How Can Increased Randomness in Stochastic Gradient Descent Improve Generalization?

Arwen V. Bradley*, Carlos A. Gómez-Uribe*

Apple
1 Infinite Loop, Cupertino, CA
{arwen_bradley, cgomezuribe}@apple.com

Abstract

Recent works report that increasing the learning rate or decreasing the minibatch size in stochastic gradient descent (SGD) can improve test set performance. We argue that this behavior is indeed expected under some conditions in models that have a loss function with multiple local minima. Our main contribution is an approximate but analytical approach inspired by methods in Physics to study the role of the SGD learning rate and batch size in generalization. We characterize test set performance under a shift between the training and test data distributions for loss functions with multiple minima. The shift between training and test can simply be due to sampling, and is therefore typically present in practical applications. We show that the resulting shift in local minima worsens test performance by picking up curvature, implying that generalization improves by selecting wide and/or little-shifted local minima. We then specialize our results to SGD, and study its test performance assuming it has reached stationarity. Because obtaining the exact stationary distribution of parameters that SGD produces is intractable, we derive a Fokker-Planck approximation of SGD and obtain its stationary distribution instead. This process shows that the learning rate divided by the minibatch size plays a role analogous to temperature in statistical mechanics, and implies that SGD, including its stationary distribution, is largely invariant to changes in learning rate or batch size that leave its temperature constant. We show that increasing SGD temperature encourages the selection of local minima with lower curvature, and can enable better generalization. We provide experiments on CIFAR10 demonstrating the temperature invariance of SGD, improvement of the test loss as SGD temperature increases, and quantifying the impact of sampling versus distribution shift in driving this effect. Finally, we present synthetic experiments showing how our theory applies in a simplified loss with two local minima.

1 Introduction

In typical machine learning applications, we seek to learn a model by fitting a training dataset that will ultimately perform well on unseen data, for which the test set is a proxy. Performance is measured by evaluating a loss function that depends on the model parameters and the data. Generalization refers to the performance of a model on the test set compared to its performance on the training set. Classical statistical theory holds that overparametrized models without sufficient regularization can overfit the training data, degrading performance on the test set. However, modern machine learning practice employs highly overparametrized deep learning models while maintaining good test performance (Nakkiran et al. 2019; Belkin 2021). This behavior may be related to the structure of the networks themselves (e.g. (Jacot, Gabriel, and Hongler 2018)), or the algorithms used to train them, or both. In this paper we focus on the latter, under the assumption that the model is complex enough that the loss function has multiple minima with respect to the model parameters.

Stochastic gradient descent (SGD) and its variants are commonly used for training deep networks. SGD is a stochastic iterative algorithm that processes only a subset of the training set (called a batch) at every iteration. Batch size directly impacts noise strength in SGD, with smaller batches resulting in more noise. Practitioners have observed that higher SGD noise can improve generalization. For example, (Smith, Elsen, and De 2020; McCandlish et al. 2018; Golmant et al. 2018; Hoffer, Hubara, and Soudry 2017) observed generalization improvements in large DNNs when SGD noise was increased by decreasing batch size or increasing learning rate. Similarly, (Shallue et al. 2018) observed that generalization suffered when batch size was increased unless additional regularization was used.

The noise in SGD affects both the rate of convergence1 (Lewkowycz et al. 2020) and the distribution of parameter values to which SGD converges; both of these are important for generalization. So increased noise could aid generalization in at least two ways: by speeding up the exploration of the loss landscape, and by encouraging SGD to sample parameter values with better generalization properties. In this

---

1The rate of convergence is related to the ‘escape time’ (or expected time to escape one basin around a local minimum of the loss, and explore another), which depends exponentially on the height of the loss (or ‘energy’1) barrier between the basins relative to the noise scale. (Van Kampen 1965; Kubo, Matsuo, and Kitahara 1973; Bovier et al. 2004; Freidlin and Weber 2004; Xie, Sato, and Sugiyama 2020). That means that with low noise, it can take a long time to explore new local minimum, consistent with observations that longer training is beneficial for generalization (Hoffer, Hubara, and Soudry 2017; Goyal et al. 2017).
paper, we focus only on the latter, under the assumption that SGD has converged to a stationary distribution. The role that SGD noise plays in generalization is an active research area: (Smith and Le 2017; Mandt, Hoffman, and Blei 2017; Ahn, Korattikara, and Welling 2012) take a Bayesian perspective, (Chaudhari and Soatto 2018) study the limiting SDE, (Belkin et al. 2019) focus on model capacity, (Martin and Mahoney 2018) apply random matrix theory, (Corneanu, Escalera, and Martinez 2020) propose persistent topology measures, (Russo and Zou 2016; Xu and Raginsky 2017) provide information-theoretic bounds, (Smith et al. 2021) perform error analysis relative to gradient flow, (Lee et al. 2017; Khan et al. 2019) connect to Gaussian processes, (Wu et al. 2019) analyze multiplicative noise, and (Zhu et al. 2018) study ‘escaping efficiency’.

Our main contribution is an approximate but analytical approach inspired by methods in Physics to study the role of the SGD learning rate and batch size in generalization. After describing our setup in Sec. 2, we obtain in Sec. 3 a novel expression that approximates model test performance under a shift between the training and test data distributions for complex losses with multiple minima when an arbitrary distribution of model parameters is provided. This shows that shifts in local minima pick up curvature that worsens test performance. Sec. 4 presents a new approximation for the shift in the local minima between training and test in terms of sampling effects and distribution shift. Next, we study test performance of SGD in Sec. 5. We find that it depends on the SGD temperature, which is equal to learning rate divided by batch size, and captures the noise strength in SGD. We show analytically in Sec. 6 that test performance can improve as SGD temperature increases when the loss function has multiple (two or more) minima, and when deeper local minimas have higher curvature. We conclude with a brief discussion in Sec. 7. Additional contributions which we believe to be novel include (i) a method for approximating a discrete-time Markov process with a continuous-time Markov process, (ii) a more explicit expression for the multi-parameter stationary SGD distribution than has been described before, as well as a Gaussian mixture approximation thereof, and (iii) experiments on CIFAR10 demonstrating improvement of the test loss as a function of temperature and offering insight into the role of sampling versus distribution shift, as well as (iv) synthetic experiments that validate our theory with a simplified loss with two local minima.

2 Setup

We consider a loss $U(x, \theta)$ that depends on the data $x$ and model parameters $\theta$ that is a log-likelihood but otherwise arbitrary, i.e., $U(x, \theta) = - \log p(x|\theta)$, where $p$ is some underlying conditional probability density that defines the model, and $\theta \in \mathbb{R}^n$. We assume we are given a training set $D_t = \{x_1^{(t)}, \ldots, x_{N_t}^{(t)}\}$ obtained from independent and identically distributed (i.i.d.) sampling from a training (or training) distribution $r_t(x)$. As a shorthand, we write $x_i^{(t)} \sim r_t(x)$ to mean that the training examples are i.i.d. samples from $r_t(x)$. Similarly, we assume we are given a test data set $D_e = \{x_1^{(e)}, \ldots, x_{N_e}^{(e)}\}$, with $x_i^{(e)} \sim r_e(x)$, where $r_e(x)$ is the evaluation (or test) distribution. We generally assume the dataset sizes to be large enough so that $N_t^{-1}$ and $N_e^{-1}$ are both small. We define the point-wise (for a given $\theta$) training and testing losses

$$L_t(\theta) = \frac{1}{N_t} \sum_{i=1}^{N_t} U(x_i^{(t)}, \theta) = \int q_t(x) U(x, \theta) dx,$$  

(1)

$$L_e(\theta) = \frac{1}{N_e} \sum_{i=1}^{N_e} U(x_i^{(e)}, \theta) = \int q_e(x) U(x, \theta) dx,$$  

(2)

where the training set and test set distributions $q_t(x)$ and $q_e(x)$ are defined through the use of the Dirac delta function\footnote{Recall that the Dirac delta function satisfies $\int \delta(x-x_0) f(x) dx = f(x_0)$ for any function $f(x)$ and an arbitrary value $x_0$ of $x$. E.g., applying this relation to the right-hand side of Eqs. 1 and 2 yields the middle expressions in the same equations.} $\delta(x)$ via $q_t(x) = \frac{1}{N_t} \sum_{i=1}^{N_t} \delta(x - x_i^{(t)})$, and $q_e(x) = \frac{1}{N_e} \sum_{i=1}^{N_e} \delta(x - x_i^{(e)})$. The dataset distributions $q_t(x)$ and $q_e(x)$ allow us to replace dataset averages by expectations, as in Eqs. 1 and 2, and will simplify our exposition. In general, $r_e(x) \neq r_t(x)$, but even when these distributions are identical, $q_t(x) \neq q_e(x)$ because of sampling, unless the data sets are infinite. We assume that $L_e(\theta)$ is a function with multiple local minima at $\theta = \theta_k$, and generally reserve $k$ as an index that runs through local minima. We let $U_k = L_e(\theta_k)$ denote the local loss, and $C_k = \partial^2 L_e(\theta_k) \in \mathbb{R}^{n \times n}$ the local curvature of the test loss at $\theta_k$. Both of these quantities are important for good model performance, as we will see. We also assume $L_e(\theta)$ has local minima at $\theta_k$, and assume there is a one-to-one mapping between local minima
of $\mathcal{L}_c(\theta)$ and $\mathcal{L}_t(\theta)$. We will see that understanding the difference $\hat{\theta}_k - \theta_k$ is important. Throughout our note, all quantities with a tilde (like $\hat{\theta}_k$) are analogous to those without a tilde but refer to the training (loss or data set or distribution) rather than to the test (loss or data set or distribution). E.g., $\dot{C}_k = \partial^2_\theta \mathcal{L}_c(\hat{\theta}_k)$ is the local curvature of the training loss. The assumptions stated are required to enable our subsequent analysis, and are the main limitations of our approach. For example, some deep learning models may have losses with local minima that are not points, but collections of points; or there may not be a one-to-one correspondence between train and test minima. Future work is needed to accommodate such situations.

Because we are interested in SGD, which returns a distribution over model parameters, assume we are given an arbitrary distribution of model parameters $\rho(\theta)$. We define the test set performance $\mathcal{L}_e$, which is ultimately how we define the performance of a model-algorithm combination, by

$$\mathcal{L}_e = \int \rho(\theta) \mathcal{L}_e(\theta) d\theta. \quad (3)$$

We specialize $\rho(\theta)$ shortly to a general mixture of Gaussians first, and then to the approximate stationary distribution produced by SGD after analyzing the training set.

## 3 Test Set Performance For Gaussian Mixture

Our goal here is to obtain an approximate expression for $\mathcal{L}_e$ when $\rho(\theta)$ is a mixture of Gaussians with one component for every local minimum of $\mathcal{L}_c(\theta)$. This form for $\rho(\theta)$ turns out to work well for SGD. We define

$$\rho(\theta) = \sum_k w_k \mathcal{N}(\mu_k, \Sigma^2_k) = \sum_k w_k \rho_k(\theta), \quad (4)$$

where $w_k, \mu_k, \Sigma^2_k$ are the weights, means, and covariances of the Gaussians. We define the local bias $b_k = \mu_k - \hat{\theta}_k$ due to the algorithm, and the (algorithm independent) shift in the local minima between the training and test loss $s_k = \hat{\theta}_k - \theta_k$.

and expand the loss about $\theta_k$:

$$U(x, \theta) = U(x, \theta_k) + \delta \partial_\theta U(x, \theta_k) + \frac{1}{2} \delta^2 \partial^2_\theta U(x, \theta_k) \delta,$$

where $\delta = \theta - \theta_k = \theta - \mu_k + b_k + s_k$.

Taking the expectation with respect to both the test set distribution $q_e(x)$ and $\rho_k(\theta)$ yields

$$E_{\rho_k} [\mathcal{L}_e(\theta)] = U_k + \frac{1}{2} E_{\rho_k} [\delta^2 C_k \delta],$$

where $E_{\rho_k} [\cdot]$ denotes expectation under $\rho_k(\theta)$. The mean and second moment of $\delta$ are easy to find:

$$E_{\rho_k} [\delta] = b_k + s_k$$

$$E_{\rho_k} [\delta^2] = \Sigma_k + (b_k + s_k) (b_k + s_k)'$$

$$\implies E_{\rho_k} [\delta^2 C_k \delta] = \text{Tr}(C_k E_{\rho_k} [\delta^2]) = \text{Tr}(C_k \Sigma_k + (b_k + s_k) C_k (b_k + s_k)). \quad (5)$$

Therefore:

$$E_{\rho_k} [\mathcal{L}_e(\theta)] = U_k + \frac{1}{2} \left[ \text{Tr}(C_k \Sigma_k + (b_k + s_k) C_k (b_k + s_k)) \right] = \text{Tr}(C_k \Sigma_k) + (b_k + s_k) C_k (b_k + s_k). \quad (6)$$

Here and elsewhere the angle brackets denote expectation under $w_k$ over any local-minima dependent quantity $f_k$, i.e., $\langle f \rangle = \sum k w_k f_k$. Eq. 6 is our main result here. It combines key quantities of different kinds: some that are determined solely by the loss (its value and curvature $U_k$ and $C_k$), others that depend on both the loss and the underlying distributions that generate the datasets (the shifts in the local minima $s_k$), and finally others that depend on the algorithm as well ($b_k, w_k$, and $\Sigma_k$). In SGD, we will find that the term in Eq. 6 proportional to $s_k C_k s_k$ is the key to understand test performance as learning rate and batch sizes change. To proceed further, then, we need expressions for the shift, and for the algorithm-dependent quantities when SGD is employed.

Some authors have suggested that generalization quality can be tied directly to curvature ($C$ in Equation 6) (Jiang et al. 2019; Keskar et al. 2016; Hochreiter and Schmidhuber 1997), but (Dinh et al. 2017) argue against this by observing that one can reparametrize $p(x|\theta)$ to obtain an identical data distribution (or model), but change the curvature of the local minima. While it is true that $C$ is not invariant to reparametrization, we show in the appendix C that just like the original point-wise losses, Equation 6 is reparametrization-invariant when SGD is used.

