A Space-Time Approach to Analyzing Stochastic Gradient Descent

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Abstract

We present a diagrammatic calculus for reasoning about the behavior, at small learning rates, of SGD and its variants. We interpret the diagrams as histories of scattering events, thus offering a new physical analogy for descent. Illustrating this technique, we construct a regularizing term that causes large-batch GD to emulate small-batch SGD, present a model-selection heuristic that depends only on statistics measured before optimization, and exhibit a counter-intuitive loss landscape wherein SGD eternally cycles counterclockwise around a circle of minima.

1. Introduction

Stochastic gradient descent (SGD) decreases an unknown objective l by performing discrete-time steepest descent on noisy estimates of l. A key question is how the noise affects the final objective value. We connect SGD dynamics to physical scattering theory, thus providing a quantitative and qualitative toolkit for answering this question.

Specifically, we derive a diagram-based formalism for reasoning about SGD via a path integral over possible interactions between weights and data. The formalism permits perturbative analysis, leading to predictions of learning curves for small η. Unlike the continuous-time limits of previous work, this framework models discrete time, and with it, the potential **non-Gaussianity** of noise. We thus obtain new results quantifying the **effect of epoch number, batch size, and momentum** on SGD test loss. We also contrast SGD against popular continuous-time approximations such as ordinary or stochastic differential equations (ODE, SDE).

Path integrals offer not only quantitative predictions but also an exciting new viewpoint — that of iterative optimization as a **scattering process**. Much as individual Feynman diagrams (see Dyson (1949a)) depict how local particle interactions compose into global outcomes, our diagrams depict

how individual SGD updates influence each other before affecting a final test loss. In fact, we import from physics tools such as **crossing symmetries** (see Dyson (1949b)) and **re-normalization** (see Gell-Mann & Goldberger (1954)) to simplify our calculations and refine our estimates. The diagrams' combinatorial properties immediately yield several precise qualitative conclusions as well, for instance that to order η^2, **inter-epoch** shuffling does not affect expected test loss.

1.1. Related Work

It was Kiefer & Wolfowitz (1952) who, in uniting gradient descent (Cauchy, 1847) with stochastic approximation (Robbins & Monro, 1951), invented SGD. Since the development of back-propagation for efficient differentiation (Werbos, 1974), SGD and its variants have been used to train connectionist models including neural networks (Bottou, 1991), in recent years to remarkable success (LeCun et al., 2015).

Several lines of work predict the overfitting of SGD-trained networks (Neyshabur et al., 2017a). For instance, Bartlett et al. (2017) controls the Rademacher complexity of deep hypothesis classes, leading to generalization bounds that are post hoc or optimizer-agnostic. However, since deep networks trained via SGD generalize despite their seeming ability to shatter large sets (Zhang et al., 2017), one infers that generalization arises from the aptness to data of not only architecture but also optimization (Neyshabur et al., 2017b). Others have focused on the implicit regularization of SGD itself, for instance by modeling descent via stochastic differential equations (e.g. Chaudhari & Soatto (2018)). However, as explained by Yaida (2019), such continuous-time analyses cannot treat covariance correctly, and so they err when interpreting results about SDEs as results about SGD.

Following Roberts (2018), we avoid making a continuous-time approximation by instead Taylor-expanding around the learning rate $\eta = 0$. In fact, we develop a diagrammatic language for evaluating each Taylor term that is similar to and inspired by the field theory methods popularized by Dyson (1949a). Using this technique, we quantify the overfitting effects of batch size and epoch number, and based on this analysis, propose a regularizing term that

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causes large-batch GD to emulate small-batch SGD, thus establishing a precise version of the Covariance-BatchSize-Generalization relationship conjectured in Jastrzębski et al. (2018).

While we make rigorous, architecture-agnostic predictions of learning curves, these predictions become vacuous for large η. Other discrete-time dynamical analyses allow large η by treating neural generalization phenomenologically, whether by fitting to an empirically-determined correlate of Rademacher bounds (Liao et al., 2018), by exhibiting generalization of local minima **flat** with respect to the standard metric (see Hoffer et al. (2017), Keskar et al. (2017), citetwa18), or by exhibiting generalization of local minima **sharp** with respect to the standard metric (see Stein (1956), Dinh et al. (2017), Wu et al. (2018)). Our work, which makes explicit the dependence of generalization on the underlying metric and on the form of noise present, provides a framework to reconcile those latter, seemingly clashing claims.

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2. Background and Notation

2.1. Gradient-Based Optimization and Generalization

We adopt the standard summation notation for Greek but not Roman indices, suppressing indices when convenient and clear. To expedite dimensional analysis, we follow (Bonnabel, 2013) in considering the learning rate as an inverse metric $\eta^{\mu\nu}$ that converts a gradient (row vector) into a displacement (column vector).

