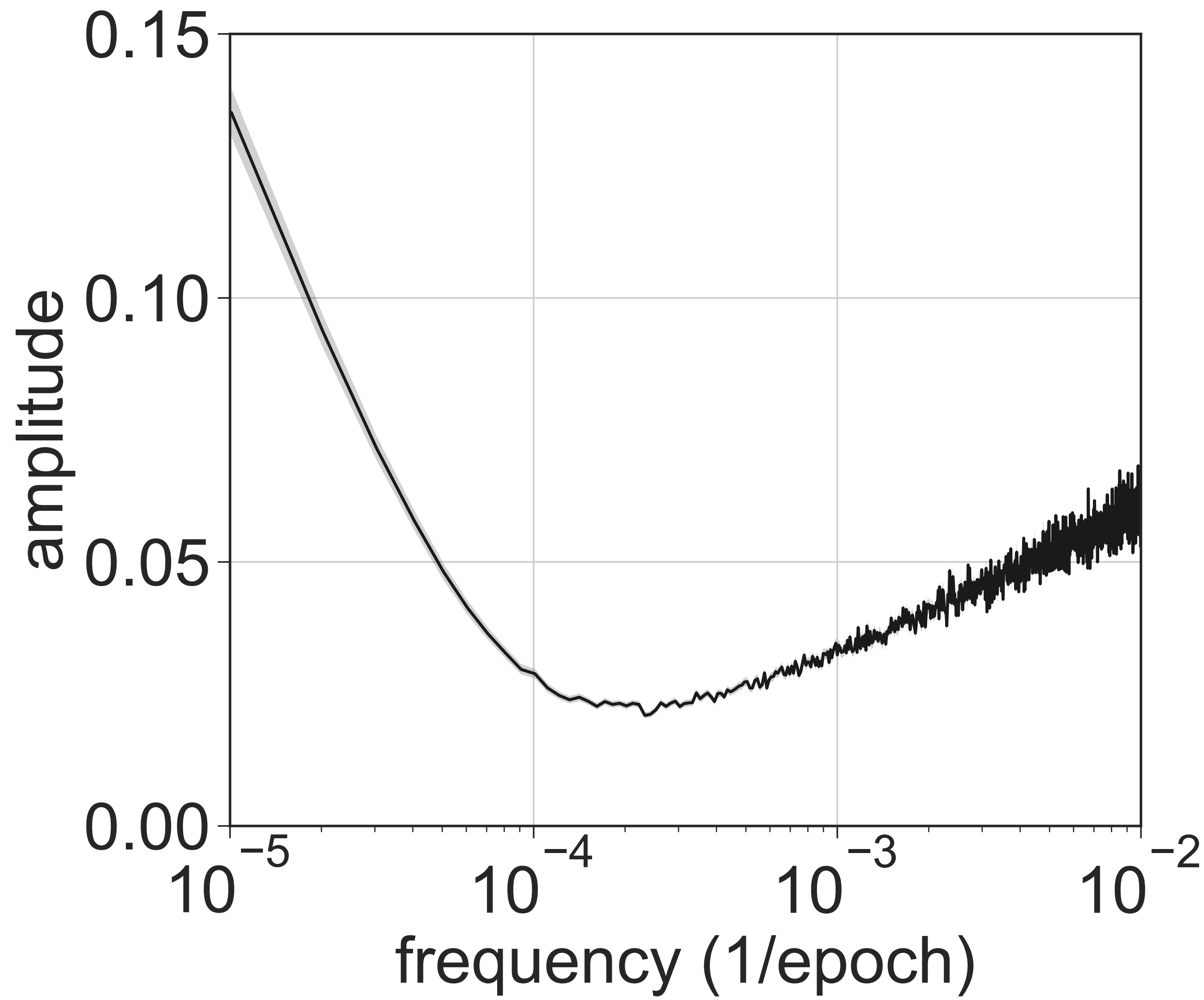
is such that

$$\mathrm{div}\, j(x) = 0.$$

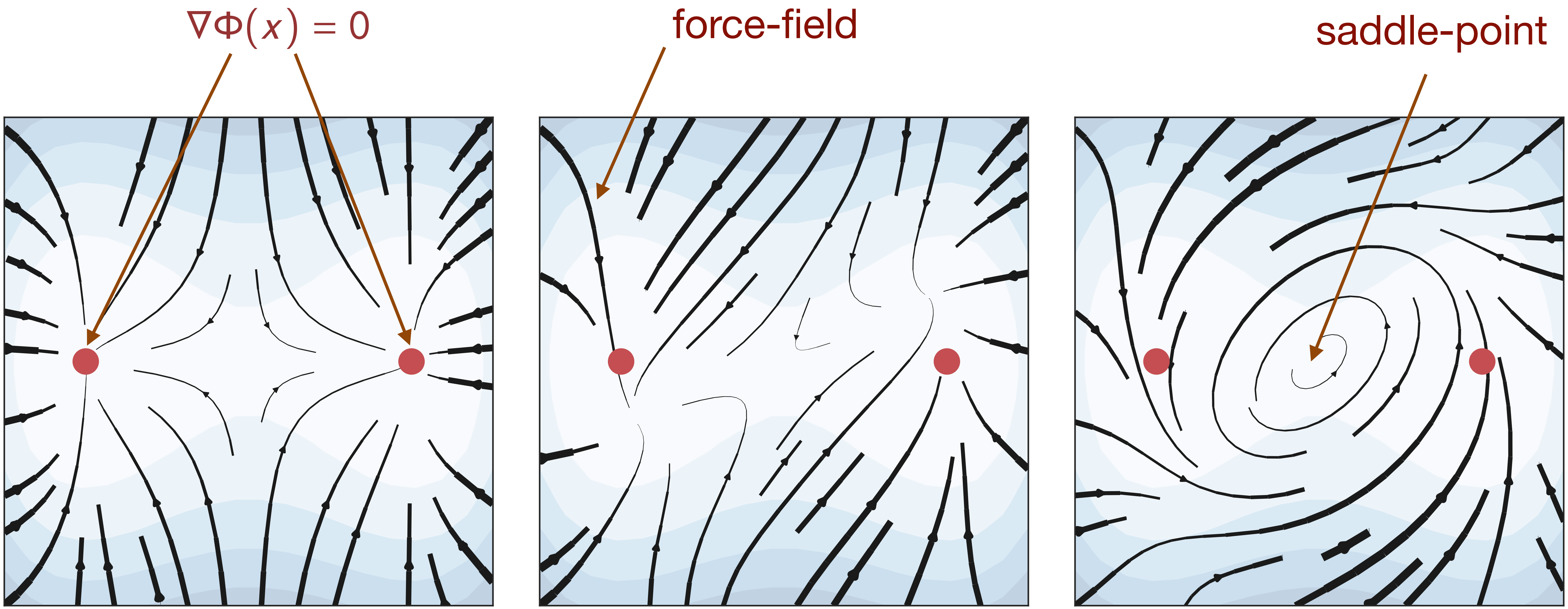
Trajectories of SGD

- Run SGD for 10^5 epochs

FFT of $x^i_{k+1} - x^i_k$



An example



$j(x) = 0$ | $|j(x)|$ is small | very large $|j(x)|$

Most likely locations are not the critical points of the original loss

Theorem [Chaudhari & Soatto, ICLR '18]