## 4 The Shifts In Local Minima

Here we find an approximate expression for the shifts $s_k$. When there is distribution shift, i.e., when the training and test distributions $r_t(x)$ and $r_r(x)$ are different, we expect the training and test losses in Eqs. 1 and 2 to be different. But even in the absence of distribution shift, the losses can differ due to the sampling that determines the test set distributions $q_e(x)$ and $q_r(x)$ that define the losses. We model shifts that arise due to either distribution shift, or sampling, as follows.

| Symbol | Definition | Notes |
|--------|------------|-------|
| $q_e(x)$ | Test data distribution | |
| $q_t(x)$ | Training data distribution | |
| $U(x, \theta)$ | Loss function | |
| $\mathcal{L}_c(\theta)$ | Expected test loss | |
| $\mathcal{L}_t(\theta)$ | Expected train loss | |
| $\theta_k$ | $\arg\min \mathcal{L}_c(\theta)$ | Test loss minima |
| $\delta$ | $\arg\min \mathcal{L}_t(\theta)$ | Training loss minima |
| $s_k$ | $\hat{\theta}_k - \theta_k$ | Train/test shift |
| $U_k$ | $\mathcal{L}_c(\theta_k)$ | Objective at local minima |
| $C_k$ | $\partial^2_\theta \mathcal{L}_c(\hat{\theta}_k)$ | Curvature at local minima |
| $D_k$ | $E_{q_e} \partial_\theta U(x, \theta_k)^2$ | Gradient variance |
| $\rho(\theta)$ | $\sum_k w_k \mathcal{N}(\mu_k, \Sigma^2_k)$ | Parameter distribution |
| $b_k$ | $\mu_k - \hat{\theta}_k$ | Biases of $\rho$ |
First, we now assume that the training and test distributions come from the same space of probability distributions, and can be parametrized, with \( r_t(x) = r(x | \eta_t) \) and \( r_r(x) = r(x | \eta_r) \), where the parameter \( \eta \in \mathbb{R}^m \). We let \( \epsilon = \eta_r - \eta_t \), assume \( \epsilon \) is small, and expand \( r_t(x) \) to first order to obtain
\[
r_t(x) = r_r(x) + \epsilon \frac{\partial}{\partial \eta} r(x | \eta_r).
\] (7)

In addition, since datasets are large, we can approximate the gradient of the losses from a sample from Gaussian random variables with a mean and covariance that are proportional to the mean and covariance of the gradients under the appropriate training and test distributions. These assumptions can be used to show that to leading order in our small parameters \( \epsilon, N^{-1}_k \) and \( N^{-1}_e \), the following approximate expression for the shift holds:
\[
s_k \approx C^{-1}_k z_k, \text{ where } z_k \sim N\left(F_k \epsilon, \frac{1}{N_{\text{eff}}} 2D_k\right),
\] (8)
so \( E[s_k] = C^{-1}_k F_k \epsilon \), and
\[
\text{Cov}(s_k) = \frac{1}{N_{\text{eff}}} 2C^{-1}_k D_k C^{-1}_k,
\] (9)
where we define
\[
N_{\text{eff}} = \frac{1}{2} \left(N^{-1}_e + N^{-1}_k\right), \quad R(x, \eta) = -\log r(x | \eta),
\]
\[
F(\theta) = \int r(x) \frac{\partial \theta}{\partial \theta} U(x, \theta) \frac{\partial}{\partial \eta} R(x, \eta) \, dx, \quad F_k = F(\theta_k),
\]
\[
D(\theta) = \text{Cov}_{\theta_k} \left( \frac{\partial \theta}{\partial \theta} U(x, \theta) \right), \quad D_k = D(\theta_k).
\] (11)

Here \( N_{\text{eff}} \) is the effective data set size; the harmonic mean of the training and test set sizes. \( F_k \in \mathbb{R}^{n \times m} \) is the covariance of gradients of \( U \) and \( R \) under \( r_r(x) \). \( E[\cdot] \) denotes expectation over data set realizations sampled from \( r_t(x) \) and \( r_r(x) \).

The local curvature \( C_k \) is related to the covariance of gradients \( D_k \), a fact we will use later. To see this, note that
\[
\frac{\partial^2}{\partial \eta^2} U(x, \theta) = \frac{\partial^2 p(x | \theta)}{p(x | \theta)} + \frac{\partial}{\partial \theta} U(x, \theta) \frac{\partial}{\partial \eta} U(x, \theta), \text{ so}
\]
\[
\Rightarrow D_k = C_k - E_k, \quad E_k := -E_{\theta_k} \left[ \frac{\partial^2 p(x | \theta_k)}{p(x | \theta_k)} \right],
\] (12)

where we took the average of the first equation with respect to \( q_r(x) \). By definition \( D_k \geq 0 \), so \( C_k - E_k \geq 0 \). Similarly, \( C_k > 0 \) by definition. If \( \theta_k \) is close to a maximum of \( p(x | \theta) \), we expect \( E_k \geq 0 \) as well.

To gain some further intuition about the shift \( s_k \), we consider the special case when all distributions belong to the same model space, data sets are infinite, and where both \( \eta \) and \( \theta \) are so-called location parameters. As shown in Appendix D, in that case \( F_k = C_k \) and \( s_k = \epsilon \). In general, Eq. 9 shows that the average shift is zero when there is no distribution shift, and is proportional to the distribution shift \( \epsilon \). Eq. 10 shows that the covariance of the shift is independent of the distribution shift, and goes to zero as the data sets become infinite. However, the shift can still impact model performance significantly for models with many parameters even when the train and test set sizes \( N_e \) and \( N_t \) are large and there is no distribution shift. Indeed, Eq. 6 shows that performance depends on the shift via \( s_k' C_k \), and
\[
E[s_k' C_k] = \text{Tr} \left( C_k \text{Cov}(s_k) \right) + E[s_k' \text{Cov}(s_k)] C_k E[s_k]
\]
\[
= \frac{2}{N_{\text{eff}}} (n - \text{Tr}(E_k C_k^{-1})) + \epsilon'_k F_k C_k^{-1} F_k \epsilon.
\] (13)

We used Eq. 12 to get the last equality. The second term on the right is quadratic in \( \epsilon \) and disappears in the absence of distribution shift. But the first one is always present in finite data sets, and can be as large as \( \frac{2n}{N_{\text{eff}}} \). The experiments in Figure 2 suggest that for the CIFAR10 dataset, sampling rather than distribution shift causes the shift \( s \).

## 5 Stochastic Gradient Descent

SGD attempts to minimize the training loss \( L_t(\theta) \) through a discrete-time stochastic process with state \( \theta_t \in \mathbb{R}^m \), where \( t \) is an integer indexing time, that changes in value by the random variable \( \Delta_t \) that depends on the training data:
\[
\theta_{t+1} = \theta_t + \Delta_t, \text{ where}
\] (14)
\[
\Delta_t = -\frac{\lambda}{B} \sum_{i=1}^{B} \frac{\partial \theta}{\partial \theta} U(x_i, \theta), \text{ where } x_i \sim q_t(x).
\] (15)

We refer to \( B \) as the mini-batch size, and to the step size \( \lambda \) as the learning rate. In order to study SGD, we construct a continuous-time Markov process that approximates an arbitrary Markov discrete-time process, and develop its Kramers-Moyal (KM) expansion. We then specialize the
\footnote{Our method validates a conjecture in (Bazant 2005) that the moments of the continuous-time process should be proportional to the cumulants of the discrete-time process.}
approximation to SGD, and see that the $i$-th term of the KM expansion scales with $T^i$, where $T = \lambda/B$ is the temperature of SGD. The typical setting for SGD, and the one we consider throughout, has $T << 1$, which justifies truncating its KM expansion to second order to obtain a Fokker-Planck (FP) equation. The FP equation depends on the gradient statistics $\partial_\theta \bar{U}(\theta)$ and $\bar{D}(\theta)$, on $T$, and on $B$:

$$\partial_t \rho(\theta, t) = BT \sum_{i=1}^n \partial_\theta \left\{ \partial_\theta \bar{U}(\theta) \rho(\theta, t) \right\} + \frac{1}{2} B^2 T^2 \sum_{i,j=1}^n \partial_{\theta_i} \partial_{\theta_j} \left\{ \bar{D}_{ij}(\theta) \rho(\theta, t) \right\},$$

where

$$\partial_\theta \bar{U}(\theta) = \int q_\theta(x) \partial_\theta U(x, \theta) dx,$$

$$\bar{D}(\theta) = \text{Cov}_{\theta \theta} \left( \partial_\theta U(x, \theta) \right).$$

This approximates SGD in the sense that $\rho(\theta, t) \approx P(\theta_\epsilon = \theta)$; Appendix A derives all results in this section. Eq. 16 has important implications. First, note that when the process reaches stationarity and $\partial_t \rho(\theta, t) = 0$, the right hand side can be divided by $B$, so that the stationary distribution depends only on $T$, hence it is unchanged if the learning rate and batch size are scaled identically. This is confirmed experimentally in Figure 1, as well as other empirical studies (Goyal et al. 2017; He, Liu, and Tao 2019). (Goyal et al. 2017) note that the temperature-dependence begins to break down for very large batch sizes (corresponding to large learning rates when temperature is held constant); this is expected, since the continuous approximation relies on an i.i.d. assumption for small time increments within an SGD step, which may be violated for large learning rates, as well as early in training when parameters are evolving rapidly.

Beyond stationarity, the time variable in Eq. 16 can be rescaled via $t' = Bt$ to remove $B$ entirely from the FP description; the resulting FP measures time in terms of epochs, and has $T$ as its only free parameter (given a training set and loss function). This predicts that one can increase the batch size to $\alpha B$, with $\alpha > 1$, to reduce the number of iterations by $1/\alpha$ while maintaining the same model performance; this has been empirically demonstrated in (Smith et al. 2017). Later we will see that $T$ is also the key parameter impacting model performance for SGD.

Proceeding, we set $\partial_t \rho(\theta, t) = 0$ and follow (Gardiner 2009) to find the steady-state solution of Equation 16:

$$\rho(\theta) \propto \exp \left\{ -\frac{1}{T} \tilde{v}(\theta) - \tilde{a}(\theta) \right\},$$

where

$$\tilde{v}(\theta) = \int \bar{D}^{-1} \partial_\theta \bar{U} \cdot d\theta, \quad \tilde{a}(\theta) = \int_0^\theta \bar{D}^{-1} (\partial_\theta \bar{D})' \cdot d\theta.$$

Here, $\tilde{v}(\theta)$ is the effective potential, which is related to the training loss (or potential) $\ell\epsilon(\theta)$, but in general not the same.\(^5\) We dropped the $\theta$ argument of $\bar{D}$ and $\partial_\theta \bar{U}$ for compactness. Eq. 19 gives a more explicit expression for the stationary SGD distribution than previously published ones, and enables the analysis we do next.

Next, we further approximate the stationary distribution of SGD in Eq. 19 by a mixture of Gaussians, i.e., as a distribution of the form in Eq. 4. Letting $\bar{v}_k = \tilde{v}(\theta_k)$, and $\bar{a}_k = \tilde{a}(\theta_k)$, we show in Appendix B through the Laplace approximation that to leading order in $T$,

$$w_k = e^{-\frac{2\bar{v}_k}{T}} e^{-\frac{\bar{a}_k}{T}} \sqrt{\frac{\bar{D}_k}{C_k}},$$

$$b_k \approx -\frac{T}{2} \bar{C}_k^{-1} (\partial_\theta \cdot \bar{D}_k),$$

$$\Sigma_k = \frac{T}{2} \bar{C}_k^{-1} \bar{D}_k,$$

$$Z = \sum_k e^{-\frac{2\bar{v}_k}{T}} e^{-\frac{\bar{a}_k}{T}} \sqrt{\frac{\bar{D}_k}{C_k}}.$$  

Note that these quantities all depend on the temperature. Before doing a more rigorous analysis, we discuss the qualitative behavior implied by Equation 20. Notice that at $T = 0$, $w$ puts all the weight of $\rho$ on the deepest minimum of $v$, but as $T$ increases, $w$ begins to transfer weight onto other minimum, generally favoring lower curvature basins due to the $\sqrt{\bar{C}_k}$ term. The intuition is that deeper basins are better for both train and test loss, but lower curvature basins tend to generalize better. We formalize this next.

6 Performance and SGD Temperature

We finally have the tools to answer our main question: can increasing SGD temperature improve test performance? Test loss improves with increasing temperature if $\partial_T \mathcal{L}_e < 0$. Appendix F shows that for any basin dependent quantity $f_k$,

$$\partial_T \langle f \rangle = \frac{2}{T^2} \text{Cov}(\bar{v}, f).$$

The covariances in this section are all with respect to the distribution over local minima $w_k$. For example, letting $f_k = \bar{v}_k$ yields $\partial_T \langle \bar{v} \rangle = \frac{2}{T^2} \text{Var}(\tilde{v})$, so the average effective potential can never decrease with increasing temperature. Applying Eq. 24 to the model performance in Eq. 6, we find:

$$\partial_T \mathcal{L}_e = \frac{2}{T^2} \text{Cov}(\bar{v}, \mathcal{U}) + \frac{1}{T^2} \text{Cov}(\bar{v}, \text{Tr}(\Sigma))$$

$$+ \frac{1}{T^2} \text{Cov}\left(\bar{v}, (b + s)^T C(b + s)\right) + \frac{1}{2} \langle \partial_T \text{Tr}(\Sigma) \rangle$$

$$+ \frac{1}{2} \langle (\partial_T (b'Cb) + S'(\partial_T b) + \partial_T b)'Cs) \rangle.$$

\(^5\)Note that when $n = 1$, $\tilde{a}(\theta) = \log(\bar{D}(\theta))$. Similarly, when $\bar{D} = \bar{d}(\theta) I$ for some scalar function $\bar{d}$ of $\theta$, then $e^{-\tilde{a}(\theta)} = \bar{d}(\theta)^{-1}$ so $\rho(\theta) \propto \bar{d}(\theta)^{-1} e^{-\tilde{v}(\theta)}$. If $\bar{d}(\theta)$ is constant, then $\tilde{v}(\theta) = \bar{d}^{-1} \mathcal{L}_e(\theta)$ and $\tilde{a} = 0$, so the effective potential is proportional to the training potential, and $\rho(\theta) \propto e^{-\frac{2}{T} \mathcal{L}_e(\theta)}$.
For SGD, \( b_k \propto T \) and \( \sigma_k^2 \propto T \) from Eqs. 21 and 22. So for small temperatures (smaller than \(|\epsilon_\eta|\)), to leading order Eq. 25 simplifies to:

\[
\partial_T \mathcal{L}_e = \frac{1}{T^2} \left[ 2\text{Cov}(\tilde{v}, U) + \text{Cov}(\tilde{v}, s'C_s) \right] + O\left(\frac{1}{T}\right).
\]

(26)

Test performance can improve with increasing temperature only when the square brackets become negative. This is possible when there are multiple basins with specific characteristics, as argued next. Although it is possible for \( \tilde{v}_k \) to reorder the minima rankings determined by \( U_k \), we generally expect the test and effective potentials \( U_k, \tilde{v}_k \) to be positively correlated. In this case, the first term in (26) is positive while the second term could be either positive or negative. Therefore, to order \( 1/T \), the test loss can only possibly improve as a function of temperature if there is a shift between the local minima, i.e., when \( s_k \neq 0 \) in such a way that the covariance of \( \tilde{v} \) and \( s'C_s \) is negative. In other words, when basins of the loss function with low effective potentials have low curvature, so that the local shifts pick up a small contribution \( s'C_{ks} \), and vice-versa. Eq. 13 can be used to study this further, but we only pursue that here in a simplified two-basin situation later. Figure 1 shows our experiments on CIFAR10 (Krizhevsky, Hinton et al. 2009) (with a VGG9 network (Simonyan and Zisserman 2014) and the training procedure of (Li et al. 2017)), demonstrating that test loss indeed improves as temperature increases, while training loss remains approximately zero.

**One basin**

Models with losses that have a single minima also have only one weight \((w_0 = 1)\), so all covariances with respect to \( w_k \) are zero. In fact, if we look at the remaining terms of Eq. 25, it is clear that to leading order (where \( T|\epsilon_\eta| \) is ignored too since \( |\epsilon_\eta| \) is also small)

\[
\partial_T \mathcal{L}_e \approx \frac{1}{2} \partial_T \text{Tr}(C\Sigma) = \text{Tr}(C\tilde{C}^{-1} \tilde{D}) \geq 0,
\]

(27)

since both the curvature \( C \) and the gradient covariance \( D \) are positive semidefinite. So we expect that the loss can only degrade with increasing temperature.

**Two basins**

When there are only two basins, with weights \( w_1 \) and \( w_0 = 1 - w_1 \), the covariance of any basin-dependent quantity \( f_i \) and \( \tilde{v}_i \) is simply

\[
\text{Cov}(\tilde{v}_i, f_i) = w_1(1 - w_1)(f_1 - f_0)(\tilde{v}_1 - \tilde{v}_0),
\]

so Eq. 26 becomes

\[
\partial_T \mathcal{L}_e \approx \frac{1}{T^2} w_1(1 - w_1)(\tilde{v}_1 - \tilde{v}_0)
\]

\[
\times \left[ 2(U_1 - U_0) + (s_1'C_1s_1 - s_0'C_0s_0) \right].
\]

Without loss of generality, we can assume that \( U_1 - U_0 > 0 \), so if the effective potential does not reverse the ranking of

\[
E[s_1'C_1s_1 - s_0'C_0s_0] \approx \frac{2}{N_{\text{eff}}} \text{Tr}(E_0C_0^{-1} - E_1C_1^{-1})
\]

\[
+ \epsilon_\eta'(F_1'C_1^{-1}F_1 - F_0'C_0^{-1}F_0)\epsilon_\eta.
\]

This is a complicated expression to interpret, partly because the matrices \( E_k \) and \( F_k \) are not well understood. But it is helpful to consider some special cases. Assuming \( E_0 \approx E_1 > 0 \), the sampling dependent term (the first one on the right) is negative when the trace of \( C_1^{-1} \) is much larger than the trace of \( C_0^{-1} \), i.e., when the shallower minimum is much deeper, i.e., if \( \tilde{v}_1 - \tilde{v}_0 > 0 \), the expression is negative when \( s_0'C_0s_0 \) is sufficiently larger than \( s_1'C_1s_1 \), i.e., when the shift of the deeper basin picks up more curvature than the shift of the shallow one. Using Eq. 13 along with Eq. 12, yields after some algebra

Figure 3: Synthetic two-basin loss with train loss shifted left or right by a constant-but-random amount relative to test loss (to model location parameters), and \( D \) constant. Top: Minimum at 1 is deeper and wider; both training and test error worsen as \( T \) increases. Bottom: Minimum at -1 is deeper but minimum at 1 is wider; test error decreases and training error increases with increasing temperature, as stationary distribution transfers weight to the wider minimum which is less sensitive to the shift.
flatter than deeper one. In the special case when $\theta$ and $\eta$ are location parameters in the same model space and data sets are infinite, we have already seen that $s_k = \epsilon_p$, so we know that the second term is just $c'(C_1 - C_0)\epsilon_p$, which is negative only if $C_0 > C_1$, i.e., again if the shallower minimum is flatter. So both terms can become negative when the deeper minimum is narrower than the shallower one, so we expect that performance can improve with increased temperature in that case. The corresponding intuition is that increasing $T$ shifts weight from the narrower-but-deeper minimum to the wider-but-shallower minimum, which can improve generalization. On the other hand, when the deepest minimum is also the widest, increasing $T$ can only hurt performance. These situations are simulated in Figure 3, where we create a synthetic two-basin loss using a weighted combination of Gaussians and model the location parameter case by shifting the train loss left or right relative to the test loss by a constant-but-random amount. Appendix H provides details, and includes similar one-basin and three-basin cases.

Finally, although it seems unlikely that $U, \tilde{v}$ would be negatively correlated in practical networks with many local minima, it is possible for this to happen in the two basin case. We show such a case in a synthetic example in Appendix H.

### Entropy Regularization

Our results are consistent with SGD performing implicit regularization. In Appendix E we show that the stationary SGD distribution in Eq. 19 solves

$$\min_{p(\hat{\theta})} 2\langle \tilde{v}(\hat{\theta}) \rangle + T\langle \hat{a}(\theta) \rangle - Th(p). \quad (28)$$

Here $p(\theta)$ denotes any continuous distribution of $\theta$, $h(p)$ is the differential entropy of $p(\theta)$, and the brackets indicate expectation with respect to $p(\theta)$, unlike in the rest of our paper. The first term is the effective potential that is related to minimizing the model loss. The third term grows linearly with $T$ and provides entropy-based regularization, as noted, e.g., by (Chaudhari and Soatto 2018). But the second term has not been previously identified as far as we know, and its magnitude also grows linearly with $T$. For models where $\theta$ is a scalar (i.e., that have a single parameter) $\hat{a}(\theta) = \log D(\theta)$, which we expect to grow monotonically with the curvature via Eq. 12. So at least then we expect this term to encourage solutions where the loss has low curvature. If this effect holds for any number of parameters, then this term may further aid model generalization as $T$ is increased (independently of whether it should be seen as providing a different regularization mechanism).

### 7 Discussion And Conclusion

We have described an approximate analytical framework to study how the learning rate and batch size in stationary SGD affect test performance for models with losses that have multiple minima. There are many interesting avenues for future work. First, a study analogous to ours that focuses on the SGD distribution before stationarity is reached could be a useful complement. Second, our framework is approximate in part because it only keeps leading terms of expressions in terms of several small parameters: the inverse effective data set size $N^{-1}_{eff}$, the (non-sampling-based) training to test distribution shift $\epsilon_p$, and for SGD, low temperature $T$. Considering the next order of terms could be useful, particularly for SGD temperature, e.g., for finding an optimal SGD temperature. Our assumption that local minima of the losses are points rather than more complex regions of parameter space is another limitation that future work could address, e.g., through reparametrization. Third, the behavior of the gradient variance $D$ and its impact on the effective potential $\tilde{v}$ is still mysterious. Under the log-likelihood model, $D$ is related to the curvature by Equation 12, but there is an additional term, $\tilde{v}$, that we do not yet understand. Our experiments with nonconstant $D$ in Appendix H suggest that $D$ can affect $\tilde{v}$ in surprising ways. The relationship between the true and effective potentials (which can possibly have different local minimum ordering) and its implications for the optimization problem that SGD actually solves, are missing pieces in our understanding. Finally, parts of our approach can be applied to other stochastic algorithms, and our results could inform the design of new training algorithms that, for example, retain SGD’s generalization benefits while allowing for higher fidelity to the original loss, or faster training.

Various techniques in statistical mechanics contribute to our approach, including a Kramers-Moyal and Fokker-Plank description of SGD dynamics to obtain the approximate stationary SGD distribution which is very similar in form to the equilibrium distribution from thermodynamics. Our derivation of the change in test performance with respect to temperature is an almost exact analog of standard thermodynamic calculations to obtain the change of measurable quantities as temperature changes. Seminal works like (Seung, Sompolinsky, and Tishby 1992; Watkin, Rau, and Biehl 1993) have studied learning from the point of view of statistical mechanics, but they differ from our approach in at least two ways. First, they inherit the state-independent diffusion matrix of statistical mechanics. The $\theta$-dependence of $D$ may play an important role in model performance, e.g., by making $\tilde{v}(\theta)$ nonzero and modifying the shift covariance. Second, these approaches account only for shifts due to sampling effects rather than (also) distribution shifts. We expect to see more Physics techniques contribute to machine learning. We hope that the results presented here can improve the community’s understanding of the role of SGD noise in generalization, and that the techniques can offer a framework for further study of this and related phenomena.

### References

Ahn, S.; Korattikara, A.; and Welling, M. 2012. Bayesian posterior sampling via stochastic gradient Fisher scoring. arXiv preprint arXiv:1206.6380.

Bazant, M. 2005. Lecture 9: Kramers-Moyal Cumulant Expansion, scribed by Jacy Bird. https://math.mit.edu/classes/18.366/lec05/lec09.pdf.
Belkin, M. 2021. Fit without fear: remarkable mathematical phenomena of deep learning through the prism of interpolation. arXiv preprint arXiv:2105.14368.

Belkin, M.; Hsu, D.; Ma, S.; and Mandal, S. 2019. Reconciling modern machine-learning practice and the classical bias–variance trade-off. Proceedings of the National Academy of Sciences, 116(32): 15849–15854.

Bovier, A.; Eckhoff, M.; Gayrard, V.; and Klein, M. 2004. Metastability in reversible diffusion processes I. Sharp asymptotics for capacities and exit times. J. Eur. Math. Soc. Chaudhari, P.; and Soatto, S. 2018. Stochastic gradient descent performs variational inference, converges to limit cycles for deep networks. In 2018 Information Theory and Applications Workshop (ITA), 1–10. IEEE.

Corneanu, C. A.; Escalera, S.; and Martinez, A. M. 2020. Computing the testing error without a testing set. In Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition, 2677–2685.

Dinh, L.; Pascanu, R.; Bengio, S.; and Bengio, Y. 2017. Sharp minima can generalize for deep nets. In Proceedings of the 34th International Conference on Machine Learning-Volume 70, 1019–1028. JMLR. org.

Freidlin, M.; and Weber, M. 2004. Random perturbations of dynamical systems and diffusion processes with conservation laws. Probability theory and related fields, 128(3): 441–466.

Gardiner, C. 2009. Stochastic methods, volume 4. Springer Berlin.

Golmant, N.; Vemuri, N.; Yao, Z.; Feinberg, V.; Gholami, A.; Rothauge, K.; Mahoney, M. W.; and Gonzalez, J. 2018. On the computational inefficiency of large batch sizes for stochastic gradient descent. arXiv preprint arXiv:1811.12941.

Goyal, P.; Dollár, P.; Girshick, R.; Noordhuis, P.; Wesolowski, I.; Kyrola, A.; Tulloch, A.; Jia, Y.; and He, K. 2017. Accurate, large minibatch sgd: Training imagenet in 1 hour. arXiv preprint arXiv:1706.02677.

He, F.; Liu, T.; and Tao, D. 2019. Control batch size and learning rate to generalize well: Theoretical and empirical evidence. Advances in Neural Information Processing Systems, 32: 1143–1152.

Hochreiter, S.; and Schmidhuber, J. 1997. Flat minima. Neural computation, 9(1): 1–42.

Hoffer, E.; Hubara, I.; and Soudry, D. 2017. Train longer, generalize better: closing the generalization gap in large batch training of neural networks. In Advances in Neural Information Processing Systems, 1731–1741.

Jacot, A.; Gabriel, F.; and Hongler, C. 2018. Neural tangent kernel: Convergence and generalization in neural networks. In Advances in neural information processing systems, 8571–8580.

Jiang, Y.; Neyshabur, B.; Mobahi, H.; Krishnan, D.; and Bengio, S. 2019. Fantastic generalization measures and where to find them. arXiv preprint arXiv:1912.02178.

Keskar, N. S.; Mudigere, D.; Nocedal, J.; Smelyanskiy, M.; and Tang, P. T. P. 2016. On large-batch training for deep learning: Generalization gap and sharp minima. arXiv preprint arXiv:1609.04836.

Khan, M. E.; Immer, A.; Abedi, E.; and Korzepa, M. 2019. Approximate Inference Turns Deep Networks into Gaussian Processes. arXiv preprint arXiv:1906.01930.

Krizhevsky, A.; Hinton, G.; et al. 2009. Learning multiple layers of features from tiny images.

Kubo, R.; Matsuo, K.; and Kitahara, K. 1973. Fluctuation and relaxation of macrovariables. Journal of Statistical Physics, 9(1): 51–96.