The Ito SDE

$$dx = -\nabla f \; dt + \sqrt{2\beta^{-1} D} \; dW(t)$$

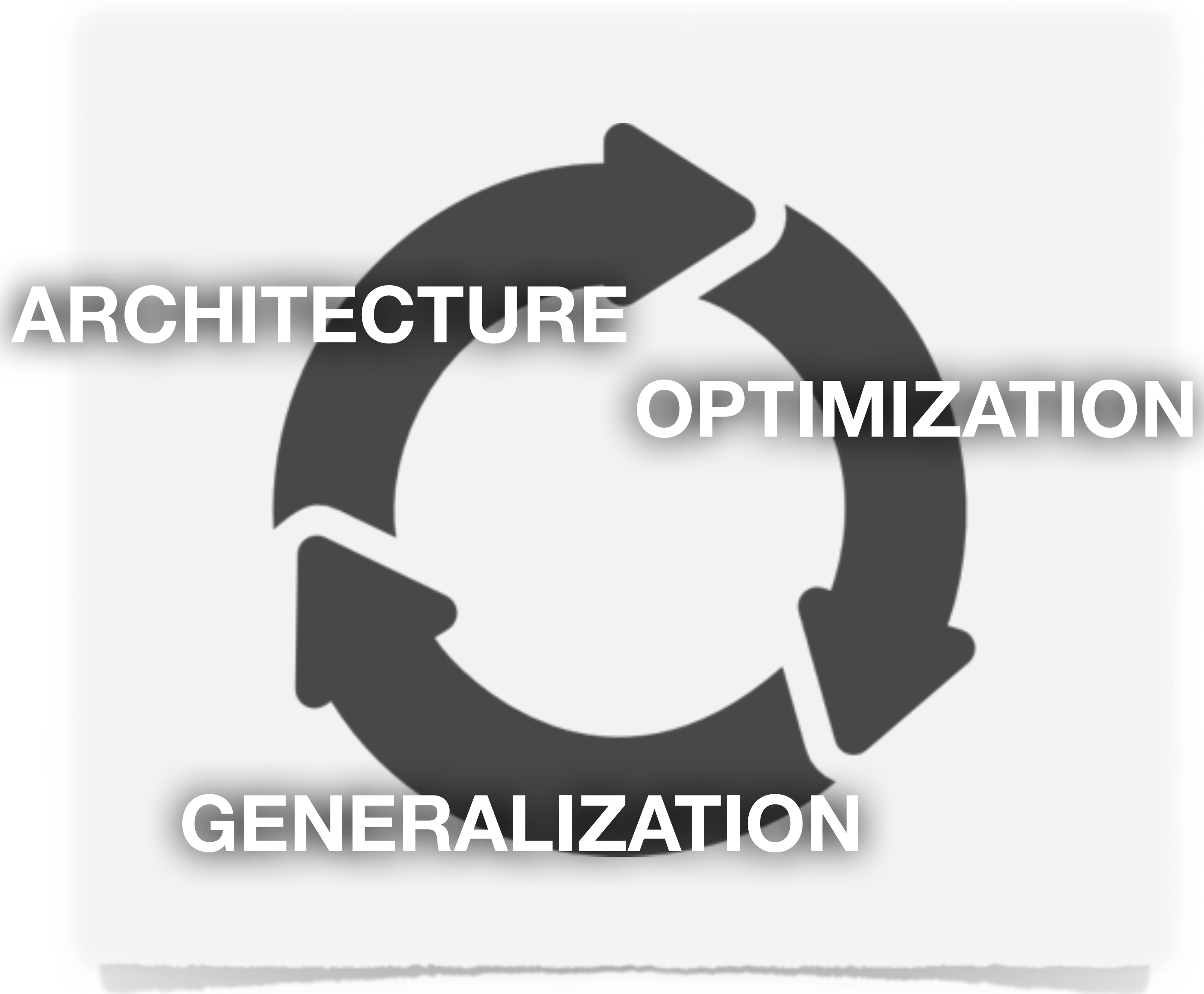
is equivalent to an A-type SDE

$$dx = -\big(D + Q\big) \; \nabla \Phi \; dt + \sqrt{2\beta^{-1} D} \; dW(t)$$

with the same steady-state $\rho^{ss} \propto e^{-\beta \Phi(x)}$ if

$$\nabla f = \big(D + Q\big) \; \nabla \Phi - \beta^{-1} \; \mathrm{div} \; \big(D + Q\big).$$

Knots in our understanding



Punchline

Is SGD special?

arXiv:1710.11029, ICLR '18

Stochastic gradient descent performs variational inference, converges to limit cycles for deep networks,
Pratik Chaudhari and Stefano Soatto.

www.pratikac.info

Thank you, questions?