Lee, J.; Bahri, Y.; Novak, R.; Schoenholz, S. S.; Pennington, J.; and Sohl-Dickstein, J. 2017. Deep neural networks as gaussian processes. arXiv preprint arXiv:1711.00165.

Lewkowycz, A.; Bahri, Y.; Dyer, E.; Sohl-Dickstein, J.; and Gur-Ari, G. 2020. The large learning rate phase of deep learning: the catapult mechanism. arXiv preprint arXiv:2003.02218.

Li, H.; Xu, Z.; Taylor, G.; Studer, C.; and Goldstein, T. 2017. Visualizing the loss landscape of neural nets. arXiv preprint arXiv:1712.09913.

Li, Q.; Tai, C.; et al. 2017. Stochastic modified equations and adaptive stochastic gradient algorithms. In Proceedings of the 34th International Conference on Machine Learning-Volume 70, 2101–2110. JMLR. org.

Mandt, S.; Hoffman, M. D.; and Blei, D. M. 2017. Stochastic gradient descent as approximate bayesian inference. The Journal of Machine Learning Research, 18(1): 4873–4907.

Martin, C. H.; and Mahoney, M. W. 2018. Implicit self-regularization in deep neural networks: Evidence from random matrix theory and implications for learning. arXiv preprint arXiv:1810.01075.

McCandlish, S.; Kaplan, J.; Amodei, D.; and Team, O. D. 2018. An empirical model of large-batch training. arXiv preprint arXiv:1812.06162.

Nakkiran, P.; Kaplun, G.; Bansal, Y.; Yang, T.; Barak, B.; and Sutskever, I. 2019. Deep double descent: Where bigger models and more data hurt. arXiv preprint arXiv:1912.02292.

Russo, D.; and Zou, J. 2016. Controlling bias in adaptive data analysis using information theory. In Artificial Intelligence and Statistics, 1232–1240. PMLR.

Seung, H. S.; Sompolinsky, H.; and Tishby, N. 1992. Statistical mechanics of learning from examples. Physical review A, 45(8): 6056.

Shalloe, C. J.; Lee, J.; Antognini, J.; Sohl-Dickstein, J.; Frostig, R.; and Dahl, G. E. 2018. Measuring the effects of data parallelism on neural network training. arXiv preprint arXiv:1811.03600.

Simonyan, K.; and Zisserman, A. 2014. Very deep convolutional networks for large-scale image recognition. arXiv preprint arXiv:1409.1556.

Smith, S.; Elsen, E.; and De, S. 2020. On the Generalization Benefit of Noise in Stochastic Gradient Descent. In International Conference on Machine Learning, 9058–9067. PMLR.
Smith, S. L.; Dherin, B.; Barrett, D. G.; and De, S. 2021. On the origin of implicit regularization in stochastic gradient descent. \textit{arXiv preprint arXiv:2101.12176.}

Smith, S. L.; Kindermans, P.-J.; Ying, C.; and Le, Q. V. 2017. Don’t decay the learning rate, increase the batch size. \textit{arXiv preprint arXiv:1711.00489.}

Smith, S. L.; and Le, Q. V. 2017. A bayesian perspective on generalization and stochastic gradient descent. \textit{arXiv preprint arXiv:1710.06451.}

Van Kampen, N. 1965. Fluctuations in nonlinear systems. \textit{Fluctuation phenomena in solids}, 139–177.

Watkin, T. L.; Rau, A.; and Biehl, M. 1993. The statistical mechanics of learning a rule. \textit{Reviews of Modern Physics}, 65(2): 499.

Wu, J.; Hu, W.; Xiong, H.; Huan, J.; and Zhu, Z. 2019. The Multiplicative Noise in Stochastic Gradient Descent: Data-Dependent Regularization, Continuous and Discrete Approximation. \textit{arXiv preprint arXiv:1906.07405.}

Xie, Z.; Sato, I.; and Sugiyama, M. 2020. A diffusion theory for deep learning dynamics: Stochastic gradient descent exponentially favors flat minima. \textit{arXiv preprint arXiv:2002.03495.}

Xu, A.; and Raginsky, M. 2017. Information-theoretic analysis of generalization capability of learning algorithms. \textit{arXiv preprint arXiv:1705.07809.}

Yaida, S. 2018. Fluctuation-dissipation relations for stochastic gradient descent. \textit{arXiv preprint arXiv:1810.00004.}

Zhu, Z.; Wu, J.; Yu, B.; Wu, L.; and Ma, J. 2018. The anisotropic noise in stochastic gradient descent: Its behavior of escaping from minima and regularization effects. \textit{arXiv preprint arXiv:1803.00195.}
A Continuous Time Approximation of SGD

A Continuous-Time Approximation Of A Discrete-Time Continuous-Space Markov Process

We consider a discrete-time stochastic process with state $\theta_j \in \mathbb{R}^n$, where $j$ indexes time, that changes in value by the random variable $\Delta_j \in \mathbb{R}^n$ i.e., the process evolves according to Eq. 14. (Note the different notation from the main text: $j$ rather than $t$ is the discrete time index here, so that we can use $t$ to represent continuous time.) We drop time index $j$ from $\theta$ and $\Delta$ for now, and use subscripts on those symbols to denote specific entries. We think of the distribution of $\Delta$ as depending on $\theta$ but otherwise completely arbitrary. Dropping the time subscript of $\theta$ for now, we let $m_\gamma(\theta) = E[\Delta^\gamma] \equiv E[\Delta_j^n \cdots \Delta_{j-1}^n]$ and $\kappa_\gamma(\theta) = \log m_\gamma(\theta)$ denote the moments and cumulants, respectively, of $\Delta$. We adopt multi-index notation, so, e.g., $\gamma \in \mathbb{N}^n$ here to match the dimension of $\Delta$. Both the moments but especially the cumulants of $\Delta$ play an important role in our method.

We imagine a continuous-time Markov process $\theta(t) \in \mathbb{R}^n$ with probability distribution $\rho(\theta, t) = P(\theta(t) = \theta)$. Our main goal is to construct the process so that $\tilde{\theta}(t)$ approximates $\theta_j$ in the following sense. We assume discrete time updates of $\theta_j$ occur every $\tau > 0$ continuous time units, where $\tau$ is arbitrary. Our goal is to construct $\tilde{\theta}(t)$ such that

$$\rho(\theta, j\tau) \equiv P(\theta(j\tau) = \theta) \approx P(\theta_j = \theta),$$

assuming identical initial conditions for $\theta_j$ and for $\tilde{\theta}(t)$.

Motivation To motivate the route we take for defining the continuous-time approximation, we begin by studying the discrete time process. Rewriting Eq. 14, repeated below for convenience, as an infinite expansion of the moments of $\Delta$:

$$\theta_{j+1} = \theta_j + \Delta_j$$

$$P(\theta_{j+1} = \theta) = \int P(\theta_j = \theta - \Delta)P(\Delta_j = \Delta_j)\theta_j = \theta - \Delta)d\Delta$$

$$\Rightarrow P(\theta_{j+1} = \theta) = \sum_{\gamma \in \mathbb{N}^n_0} \frac{(-1)^\gamma}{\gamma!} \partial_\theta^\gamma \left\{ P(\theta_j = \theta) \int \Delta^\gamma P(\Delta_j = \Delta_j)\theta_j = \theta)d\Delta \right\}$$

$$= \sum_{\gamma \in \mathbb{N}^n_0} \frac{(-1)^\gamma}{\gamma!} \partial_\theta^\gamma \left\{ m_\gamma(\theta)P(\theta_j = \theta) \right\},$$

(3)

Here, $\mathbb{N}^n_0, \mathbb{N}^n_1$ denote the $n$-dimensional sets of integers $\geq 0$ and $\geq 1$, respectively, and $\partial_\theta^\gamma f(\theta) = \partial_\theta^{\gamma_0} \cdots \partial_\theta^{\gamma_{n-1}} f(\theta)$ for an arbitrary function $f(\theta)$. The first line is the discrete-time Chapman-Kolmogorov equation for a Markov process. The second line follows by Taylor expansion, i.e.,

$$f(\theta + h) = \sum_{\gamma \in \mathbb{N}^n_0} \frac{\partial_\theta^\gamma f(\theta)}{\gamma!} h^\gamma,$$

and the third assumes one can interchange the integration with respect to $\Delta$ with $\partial_\theta^\gamma$.

Assuming Eq. 1 holds for now, we can substitute $\rho(\theta, j\tau)$ for $P(\theta_j = \theta)$ in equation 3, rearrange, and divide by $\tau$, to obtain

$$\frac{\rho(\theta, t + \tau) - \rho(\theta, t)}{\tau} = \sum_{\gamma \in \mathbb{N}^n_0} (-1)^\gamma \frac{m_\gamma(\theta, \tau)}{\gamma!\tau} \rho(\theta, t).$$

(4)

Note that we now wrote $m_\gamma(\theta, \tau)$ explicitly as a function of $\tau$ to remind us that these moments correspond to increments during an interval of time of length $\tau$. Equation 4, after imagining one could take the limit of $\tau \to 0$, is highly suggestive of the main Kramers-Moyal equation we seek for $\theta$, and that we derive next.

Final Results We state the final results of our method first, and justify them afterwards. The Markov assumption for $\tilde{\theta}(t)$ implies the continuous-time Chapman Kolmogorov equation

$$\rho(\theta, t') = \int \rho(\theta - \Delta, t)W(\Delta, t'|\theta - \Delta, t)d\Delta,$$

(5)

where $W(\Delta, t'|\theta, t) = P(\tilde{\theta}(t') = \theta + \Delta|\tilde{\theta}(t) = \theta)$ is the transition probability function, and $t' \geq t$. Our approach will consist of defining this probability distribution when $t' - t = dt$ is infinitesimally small, i.e., we focus on specifying the random variable $\Delta(dt)$, and then showing that the resulting process $\tilde{\theta}(t)$ has increments over finite time intervals of arbitrary length $\tau$ that match the distribution of $\Delta_j$ in SGD.
To define $\tilde{\theta}$, we let $\tilde{\Delta}(t' - t) = \tilde{\theta}(t') - \tilde{\theta}(t)$ be the random variable that defines the increment between any two times $t' \geq t$. Note that the Markov property implies that the increment only depends on the time difference $t' - t$ when the value of $\tilde{\theta}(t)$ is known. Importantly, specifying the probability distribution for $\Delta(t' - t)$ would complete the description of our process. As is typical, we only define this probability distribution when $t' - t = dt$ is infinitesimally small, since that is sufficient to specify the process.

We define $P(\tilde{\Delta}(dt))$ through its moments

$$E[\tilde{\Delta}(dt)^\gamma] = \frac{\kappa_\gamma(\tilde{\theta}(t))}{\tau} dt,$$

with $\gamma \in \mathbb{N}_0^n$ a set of $n$ non-negative integers. In words, the moments of the small-time increments of $\tilde{\theta}(t)$ are directly proportional to the cumulants of the discrete time process $\theta_j$, it seeks to approximate. We expect the resulting process will approximate the discrete one well when $\kappa_\gamma(\tilde{\theta}(t))$ does not change much in value within each $\tau$ time increment, so that the small time increments during that time period are approximately independent and identically distributed.

Now that $\tilde{\theta}(t)$ is defined, and setting $\tau = 1$ for simplicity now, the following Kramers-Moyal expansion describes its distribution.

$$\partial_t \rho(\theta, t) = \sum_{\gamma \in \mathbb{N}_0^n} \frac{(-1)^\gamma}{\gamma!} \partial_\gamma \{ \kappa_\gamma(\theta) \rho(\theta, t) \}.$$  \hspace{1cm} (7)

**Moments of the continuous time process in terms of cumulants of the discrete time process**  
Our goal in this section is to justify Eq. 6. Let $dt = \tau/K$ for some positive integer $K$, and define $t_j = jdt$ for $j = 0, \ldots, K$, and $dt_j = t_{j+1} - t_j = dt$. Recall that $\Delta(dt_j)$ is the small time increment of our continuous process between $t_{j-1}$ and $t_j$, so that $\tilde{\Delta}(\tau, K) = \sum_{j=1}^K \Delta(dt_j)$ is the total change in our process over $\tau$ time units when breaking the temporal interval into $K$ equal-sized increments. We want to determine the moments of $\Delta(dt_j)$ so that $E[\tilde{\Delta}(\tau)^\gamma] = \lim_{K \to \infty} E[\tilde{\Delta}(\tau, K)^\gamma]$ matches the corresponding moment of the discrete SGD step $E[\Delta(\theta)]$. Assuming the increments $\Delta(dt_j)$ are approximately i.i.d. within each time interval of length $\tau$, we can approximate $\tilde{\Delta}(\tau, K)$ as a sum of i.i.d. random variables.

With simplified notation, we model the problem as follows. Consider a sum

$$S_K = \sum_{i=1}^K X_i,$$

where $X_i$ are i.i.d. random variables (each in $\mathbb{R}^n$). Suppose that we know the ‘desired’ limiting random variable $S$, along with its cumulants. We want to find the moments of the i.i.d. random variables $X$ so that $\lim_{K \to \infty} \tilde{S}_K = S$.

We will use the following definitions. Let $m_X^\gamma$ and $\kappa_X^\gamma$ denote the moments and cumulants of an arbitrary random variable $X$. Let $M_X(t) = E[e^{tX}]$ be the moment generating function of $X$, and $C_X(t) = \log M_X(t)$ the cumulant generating function, so that $m_X^\gamma = \partial^\gamma M_X(0)$ and $\kappa_X^\gamma = \partial^\gamma C_X(0)$. We will also use the identity:

$$e^x = \lim_{K \to \infty} \left( 1 + \frac{x}{K} \right)^K.$$  \hspace{1cm} (8)

To restate the problem more precisely in this notation, we want to find $m_X^\gamma$ such that $\lim_{K \to \infty} C_{S_K}(t) = C_S(t)$. Using the i.i.d. assumption and identity 8, we obtain:

$$M_{S_K}(t) = E[e^{tS_K}] = \prod_{i=1}^K E[e^{tX_i}] = (M_X)^K$$

$$\implies \lim_{K \to \infty} M_{S_K}(t) = \lim_{K \to \infty} (M_X)^K = \lim_{K \to \infty} (1 + \xi/K)^K \text{ where } \xi \text{ satisfies } M_X \equiv 1 + \xi/K$$

$$= e^\xi$$

$$\implies \lim_{K \to \infty} C_{S_K}(t) = \xi$$

Since we want $\lim_{K \to \infty} C_{S_K}(t) = C_S(t)$, we equate $\xi = C_S(t)$. Hence:

$$M_X(t) = 1 + C_S(t)/K$$

$$\implies m_X^\gamma = \partial^\gamma M_X(t) |_{t=0} = \frac{1}{K} \partial^\gamma C_S(t) |_{t=0} = \frac{1}{K} \kappa_S^\gamma$$
So, in order to achieve the desired limit, we need the moments of the i.i.d. variables $X$ to be equal to $1/K$ times the cumulants of the desired limiting distribution $S$.

To explicitly connect this result back to the continuous approximation of SGD, we associate $X_i = \hat{\Delta}(dt_i), S_j = \hat{\Delta}(\tau, K), S = \Delta(\theta)$, and $dt = \tau/K$. Then $m_X^j = \frac{1}{K} \kappa^j_S$ translates to equation 6, as we desired.

Note that the i.i.d. assumption on the increments $\Delta(dt_j)$ is an approximation that introduces error into result 6. In the approximation, we assume that $P(\Delta(dt_j)) \approx P(\Delta(dt_0))$ for $t_j = jdt, j = 1, \ldots, K, dt = \tau/K$. If $\tau$ is small and $\hat{\Delta}$ varies slowly, then this condition will approximately hold.

The continuous Kramers-Moyal Expansion We start from equation 5. Substituting $t' = t + dt$, and using our definition of $\Delta$.

$$
\rho(\theta, t + dt) = \int \rho(\theta - \Delta, t)W(\Delta, t + dt|\theta - \Delta, t)d\Delta,$$

where $W(\Delta, t + dt|\theta, t) = P(\hat{\Delta}(dt) = \Delta(\theta(t)) = \theta).$ (9)

Similar to the discrete version in equation 3, we can Taylor expand in $\Delta$ and take the limit as $dt \to 0$ to obtain the Kramers-Moyal expansion claimed in equation 7:

$$
\rho(\theta, t + dt) = \sum_{\gamma \in \mathbb{N}_0} \frac{(-\Delta)^\gamma}{\gamma!} \partial_\theta^{\gamma} \left( \rho(\theta, t)W(\Delta, t + dt|\theta, t) \right) d\Delta
$$

$$
= \sum_{\gamma \in \mathbb{N}_0} \frac{(-1)^\gamma}{\gamma!} \partial_\theta^{\gamma} \left( \rho(\theta, t) \int \Delta^\gamma W(\Delta, t + dt|\theta, t) d\Delta \right)
$$

$$
= \sum_{\gamma \in \mathbb{N}_0} \frac{(-1)^\gamma}{\gamma!} \partial_\theta^{\gamma} \left( \rho(\theta, t)E[\hat{\Delta}(dt)\gamma] \right)
$$

$$
= \rho(\theta, t) + \sum_{\gamma \in \mathbb{N}_0} \frac{(-1)^\gamma}{\gamma!} \partial_\theta^{\gamma} \left( \rho(\theta, t)E[\hat{\Delta}(dt)^\gamma] \right)
$$

$$
\Rightarrow \partial_t \rho(\theta, t) = \lim_{dt \to 0} \frac{\rho(\theta + \Delta, t + dt) - \rho(\theta + \Delta, t)}{dt}
$$

$$
= \sum_{\gamma \in \mathbb{N}_0} \frac{(-1)^\gamma}{\gamma!} \partial_\theta^{\gamma} \left( \rho(\theta, t) \lim_{dt \to 0} \frac{E[\hat{\Delta}(dt)^\gamma]}{dt} \right)
$$

$$
= \sum_{\gamma \in \mathbb{N}_0} \frac{(-1)^\gamma}{\gamma!} \partial_\theta^{\gamma} \left\{ \kappa_{\gamma}(\theta)\rho(\theta, t) \right\},
$$

where in the last line we used equation 6. To connect back to our initial motivation, note that this equation is in fact the small-time limit of equation 4 that replaces $\tau$ there by $dt$ and then takes $dt$ to zero.

The continuous process approximates the discrete process Now that we have defined $\hat{\theta}$ via equation 7 we need to check that it actually approximates SGD in the sense of equation 1, i.e. we want to show that $\rho(\theta, j\tau) \approx P(\theta_j = \theta)$. We seek to understand the approximation error in terms of the difference between $\hat{\theta}_{\gamma}(\theta)$ and $m_{\gamma}(\theta)$. The error arises because our expression for $\hat{\theta}_{\gamma}(\theta)$ relies on the approximation that small-time increments of $\hat{\theta}(t)$ are i.i.d.. We assume that $\rho(\theta, t) = P(\theta_j = \theta)$, and then study $\rho(\theta, t + \tau)$, starting from the Chapman-Kolmogorov for $\hat{\theta}(t)$ (equation 5):

$$
\rho(\theta, t + \tau) = \int \rho(\theta - \Delta, t)W(\Delta, t + \tau|\theta - \Delta, t)d\Delta
$$

$$
= \int P(\theta_j = \theta - \Delta) \left( P(\Delta_j = \Delta|\theta_j = \theta - \Delta) + \{W(\Delta, t + \tau|\theta - \Delta, t) - P(\Delta_j = \Delta|\theta_j = \theta - \Delta)\} \right) d\Delta
$$

$$
= P(\theta_{j+1} = \theta) + \int P(\theta_j = \theta - \Delta) \{W(\Delta, t + \tau|\theta - \Delta, t) - P(\Delta_j = \Delta|\theta_j = \theta - \Delta)\} d\Delta
$$

$$
= P(\theta_{j+1} = \theta) + \int \rho(\theta - \Delta, t)W(\Delta, t + \tau|\theta - \Delta, t)d\Delta - \int P(\theta_j = \theta - \Delta)P(\Delta_j = \Delta|\theta_j = \theta - \Delta)d\Delta.
$$

(10)
The two integrals above can be Taylor-expanded in the same way as our derivation of the Kramers-Moyal expansions to yield

\[ e(\theta) = \rho(\theta, t + \tau) - P(\theta_{j+1} = \theta) \]

\[ = \sum_{\gamma \in \mathbb{N}_0^2} \frac{(-1)^\gamma}{\gamma!} \partial^\gamma_{\theta} \left\{ \rho(\theta, t)E[\Delta(\tau)^\gamma] - P(\theta_j = \theta)E[\Delta_j^\gamma] \right\} \]

\[ = \sum_{\gamma \in \mathbb{N}_0^2} \frac{(-1)^\gamma}{\gamma!} \partial^\gamma_{\theta} \left\{ \rho(\theta, t)(\hat{m}_\gamma(\theta) - m_\gamma(\theta)) \right\} \]

(11)

\[ = \sum_{\gamma \in \mathbb{N}_0^2} \frac{(-1)^\gamma}{\gamma!} \partial^\gamma_{\theta} \left\{ \rho(\theta, t)e_\gamma(\theta) \right\}, \]

(12)

where we define the error in the \( \gamma \)-th moment to be \( e_\gamma(\theta) = \hat{m}_\gamma(\theta) - m_\gamma(\theta) \). So, e.g.,

\[ \int |e(\theta)|d\theta \leq \sum_{\gamma \in \mathbb{N}_0^2} \frac{1}{\gamma!} |\partial^\gamma_{\theta} \left\{ \rho(\theta, t)e_\gamma(\theta) \right\}|. \]

(13)

Recall that the errors \( e_\gamma(\theta) \) are due to the i.i.d. assumption on the infinitesimal increments in the continuous approximation; that is, the assumption that the distribution of \( \Delta \) is approximately constant in an interval of length \( \tau \). Therefore, if \( \Delta \) varies slowly relatively to the timescale \( \tau \), the approximation will be close.

**Fokker-Planck Approximation Of SGD**

We now choose \( \Delta_j \) to be as in Eq. 15 to study SGD. Our goal here is to approximate SGD with a continuous-time process. Because cumulants of independent random variables are additive, and letting \( \omega_\gamma(\theta) \) be the \( \gamma \)-th cumulant of \( \partial_\theta U(x, \theta) \) (a single gradient sample), we find that the cumulant for the full batch \( \delta \) is

\[ \kappa_\omega(\theta) = (-T)^{\gamma}B \omega_\gamma(\theta). \]

So the KM expansion (equation 7) of the continuous-time SGD approximation then becomes:

\[ \partial_t \rho(\theta, t) = B \sum_{\gamma \in \mathbb{N}_0^2} \frac{T^\gamma}{\gamma!} \partial^\gamma_{\theta} \left( \omega_\gamma(\theta) \rho(\theta, t) \right). \]

(14)

Clearly, then, as \( T \) gets small, fewer terms in the expansion matter. The first two cumulants for SGD are the mean and variance of the gradients of \( U \) over the training distribution, respectively:

\[ \omega_1(\theta) = E_{x \sim q_{tr}}[\partial_\theta U(x, \theta)] \]

(15)

\[ \omega_2(\theta) = \text{Cov}_{x \sim q_{tr}}[\partial_\theta U(x, \theta)] \]

(16)

When \( T \) is small enough, or when the cumulants \( \omega_\gamma(\theta) \) are small for \( |\gamma| > 2 \) (e.g., when \( \partial_\theta U(x, \theta) \) is Gaussian, cumulants higher than 2 are zero), we can approximate the Kramers-Moyal expansion (14) by the Fokker-Planck (FP) equation that retains only the first two terms in the expansion. Switching to the notation of the main text:

\[ \omega_1(\theta) = \partial_\theta \tilde{U}(\theta), \quad \omega_2(\theta) = \tilde{D}(\theta), \]

(17)

(so \( \tilde{D}(\theta) = \omega_2(\theta) \in \mathbb{R}^{n \times n} \) is now the empirical covariance matrix of the gradients in the training, or diffusion matrix, and we let \( \tilde{U}(\theta) = L_\ell(\theta) \) to streamline notation), we obtain Equation 16 in the main text:

\[ \partial_t \rho(\theta, t) := BT \sum_{i=1}^n \partial_{\theta_i} \left\{ \partial_{\theta_i} \tilde{U}(\theta) \rho(\theta, t) \right\} + \frac{1}{2} BT^2 \sum_{i,j=1}^n \partial^2_{\theta_i, \theta_j} \left\{ \tilde{D}_{ij}(\theta) \rho(\theta, t) \right\}. \]

Equation 16 has the steady-state solution given by equation 19 in the main text:

\[ \rho(\theta) \propto \exp \left\{ -\frac{2}{T} \tilde{v}(\theta) \right\}, \]

where

\[ \tilde{v}(\theta) = \int \left( \tilde{D}(\omega)^{-1} \partial_{\theta_0} \tilde{U}(\omega) + \frac{T}{2} \tilde{D}(\omega)^{-1} (\partial_{\theta_0} \tilde{D}(\omega))' \right) \cdot d\omega \]
\( \dot{v}(\theta) \) is the effective potential that SGD minimizes. Here, the integrals are line integrals, \( \cdot \) denotes the dot product, and \( \partial_\theta \cdot \tilde{D}(\theta) \) is the divergence of a matrix, assumed to yield a column vector (consistent with most notation elsewhere), and \( \omega \) is a dummy integration variable.

To show Eq. 19 is the stationary solution of Eq. 16, we follow (Gardiner 2009) (section 6.2). Rewrite Eq. 16 as

\[
\partial_t \rho(\theta, t) = BT (\partial_\theta \cdot J),
\]

where

\[
J = \rho(\theta, t) \partial_\theta \tilde{U}(\theta) + \rho(\theta, t) \frac{T}{2} (\partial_\theta \cdot \tilde{D}(\theta)) + \frac{T}{2} \tilde{D}(\theta) \partial_\theta \rho(\theta, t)
\]

is the probability current (vector). At steady-state, \( \partial_\theta \cdot J = 0 \) everywhere, so we seek a solution \( \rho(\theta) \) where \( J \) is constant. We also require \( \rho(\theta) \) being zero at infinity, making \( J = 0 \) everywhere. Setting Eq. 17 equal to zero yields after some algebra

\[
\frac{\partial_\theta \rho(\theta)}{\rho(\theta)} = \frac{2}{T} \tilde{D}(\theta)^{-1} \partial_\theta \tilde{U}(\theta) - \tilde{D}^{-1}(\theta) (\partial_\theta \cdot \tilde{D}(\theta)) = -Z
\]

\[
\implies \int^\theta_0 \partial_\theta \log(\rho) \cdot d\omega = -\int^\theta_0 Z \cdot d\omega := -\frac{2}{T} \tilde{g}(\theta, T), \text{ where } \tilde{g}(\theta, T) = \dot{v}(\theta) + \frac{T}{2} \tilde{a}(\theta).
\]

Applying the divergence theorem immediately results in the stationary distribution stated above, which can be also written as \( \rho(\theta) \propto \exp\{-\frac{2}{T} \tilde{g}(\theta, T)\} \) (though we often drop the \( T \) argument from \( g(\cdot) \) to reduce notational clutter). Because \( Z \) is defined as \(-\partial_\theta \log(\rho(\theta))\), the equation above can only be satisfied if \( Z \) is a gradient; a necessary and sufficient condition for this is the vanishing of the curl or so-called potential conditions

\[
\frac{\partial}{\partial \theta_i} Z_j = \frac{\partial}{\partial \theta_j} Z_i,
\]

where \( Z_i \) denotes the \( i \)-th entry of \( Z \). We assume that \( \tilde{D}(\theta) \) and \( \partial_\theta \tilde{U}(\theta) \) are such that these conditions indeed hold.

**When is the approximation accurate?** The Fokker-Planck approximation of SGD follows from two approximations. First, we need the increments \( \tilde{\Delta}(dt) \) within a time interval of \( \tau \) (corresponding to a single SGD update) to be i.i.d., so that the KM expansion in Eq. 7 is an accurate approximation of the discrete time SGD process. Second, we need the terms of order \( |\gamma| > 2 \) in the KM expansion to be small (relative to the \(|\gamma| \leq 2 \) terms), so that the truncation that yields the FP equation is appropriate. The latter is satisfied when \( T \) is small, and/or the third and higher cumulants of the gradients (i.e., \( \omega_3(\theta) \) for \(|\gamma| > 2 \)) are small. The former needs the product of the expected change in \( \theta \) during a single update and of the derivative w.r.t. \( \theta \) of the density of any small increment to be small. \(^1\)

Furthermore, our analysis relies on the distribution having reached steady-state, and the number of SGD steps required to reach steady-state scales inversely with batch size, so in practice with small batch size the steady-state could be difficult to attain. Therefore, practically speaking, our conclusions start to break down for large \( T \) (i.e. large ratio of LR to batch size), but can also break down for fixed small \( T \) at extreme (very small or very large) learning rates or batch sizes. A large learning rate makes the expected change in \( \theta \) in a single update large, potentially violating the i.i.d. assumption of the small time increments, while a large batch size at small fixed temperature also implies a large learning rate, and has the same effect. We similarly expect the mean change in an SGD update to be large at the beginning of an SGD run, and our FP approximation to not be valid during some initial transient period. Lastly, the i.i.d. assumption can be violated when the derivative of the mean and covariance of a single SGD update with respect to \( \theta \) is large.

\(^1\)To see this, consider the joint probability of two infinitesimal updates within the same time period of length \( \tau \), i.e.,

\[
P(\Delta(dt) = x_0, \Delta(dt) = x_j) = P(\Delta(dt_0) = x_0) P(\Delta(dt) = x_j|\Delta(dt_0) = x_0),\text{ where } j > 0,
\]

and assume \( \theta = \theta_0 \) at the beginning of the \( dt_0 \) interval. We can write the latter probability as

\[
P(\Delta(dt) = x_j|\Delta(dt_0) = x_0) = E_W [P(\Delta(dt_j) = x_j|\theta_{j-1} = \theta_0 + W)], \text{ and } W = x_0 + \Delta(t_1, t_{k-1})
\]

is a random variable describing the increment since the start of the \( \tau \) time interval until the beginning of the \( k \)-th infinitesimal increment at \( k \)-1. Letting \( \mu_w \) denote the mean of \( W \), we can Taylor expand to first order around \( W = 0 \) to find that

\[
E_W [P(\Delta(dt) = x_j|\theta_{j-1} = \theta_0 + W)] \approx P(\Delta(dt_j) = x_j|\theta_{j-1} = \theta_0) + \mu_w \partial_{\theta_{j-1}} P(\Delta(dt_j) = x_j|\theta_{j-1} = \theta_0)
\]

plus higher order terms. When the second term above is small compared to the first, we can finally write that \( P(\Delta(dt_0) = x_0, \Delta(dt_j) = x_j) = P(\Delta(dt_0) = x_0) P(\Delta(dt) = x_j), \) and since \(|dt_j| = |dt_0| = dt \), and these increments only depend on these magnitudes and on \( \theta \) at the beginning of each increment (both equal to \( \theta_0 \) in our expansion above), then the i.i.d. assumption is satisfied. Conversely, when \( \mu_w \) and/or \( \partial_{\theta_j} P(\Delta(dt_j) = x_j|\theta = \theta_0) \) are large we expect the increments not to be i.i.d., and the KM expansion to not approximate the discrete process well.
**B Gaussian Mixture Approximation of SGD Stationary Distribution**

We further approximate the stationary distribution of SGD in Eq. 19 by a mixture of Gaussians, i.e., as a distribution of the form Eq.4, so we need to find the means and covariances $\mu_k$ and $\Sigma_k$, and the weights $w_k$. Throughout, we assume that $T$ is small, and of the same order as $\epsilon_0$, and keep only leading terms in either $T$ or $\epsilon_1$. What follows is essentially the Laplace approximation.

The test performance $\mathcal{L}_e$ only depends on the mean $\mu_k$ through the bias $b_k$. Recall that $\mu_k = \tilde{\theta}_k + b_k$. We define $\mu_k$ to be the local minima of $\tilde{g}(\theta) = \tilde{v}(\theta) + \frac{T}{2}\tilde{a}(\theta)$ that is close to the local minima $\tilde{\theta}_k$ of $\mathcal{L}_e(\theta)$. Since

$$\partial_\theta \tilde{g}(\theta) = \tilde{D}^{-1}(\theta) \left[ \partial_\theta \tilde{U}(\theta) + \frac{T}{2} \partial_\theta \cdot \tilde{D}(\theta) \right],$$

we have that

$$\partial_\theta \tilde{g}(\mu_k) = 0 \implies 0 = \partial_\theta \tilde{U}(\mu_k) + \frac{T}{2} \partial_\theta \cdot \tilde{D}(\mu_k)$$

$$0 = \tilde{U}(\tilde{\theta}_k) + \tilde{C}_k b_k + \frac{T}{2} \partial_\theta \cdot \tilde{D}_k$$

plus second-order terms, and where $\tilde{C}_k = \partial_\theta^2 \tilde{U}(\tilde{\theta}_k)$ and $\tilde{D}_k = \tilde{D}(\tilde{\theta}_k)$ are the local curvature and gradient covariance of the training objective at the $k$ local minima. A bit of algebra then leads to

$$b_k = -\frac{T}{2} \tilde{C}_k^{-1}(\partial_\theta \cdot \tilde{D}_k). \tag{21}$$

So the bias is proportional to the temperature. Next, we find $\Sigma_k$ and $w_k$, and we start by approximating $\rho(\theta)$ locally around a neighborhood $B_k$ of $\mu_k$ by Taylor expanding $\tilde{g}(\theta)$ around $\mu_k$. So

$$\rho(\theta) \propto e^{-\frac{1}{2} \tilde{g}(\mu_k)} e^{-\frac{1}{4}(\theta - \mu_k)^T \partial_\theta^2 \tilde{g}(\mu_k)(\theta - \mu_k)}$$

$$\propto e^{-\frac{1}{2} \tilde{g}(\mu_k)} \sqrt{|\Sigma_k|} \mathcal{N}(\mu_k, \Sigma_k), \text{ where } \Sigma_k = \frac{T}{2} (\partial_\theta^2 \tilde{g}(\mu_k))^{-1}. \tag{22}$$

Assuming $B_k$ is large enough to cover most of the probability mass of $\mathcal{N}(\mu_k, \Sigma_k)$, we then have that $w_k \propto e^{-\frac{1}{2} \tilde{g}(\mu_k)} \sqrt{|\Sigma_k|}$. We now find an explicit expression for $\Sigma_k$:

$$\partial_\theta^2 \tilde{g}(\theta) = \tilde{D}^{-1}(\theta) \left[ \partial_\theta^2 \tilde{U}(\theta) + \frac{T}{2} \partial_\theta(\partial_\theta \cdot \tilde{D}(\theta)) \right] - \tilde{D}^{-1}(\theta)(\partial_\theta D(\theta)) \partial_\theta \tilde{g}(\theta).$$

We want the matrix above when $\theta = \mu_k$. The quantity $\partial_\theta \cdot \tilde{D}(\theta)$ in the second term on the right is a tensor, but we do not need to understand it because when $\theta = \mu_k$, $\partial_\theta \tilde{g}(\mu_k) = 0$, so the second term drops out. In addition, since we only want leading terms in $T$ in our expression for $\Sigma_k$, we have that

$$\partial_\theta^2 \tilde{g}(\mu_k) \approx \tilde{D}^{-1}(\mu_k) \partial_\theta^2 \tilde{U}(\mu_k) \approx \tilde{D}_k^{-1} \tilde{C}_k,$$

where the last equality follows from $b_k$ being small and of order $T$. Inverting the last equation, we find the covariance

$$\Sigma_k = \frac{T}{2} \tilde{C}_k^{-1} \tilde{D}_k = \frac{T}{2} (I - \tilde{C}_k^{-1} \tilde{E}_k), \tag{23}$$

which is also proportional to the temperature. Here $I$ is the identity matrix. Finally, we clean up our expression for $w_k$. We let $\tilde{v}_k = \tilde{v}(\tilde{\theta}_k)$, and note that $e^{-\frac{1}{2} \tilde{g}(\mu_k)} = e^{-\frac{1}{2} \tilde{v}_k - \tilde{a}_k}$ to leading order (in $T$ and our other small parameters, $\epsilon_1$ and $N$), and that $|\Sigma_k| \propto |\tilde{C}_k^{-1} \tilde{D}_k|$, so

$$w_k = e^{-\frac{2\tilde{v}_k}{Z}} e^{-\tilde{a}_k} \sqrt{|\tilde{D}_k|/|\tilde{C}_k|} = e^{-\frac{2\tilde{v}_k}{Z}} e^{-\tilde{a}_k} \sqrt{|I - \tilde{C}_k^{-1} \tilde{E}_k|}, \text{ where } \tag{24}$$

$$Z = \sum_j e^{-\frac{2\tilde{v}_j}{Z}} e^{-\tilde{a}_j} \sqrt{|\tilde{D}_j|/|\tilde{C}_j|} \tag{25}$$

is the partition function. This distribution is essentially in the same form as the equilibrium distribution over states in thermodynamics. Indeed, we follow the process used in thermodynamics to understand how different quantities change with temperature, to understand how the test performance depends on SGD temperature.
We want to show that the model performance in Eq. 6, i.e.,

\[ \mathcal{L}_e = \langle \mathcal{L}_e(\theta) \rangle = (U) + \frac{1}{2} \left( \text{Tr}(C\Sigma) + ((b + s)'C(b + s)) \right), \]

(where \( f = \sum_k w_k f_k \)),

is approximately reparametrization-invariant, for any distribution \( \rho(\theta) = \sum_k w_k \mathcal{N}(\mu_k, \Sigma_k) \) that approximates a distribution of the form \( \rho(\theta) \propto e^{-\frac{1}{2} \tilde{g}(\theta, T)} \), such that \( \mu_k \approx \theta_k \), i.e. the peaks of \( \rho(\theta) \) are approximately located at the local minima \( \theta_k \) of \( U \).

Specifically, we assume that \( b_k = \mu_k - \theta_k = O(T) \), where \( T \) is small. The SGD stationary distribution satisfies this condition.

To reduce clutter, we do not write the argument \( e \) to simplify notation. Some of the dimensions of the other quantities here are:

- \( \partial_y f(r(y)) \in \mathbb{R}^n \),
- \( \partial^2_y f(r(y)) \in \mathbb{R}^{n \times n} \),
- \( \partial_\theta f \in \mathbb{R}^n \),
- \( \partial^2_\theta f \in \mathbb{R}^{n \times n} \).

We can use these to help with the terms in \( \mathcal{L}_e(\theta_k) \):

Consider a reparametrization \( y = r^{-1}(\theta) \) of \( \theta \) (with \( \theta, y \in \mathbb{R}^n \)), where \( r : \mathbb{R}^n \rightarrow \mathbb{R}^n \) is invertible. For an arbitrary function \( f(\theta) \), we define the reparametrized version by \( f'(y) = f(r(y)) = f(\theta) \). With this notation, we want to show that \( w^e_k = w_k \) and \( \mathcal{L}_e(y_k) = \mathcal{L}_e(\theta_k) \), where \( y_k = r^{-1}(\theta_k) \).

First, we recall from Equation 22 that any distribution of the form \( \rho(\theta) \propto e^{-\frac{1}{2} \tilde{g}(\theta)} \) can be approximated as a Gaussian mixture

\[ \rho(\theta) \propto e^{-\frac{1}{2} \tilde{g}(\mu_k)} \sqrt{\det \Sigma_k} \mathcal{N}(\mu_k, \Sigma_k), \]

where \( \Sigma_k = \frac{T}{2} (\partial_\theta \tilde{g}(\mu_k))^{-1} \).

First we want to show that the weights \( w_k \) are reparametrization invariant. These are defined as: \( w_k = \int_{N_k} \rho(\theta) d\theta \), where \( N_k \) is the basin around \( \theta_k \). Letting \( \rho^\mu(y) \) denote the p.d.f. of \( y = r^{-1}(\theta) \), and noting that \( \rho^\mu(y) = \rho(\theta) |\det dr(y)| \), where \( dr \in \mathbb{R}^{n \times n} \) is the Jacobian of \( r \), (by applying a general formula for invertible functions of random variables), we have:

\[
\begin{align*}
    w_k &= \int_{N_k} \rho(\theta) d\theta \\
    &= \int_{r^{-1}(N_k)} |\det dr(y)| \rho(r(y)) dy \\
    &= \int_{N_k} \rho^\mu(y) dy = w_k.
\end{align*}
\]

Next we want to show that \( \mathcal{L}_e(\theta_k) \), defined as:

\[ \mathcal{L}_e(\theta_k) = U_k + \frac{1}{2} \left( \text{Tr}(C_k \Sigma_k) + (b_k + s_k)'C_k(b_k + s_k) \right), \]

is approximately reparametrization-invariant. First note that for any \( f : \mathbb{R}^n \rightarrow \mathbb{R} \), the first two derivatives of \( f' \) are:

\[
\begin{align*}
    \partial_y f(r(y)) &= \partial_y r(y)' \partial_\theta f(\theta), \\
    \partial^2_y f(r(y)) &= \partial_y r(y)' \partial^2_\theta f(\theta) \partial_\theta r(y) + \partial^2_\theta r(y) \partial_\theta f(\theta) \\
    &= \partial_\theta f(\theta) \partial_\theta r(y), \text{ if } \theta \text{ is a local extremum of } f.
\end{align*}
\]

Here \( \partial^2_\theta r(y) \) is a tensor, so the way we wrote it does not quite make sense, but it does not pay to introduce tensor notation since it gets multiplied by \( \partial_\theta f(\theta_k) \), which is a vector of zeros, when we use the above. So the tensor never plays a role in our subsequent computations. Some of the dimensions of the other quantities here are \( \partial_\theta r(y) \in \mathbb{R}^n \), with its \( i,j \)-th entry being \( \frac{\partial}{\partial \theta_i} \theta_j \), \( \partial_\theta f(r(y)) \in \mathbb{R}^n \), \( \partial^2_\theta f(r(y)) \in \mathbb{R}^{n \times n} \), \( \partial_\theta f \in \mathbb{R}^n \), \( \partial^2_\theta f \in \mathbb{R}^{n \times n} \). We can use these to help with the terms in \( \mathcal{L}_e(\theta_k) \):
\[ U_k^r = U(r(y_k)) \equiv U(\theta_k) = U_k \]  
\[ C_k^r = \partial^2_y U(r(y_k)) \]  
\[ = \partial_y r(y_k) \partial^2_y U(\theta_k) \partial_y r(y_k) \quad \text{since } \partial_\theta U(\theta_k) = 0 \]  
\[ = \partial_y r(y_k) C_k \partial_y r(y_k) \]  
\[ s_k^r = \hat{y}_k - y_k \]  
\[ \approx \partial_y r(y_k)^{-1}(\hat{\theta}_k - \theta_k) + O((\hat{y}_k - y_k)^2) \quad \text{since } \Delta \theta \approx (\partial_y r) \Delta y + O(\Delta y^2) \]  
\[ = \partial_y r(y_k)^{-1} s_k + O(s_k^2) \]  
\[ \Sigma_k^r = \frac{T}{2} \left( \partial^2_y g(r(y_k^r)) \right)^{-1} \]  
\[ = \frac{T}{2} \partial_y r(y_k^r)^{-1} \left( \partial^2_y g(\mu_k) \right)^{-1} \partial_y r(y_k^r)^{-1} \]  
\[ = \frac{T}{2} \partial_y r(y_k)^{-1} \left( \partial^2_y g(\theta_k) \right)^{-1} \partial_y r(y_k)^{-1} + O(T^2), \quad \text{since } b_k, y_k^r - y_k = O(T) \]  
\[ = \partial_y r(y_k)^{-1} \Sigma_k^{-1} \partial_y r(y_k)^{-1} + O(T^2) \]  
\[ \Rightarrow \mathcal{L}_c(y_k) = U_k^r + \frac{1}{2} \left( \text{Tr}(C_k^r \Sigma_k^r) + (b_k^r + s_k^r)^T C_k^r (b_k^r + s_k^r) \right) \]  
\[ U_k^r = U_k \]  
\[ \text{Tr}(C_k^r \Sigma_k^r) = \text{Tr} \left( \partial_y r(y_k)^T C_k \partial_y r(y_k) \partial_y r(y_k)^{-1} \Sigma_k^{-1} \partial_y r(y_k)^{-1} \right) + O(T^2) \]  
\[ = \text{Tr} \left( C_k \Sigma_k^{-1} \right) + O(T^2) \]  
\[ b_k^r C_k s_k^r = O(T^2), \quad \text{since } b_k \text{ is } O(T) \]  
\[ s_k^r C_k s_k^r = \Sigma_k^{-1} \partial_y r(y_k)^{-1} \partial_y r(y_k)^{-1} \]  
\[ = \Sigma_k^{-1} \partial_y r(y_k)^{-1} + O(s_k^2) \]  
\[ \Rightarrow \mathcal{L}_c(y_k) = \mathcal{L}_c(\theta_k) + O(T^2 + s_k^2). \]  

Since \( w_k \) and \( \mathcal{L}_c(\theta_k) \) are reparametrization invariant, so is \( \mathcal{L}_c \).

**D  Shift between local minima of train and test losses**

Here we find an approximate expression for the shifts \( s_k \). We model shifts that arise due to either distribution shift, or sampling, or both. First, we now assume that the training and test distributions can be parametrized as \( r_e(x) = r(x|\eta_e) \) and \( r_r(x) = r(x|\eta_r) \), where the parameter \( \eta \in \mathbb{R}^m \). We let \( \epsilon_\eta = \eta - \eta_e \), assume \( \epsilon_\eta \) is small, and expand \( r_e(x) \) to first order to obtain
\[ r_e(x) = r_e(x) + \epsilon_\eta \partial_\eta r(x|\eta_e). \]  
Defining
\[ \partial_\theta U(\theta) := \int r_e(x) \partial_\theta U(x, \theta) dx, \quad \text{and} \quad \partial_\theta \tilde{U}(\theta) = \int r_t(x) \partial_\theta U(x, \theta) dx, \]  
we have:
\[ E[\partial_\theta \mathcal{L}_c(\theta)] := \int r_e(x) \partial_\theta \mathcal{L}_c(x, \theta) dx = \int r_e(x) \partial_\theta U(x, \theta) dx = \partial_\theta U(\theta), \]  
and similarly,
\[ E[\partial_\theta \mathcal{L}_t(\theta)] = \int r_t(x) \partial_\theta U(x, \theta) dx = \partial_\theta \tilde{U}(\theta), \]  
where \( E[\cdot] \) means expectation with respect to realizations of data sets from \( r_e(x) \) and \( r_t(x) \), keeping \( N_e \) and \( N_t \) fixed.
Using equation 37, we can write:
\[ \partial \tilde{U}(\theta) = \int (r_e(x) + \epsilon'_q \partial \eta r(x|\eta_e)) \partial \theta U(x, \theta) dx \]  
(41)

where \( F(\theta) = \int r_e(x) \partial \theta U(x, \theta) \partial \eta R(x, \eta_e)' dx, \quad R(x, \eta) = -\log r(x|\eta). \)  
(43)

Since datasets are large, we can approximate the gradient of the losses as a sample from a Gaussian random variable
\[ \partial \mathcal{L}_c(\theta) = z_\ell \sim \mathcal{N}(\partial \mathcal{L}_c(\theta), \frac{1}{N_\ell} \hat{D}(\theta)), \quad \text{and} \]
\[ \partial \mathcal{L}_e(\theta) = z_x \sim \mathcal{N}(\partial \tilde{U}(\theta), \frac{1}{N_e} \tilde{D}(\theta)). \]
(44)

where
\[
\hat{D}(\theta) = \text{Cov}_{r_e}(\partial \mathcal{L}_c(\theta)), \quad \tilde{D}(\theta) = \text{Cov}_{r}(\partial \mathcal{L}_c(\theta)), \quad D(\theta) = \text{Cov}_{q_e}(\partial \theta U(x, \theta)), \quad \tilde{D}(\theta) = \text{Cov}_{q}(\partial \theta U(x, \theta)).
\]
(46)

are the gradient covariance matrix under the specified distributions for \( x \). Also, Eq. 37 implies that \( \hat{D}(\theta) = \tilde{D}(\theta) + \frac{c}{N_e} \times \text{tensor} \), so we can write \( \hat{D}(\theta) \approx \tilde{D}(\theta) \) to leading order (since both \( \epsilon_q \) and \( N^{-1} \) are small), so we do not need to specify the tensor. Lastly, we replace \( \tilde{D}(\theta) \) with its (unbiased) sample estimate \( D(\theta) \), since that is what we have access to. All this means that
\[ \Delta_\ell(\theta) := \partial \mathcal{L}_c(\theta) - \partial \mathcal{L}_e(\theta) \sim \mathcal{N}(F(\theta) \epsilon_q, \frac{1}{N_{\text{eff}}} 2D(\theta)), \]  \quad \text{where} \quad N_{\text{eff}}^{-1} = \frac{1}{2} \left( N_e^{-1} + N_\ell^{-1} \right) \]
(47)

is the harmonic mean of the data set sizes. Next, we look at a local minima of the training function, to obtain
\[ 0 = \partial \mathcal{L}_c(\tilde{\theta}_k) = \partial \mathcal{L}_c(\theta_k) - \Delta_\ell(\tilde{\theta}_k) \approx \partial \mathcal{L}_c(\theta_k) + C_k s_k - \Delta_\ell(\theta_k) \]
(48)

\[ \implies s_k \approx C_k^{-1} \Delta_\ell(\tilde{\theta}_k) \sim \mathcal{N}(C_k^{-1}F(\tilde{\theta}_k) \epsilon_q, \frac{1}{N_{\text{eff}}} 2C_k^{-1}D(\tilde{\theta}_k)C_k^{-1}) \approx \mathcal{N}(C_k^{-1}F_k \epsilon_q, \frac{1}{N_{\text{eff}}} 2C_k^{-1}D_k C_k^{-1}). \]
(49)

Here, in the last approximation we set \( \Delta_\ell(\tilde{\theta}_k) \approx \Delta_\ell(\theta_k) \), which means ignoring a term of order \( |\partial \theta F(\theta_k)||s_k| \) in the mean, and a term of order \( |\partial \theta D(\theta_k)||s_k| \) in the covariance, under the assumption that they are smaller than the terms we keep. We can use the above to rewrite
\[ E[s_k' C_k s_k] = E[\text{Tr}(s_k' C_k s_k)] = \text{Tr}(E[C_k]E[s_k' s_k']) \approx \text{Tr}
\]
\[ C_k (\text{Cov}(s_k) + E[s_k]E[s_k']) \]
(50)

\[ = \frac{2}{N_{\text{eff}} \text{Tr}(D_k C_k^{-1}) + E[s_k' C_k E[s_k]] = \frac{2}{N_{\text{eff}}} (n - \text{Tr}(E_k C_k^{-1})) + \epsilon_q F_k C_k^{-1} F_k \epsilon_q, \]

where the approximation \( E[C_k] \approx C_k \) was used (replacing the curvature relative to \( r_e(x) \) with its empirical estimate which is relative to \( q_e(x) \)), and where the last line used \( D_k = C_k - E_k \) from Eq. 12 in the main text.

**Shift assuming location parameters**

If \( \theta \) and \( \eta \) are both location parameters, i.e. \( p(x|\theta) = p(x|\theta - \cdot), r(x|\eta) = r(x - \cdot | \eta) \) hence \( \partial \cdot = -\partial x, \partial \eta = -\partial x \) then (integrating by parts and assuming that the distributions go to zero at infinity i.e. \( \lim_{x \to \pm \infty} p(x|\theta), r(x|\eta) = 0 \):
\[ F(\theta) = -\int \partial \theta U(x, \theta) \partial \eta r(x|\eta_e) dx = -\int \partial x r(x|\eta_e) \partial \eta U(x, \theta) dx \]
(51)

\[ = \int r(x|\eta_e) \partial^2 x U(x, \theta) dx = \int r(x|\eta_e) \partial^2 \theta U(x, \theta) dx \]
(52)

\[ = E[C_k] \approx C_k \]
(53)

\[ \implies E[s_k] = \epsilon_q \]
(54)

\[ E[s_k' C_k s_k] = \frac{2}{N_{\text{eff}}} (n - \text{Tr}(E_k C_k^{-1})) + \epsilon_q C_k \epsilon_q. \]
(55)
E SGD implicit objective

We can show that the stationary distribution of SGD $\rho(\theta)$ solves the following optimization problem:

$$ \rho(\theta) = \arg \min_{\rho(\theta)} \mathcal{F}(\rho), \quad \text{where} $$

$$ \mathcal{F}(\rho) = \langle \tilde{v}(\theta) \rangle_{\rho} + \frac{T}{2} \langle \tilde{a}(\theta) \rangle_{\rho} - \frac{T}{2} h(\rho). $$

(56)

Here, $\langle \cdot \rangle_{\rho}$ denotes expectation under $\rho(\theta)$, and $\mathcal{F}(\rho)$ is the Helmholtz free energy from statistical physics (that determines the effective thermodynamic potential), and achieves its minimum value $\mathcal{F}(\rho) = -T \log Z$. The entropy of $\rho(\theta)$ is denoted by $h(\rho)$. Eq. 56 shows that SGD solves a related but different problem than the model test performance $\mathcal{L}_e$. The first term in Eq. 56 would proportional to test performance if $\hat{D}(\theta)$ were proportional to the identity. We see that SGD also attempts to maximize entropy and minimize $\tilde{a}(\theta)$, and focuses more on these two objectives as $T$ increases.

To derive Eqs. 56 and 57, we let $q(\theta) = \frac{1}{Z} \exp\{-g(\theta)\}$ be a distribution with the stated form but with arbitrary $g(\theta)$. Note that $\log q(\theta) = -\log Z - g(\theta)$. Consider the KL distance between a completely arbitrary distribution, $p(\theta)$, and $q(\theta)$:

$$ KL(p, q) = \int p(\theta) \log \frac{p(\theta)}{q(\theta)} d\theta = -h(p) - \int p(\theta) \log q(\theta) d\theta $$

$$ = \log Z + E_{\theta \sim p}[g(\theta)] - h(p). $$

(58)

Since $\log Z$ is independent of $p(\theta)$, minimizing $KL(p, q)$ with respect to $p(\theta)$ is equivalent to minimizing $E_{\theta \sim p}[g(\theta)] - h(p)$. Similarly, since $p(\theta) = q(\theta)$ minimizes this KL distance, and since $KL(p, p) = 0$, we also have that

$$ -\log Z = E_{\theta \sim p}[g(\theta)] - h(p). $$

(59)

Applying these results when $q(\theta)$ is the stationary SGD distribution from Eq. 19 results after some simple algebra in Eqs. 56 and 57. A similar argument can be made to define the optimization problem that (the discrete SGD distribution) $w_k$ solves.

F Additional calculations

Temperature derivatives (equation 24)

Here we derive equation 24. Eq. 6 expresses the test performance as a function of averages under $w_k$ of local quantities of each local minima of $\mathcal{L}_e(\theta)$. To understand how test performance changes with temperature, we need to understand how these averages do, recognizing that $w_k$ changes with temperature as specified by Eq. 20. We follow standard calculations for the canonical ensemble from Physics. Let $f_k$ denote a scalar quantity corresponding to local minima $k$, like $U_k$, $\tilde{v}_k$, etc. We let $\beta = T^{-1}$, and study the derivatives of $Z$, $\log Z$, $w_k$, and $\langle f \rangle$ with respect to $\beta$.

Recalling the definitions of $\tilde{v}(\theta)$, $\tilde{a}(\theta)$ from equation 19, we can write:

$$ e^{-2\beta \tilde{a}_j} = e^{-2\beta \tilde{v}_j - \tilde{a}_j} $$

(60)

$$ \Rightarrow \partial_\beta e^{-2\beta \tilde{a}_j} = -2 \tilde{v}_j e^{-2\beta \tilde{a}_j} $$

(61)

$$ \Rightarrow \partial_\beta \log Z = -2 \langle \tilde{v} \rangle $$

(62)

$$ \Rightarrow \partial_\beta w_k = -2 \tilde{v}_k w_k - w_k \partial_\beta \log Z = -2 w_k \langle \tilde{v} \rangle - \tilde{v}_k $$

(63)

$$ \Rightarrow \partial_\beta \langle f \rangle = \sum \partial_\beta w_k f_k = -2 \sum w_k f_k \langle \tilde{v} \rangle - \tilde{v}_k $$

(64)

$$ = 2 \text{Cov}(\tilde{v}, f) $$

(65)

Using the chain rule then gives the derivative of the average of $f_k$ with respect to $T$:

$$ \partial_T \langle f \rangle = \frac{2}{T^2} \text{Cov}(\tilde{v}, f). $$

(67)

Entropy calculations

KL/entropy decomposition of $U$:

$$ U(\theta) = -E_{x \sim p(x|\theta^*)} [\log p(x|\theta)] $$

$$ = -\int p(x|\theta^*) \log p(x|\theta) dx $$

$$ = h(\theta^*) + KL(\theta^*, \theta) $$

where $h(\theta^*)$ is the differential entropy of $p(x|\theta^*)$ and $KL(\theta^*, \theta) = \int p(x|\theta^*) \log \frac{p(x|\theta^*)}{p(x|\theta)} dx$ is the KL distance between $p(x|\theta^*)$ and $p(x|\theta)$. 
G CIFAR10 experiments

We ran experiments on CIFAR10 (Krizhevsky, Hinton et al. 2009) to demonstrate the phenomenon of generalization improving with temperature, as well as to understand the shift between and training and test sets for CIFAR10. For all experiments, we used the VGG9 network (Simonyan and Zisserman 2014) and the training procedure of (Li et al. 2017) (but with no momentum).

The temperature experiment is shown in Figure 1. We first trained a network using a large batch size (4096) and decreasing learning rate schedule (starting from 0.1, scaled by 0.1 at 0.5, 0.75 of total epochs, ending with LR 0.001) until the training converged. Then, we continued training from that initialization with a variety of batch sizes and learning rates (all LRs held constant in second stage), for 1000 epochs (regardless of batch size). For each second-stage run, we took the median of the last 100 steps (to eliminate spiky outliers) as the ‘final loss’. We repeated this two-stage experiment 10 times (with different initializations), and plotted the mean and variance of the final test loss as a function of temperature (learning rate divided by batch size) in Figure 1 (selected trajectories of the two stages are shown in 1). Our results show that both the train loss and test loss depend primarily on the temperature, and test loss decreases with increasing temperature while train loss remains roughly constant. For small batches (50 and 100), train loss was higher at the beginning of the second stage for all LRs; train loss dropped significantly by the end of training with large LRs but remained high with small LRs. We believe this was due to mismatched batchnorm statistics and parameters (parameters learned for bs 4096 but applied to bs 50 or 100); with larger LRs the network was able to retrain the batchnorm parameters, but smaller LRs did not allow sufficient progress.

Next, we ran experiments to help understand the shift between and training and test sets for CIFAR10 (Figure 2). Our analysis suggests that the generalization benefit of noise in SGD depends on a shift between the train and test sets, as captured

$$\epsilon = \eta - \eta_e$$

where $r(x|\eta)$ and $r(x|\eta_e)$ are the training and test distributions. As we discussed previously, such a shift could be due to distribution shift or finite samples (or both). To determine which of these is more likely in the case of the CIFAR10, we have run two experiments.

To study distribution shift, we merge the train and test sets, reshaple them to create a single dataset, and then randomly split the data into training and test at each trial. If there were a distribution shift between the default train and test split in the CIFAR data, the process would remove it, and we would expect the generalization gap to decrease, leaving only the shift based on finite samples. Our experiment shows that there is no significant difference in the generalization gap for different shufflings of the train and test sets, suggesting that distribution shift is not present, only finite sample shift.

To better understand the role of finite sampling, we take subsamples of the complete dataset of different sizes, still split proportionally into train and test. If finite sampling were causing the shift between the training and test distributions, we would expect smaller sample sizes to exacerbate the difference (since sampled distributions generally become closer to the underlying distribution as the sample size grows). Our experiment shows that the generalization gap increases as the sample size decreases, consistent with finite sampling as the source of distribution shift.

H Synthetic experiments

Experiment details

The objective plots show the synthetic train and test objective (loss) functions $\hat{U}(\theta)$ and $U(\theta)$. For the stationary distribution plots, we plug the train loss $\hat{U}(\theta)$, the gradient variance $\hat{D}(\theta)$, and the current temperature into Equation 19, and evaluate as a function of $\theta$. For the probability of each basin plots, we integrate the stationary distribution over the basin of each minimum (i.e., between the two local maxima adjacent to the minimum, or the range endpoint – noting that $\rho \to 0$ at the range endpoints);
Figure 2: Left: Synthetic one-basin experiment with the same setup as in Figure 3. Train and test error both increase as temperature increases. Right: Synthetic three-basin experiment with the same setup as in Figure 3. Minimum at 0 is deeper but narrower than minima at −1 and 1; −1 and 1 are equally deep but 1 is wider. Generalization improves (test error decreases while training error increases) with increasing temperature, as the stationary distribution moves probability mass from the narrower deeper minimum at 0 toward the wider minima, with a preference for the widest minimum at 1.

do the probabilities are plotted as a function of temperature. Finally, the train vs. test loss plots show the train and test losses as a function of temperature, e.g. train loss is computed as $\int \rho(\theta)\tilde{U}(\theta)d\theta$ (where $\rho(\theta)$ depends on the temperature per Eq. 19).

One and Three basin

Figures 2 shows 1-basin and 3-basin experiments analogous to the 2-basin experiment in Figure 3. In the 1-basin example, both train and test error increase with increasing temperature. The 3-basin example shows qualitatively similar behavior to the 2-basin case and confirms the SGD stationary distribution’s preference for wider minima when the depths are similar.

Two basin: when effective potential reorders minima

There are two ways the effective potential $\tilde{v}$ could reorder the minima relative to the test potential $U$. The first is if the training loss reorders the minima relative to the test loss (since $\tilde{v}$ is derived from the train loss). If the training and test set differ only due to sampling, this reordering is unlikely to happen consistently over multiple different samplings – although it might if there is a distribution shift. This situation is shown in Figure 3.

The second way the reordering can happen is if the gradient variance ($D$) is nonconstant and affects the integral in $\tilde{v}$. Some experiments are shown in Figure 4. More research is needed on this topic.

A note on formality

Regarding the following points:

• All assumptions and restrictions are stated clearly and formally
• All novel claims are stated formally (e.g., in theorem statements),

we have deliberately chosen to write our paper without formal theorem statements, although we clearly state our results, assumptions, and restrictions. We feel that formal language obscures understanding and makes it more difficult to engage a broader academic audience.

Source code and infrastructure notes

The code used for the CIFAR10 experiments was a slightly modified version of the code accompanying (Li et al. 2017), publicly available on the authors’ github. The modifications we made were primarily to allow it to run on our cluster, plus minor changes to enable our specific experiments, namely:

• Change to the learning rate schedule:

```python
- if int(epoch) == 150 or int(epoch) == 225 or int(epoch) == 275:
+ if int(epoch) == int(0.5 * args.epochs) or
  int(epoch) == int(0.75 * args.epochs) or
```
Figure 3: The situation is the same as in Figure 3, except that in addition to the left-right shift $s$, the depths of the minima are also shifted by $(+\xi, -\xi)$, respectively. Since $d$ is constant (so the effective potential is proportional to the true potential), the reordering of depths of minima can only occur when the sampling actually reorders the minima (otherwise we end up with cases shown in Figure 3. Left: $U$ (test) has minimum at 1 both deeper and wider, but $\tilde{v}(U)$ (train) reorders the minima so that minimum at $-1$ is deeper. Generalization improves (test error decreases while training error increases) with increasing temperature as weight gets transferred from $-1$ to 1. Right: $U$ (test) has minimum at $-1$ deeper but 1 narrower, while effective potential (train) reorders so that $-1$ is deeper. Both training and test error worsen with increasing temperature, as weight gets transferred from 1 to $-1$.

```
int(epoch) == int(0.9 * args.epochs):

  • Option to set a specific seed for weight initialization
  • Option to reshuffle training and test sets with a specific seed (in dataloader)
  • Option to use a subsample of full dataset (in dataloader)
```

The synthetic (1, 2, 3 basin) experiments were run on a 2018 MacBookPro running MacOS 11.1, using Python3.6. The CIFAR10 experiments were run on a cluster, where we were allocated 1 GPU (V100) and 2 CPUs, Disk 60GB, Memory 50GB, and running Python3.6 with Pytorch1.0.1.

**Experiment hyperparameter notes**

- **Figure 1 Stage 1:**
  - rand_seed: range(0, 10)
  - batch_size: 4096
  - lr: 0.1
  - lr_decay: 0.1
  - epochs: 300
  - weight_decay: 0.0005
  - momentum: 0

- **Figure 1 Stage 2:**
  - resume_run_id: all runs from Stage 1
  - resume_epoch: 1200
  - rand_seed: -1
  - batch_size: [1, 50, 100, 500, 1000, 2000, 3000, 4000]
  - lr: (batch_size/4096) * np.hstack((np.arange(0.0001, 0.001, 0.0001),
         np.arange(0.001, 0.01, 0.001),
         np.arange(0.01, 0.2, 0.01)))
  - lr_decay: 1.0
  - epochs: 2200
  - weight_decay: 0.0005
  - momentum: 0
In this experiment, we actually sample over $x$ from $U(x, \theta)$, where $U(x, \theta)$ is a two-basin potential depending on both $x$ and $\theta$. We estimate the gradient variance $\tilde{D}(\theta)$ as the variance of the gradient samples. In both panes (using different models of $U(x, \theta)$), the minimum of $U$ at $-1$ narrower but much deeper than the one at $1$, but the minimum at $1$ is deeper in the effective potential, that is, the effective potential reorders the minima. Left: $U(x, \theta) = -(w_1 + x)f_{\mu_1, \sigma_1}(\theta) - (w_2 + x)f_{\mu_2, \sigma_2}(\theta) + c\theta^2$. The train and test losses both improve with increasing temperature up to a threshold, as weight is transferred from $1$ to $-1$. This is a perhaps-surprising case where the loss can improve by moving weight from a wider to a narrower minimum – if that narrow minimum is much deeper. Right: $U(x, \theta) = -w_1 f_{\mu_1+x, \sigma_1}(\theta) - w_2 f_{\mu_2+x, \sigma_2}(\theta) + c\theta^2$. The train and test losses both degrade with increasing temperature in this case.

It is unclear to us whether either model of $U(x, \theta)$ is representative of actual losses; our only conclusion from these experiments is that further study of the impact of $\tilde{D}$ on the effective potential is needed, ideally with actual loss functions $U(x, \theta)$ arising from real networks and data (or more realistic models thereof than those explored here).

**Figure 2**

- rand_seed: -1
- batch_size: 3000
- lr: 0.1
- lr_decay: 0.1
- epochs: 2000
- weight_decay: 0.0005
- momentum: 0
- shuffle_seed: None (sample size); range(0, 25) (reshuffle)
- sample_size: [50000, 40000, 30000, 20000, 10000] (sample size); 50000 (reshuffle)

**Figure 3 Top 2-basin experiment:**

- seed = 0
- minima = [-1 1]
- weights = [0.019 0.1 ]
- sigmas = [0.1 0.5]
- c = 0.001
- stddev_shift = 0.1
- lscale = 1.0
- wscale = 0.0
• Figure 3 Bottom, 2-basin experiment:

seed = 0
minima = [-1 1]
weights = [0.021 0.1 ]
sigmas = [0.1 0.5]
c = 0.001
stddev_shift = 0.1
lscale = 1.0
wscale = 0.0

• Figure H.2 Left, 1-basin experiment:

seed = 0
minima = [0]
weights = [0.1]
sigmas = [0.1]
c = 0.001
stddev_shift = 0.03
lscale = 1.0
wscale = 0.0

• Figure H.2 Right, 3-basin experiment:

seed = 0
minima = [-1 0 1]
weights = [0.1 0.051 0.3 ]
sigmas = [0.1 0.05 0.3 ]
c = 0.001
stddev_shift = 0.1
lscale = 1.0
wscale = 0.0

• Figure H.3 Left, 2-basin experiment:

seed = 0
minima = [-1 1]
weights = [0.0195 0.1 ]
sigmas = [0.1 0.5]
c = 0.001
stddev_shift = 0.1
lscale = 1.0
wscale = 0.01

• Figure H.3 Right, 2-basin experiment:

seed = 13
minima = [-1 1]
weights = [0.0201 0.1 ]
sigmas = [0.1 0.5]
c = 0.001
stddev_shift = 0.1
lscale = 1.0
wscale = 0.01

• Figure H.4 Left, 2-basin sampling experiment:

seed_test = 1
seed_train = 2
num_samples = 10
minima = [-1 1]
weights = [0.065 0.1 ]
sigmas = [0.1 0.5]
c = 0.001
stddev_x = 1e-2
lscale = 0.0
wscale = 1.0

• Figure H.4 Right, 2-basin sampling experiment:

  seed_test = 1
  seed_train = 2
  num_samples = 10
  minima = [-1 1]
  weights = [0.05 0.1]
  sigmas = [0.1 0.5]
  c = 0.001
  stddev_x = 5e-2
  lscale = 1.0
  wscale = 0.0