Then SGD with learning rate $\eta^{\mu\nu}$ decreases an objective l by updating on a sequence of smooth, unbiased i.i.d. estimates $(l_n : 0 \leq n < N)$ of l:

$$\theta_{t+1} := \theta_t - \eta^{\mu\nu}\nabla_\mu l_t(\theta_t) \qquad (0 \leq t < T = N) \quad (1)$$

This 1-epoch, size-1 batch formulation we call **vanilla SGD**. When we later generalize to GD or multi-epoch SGD, the l_n but not the l_t will be independent.

We assume throughout that every polynomial of derivatives of the l_n, considered as random function on weight space, is smooth.

2.2. Motivating Example

Intuitively, each descent step displaces θ by $-\eta\nabla l$ and hence decreases the loss $l(\theta)$ by $\eta(\nabla l)^2$; thus, we expect after T steps a net decrease of $T\eta(\nabla l)^2$:

$$l(\theta_T) \approx l(\theta_0) - T \cdot \eta \cdot (\nabla l(\theta_0))^2 \quad (2)$$

This intuition fails to capture two crucial facts: **curvature** — that as θ changes during training, so may $\nabla l(\theta)$ — and **noise** — that l_n and l may differ.

To account for noise, we should replace each $(\nabla l_t)(\nabla l)$ by an expectation. If we are interested in train instead of test loss, We get some expectations of the form $(\nabla l_t)(\nabla l_t)$, and hence obtain a different result than for test loss.

We may account for curvature, i.e. $\nabla l(\theta)$'s evolution, in analogy with (2)'s estimate of $l(\theta)$'s evolution: each step displaces θ by $-\eta(\nabla l)$ and hence changes $\nabla l(\theta)$ by $-\eta(\nabla^2 l)(\nabla l)$; thus, we expect that $\nabla l(\theta_t)$ differs from $l(\theta_0)$ by $-t\eta(\nabla^2 l)(\nabla l)$. Recalling that $\sum_{0 \leq t < T} t = \binom{T}{2}$, we estimate the net displacement of θ as $\Delta\theta = -T\eta\nabla l + \binom{T}{2}\eta^2(\nabla^2 l)(\nabla l)$. We thus refine (2) by substituting $\Delta\theta$ into a Taylor expansion of l at θ_0 ($l, \cdots$ unadorned are evaluated at θ_0):

$$l(\theta_T) \approx l + \left(-T\eta\nabla l + \binom{T}{2}\eta^2(\nabla^2 l)(\nabla l)\right)\nabla l \quad (3)$$

$$+ \frac{1}{2}\left(-T\eta\nabla l + \binom{T}{2}\eta^2(\nabla^2 l)(\nabla l)\right)^2 \nabla l^2 \quad (4)$$

$$\approx l - T \cdot \eta \cdot (\nabla l)^2 \quad (5)$$

$$+ T\left(T - \frac{1}{2}\right) \cdot \eta^2 \cdot \nabla^2 l(\nabla l)^2 \quad (6)$$

So far, we have essentially recovered Theorem 2.1.14 of Nesterov (2004).

After establishing some general-purpose results, we will be able to derive these and analogous results simply, clearly, and harmoniously, using diagrams. The more complicated the direct computation, the greater the savings of using diagrams.

3. Diagram Calculus for SGD

3.1. Role of Diagrams

Suppose s is smooth on weight space; for example, s may be a test or train loss. We may track $s(\theta)$ as θ is updated by SGD as follows:

Proposition 1. *The formal Maclaurin series of $s(\theta_T)$ with*

respect to η is:

$$\sum_{\substack{0\le d<\infty}} (-\eta)^d \sum_{\substack{(d_t:0\le t<T)\\ \sum_t d_t=d}} \left(\prod_{0\le t<T} \frac{(g\nabla)^{d_t}}{d_t!}\Bigg|_{g=\nabla l_t(\theta)}\right) s(\theta_0)$$

In averaging over training sets (and hence over the sequence $(l_t : 0 \le t < T)$ considered as a random variable), we may factor the expectation of the above product according to independence relations between the l_t. We view various training procedures (e.g. GD, SGD with(out) inter-epoch shuffling) as **prescribing different independence relations** that lead to different factorizations and hence to potentially different generalization behavior at each order of η.

An instance of the above product (for $s = l_a$ drawn from a test set and $0 \le c \le b < T$) is

$$
\begin{aligned}
\eta^3(\nabla l_c\nabla)^2(\nabla l_b\nabla)l_a = \quad & (\nabla^\lambda l_c)(\nabla^\mu l_c)(\nabla_\lambda\nabla_\mu\nabla^\nu l_b)(\nabla_\nu l_a) \\
+ \quad & (\nabla^\lambda l_c)(\nabla^\mu l_c)(\nabla_\lambda\nabla^\nu l_b)(\nabla_\mu\nabla_\nu l_a) \\
+ \quad & (\nabla^\lambda l_c)(\nabla^\mu l_c)(\nabla_\mu\nabla^\nu l_b)(\nabla_\lambda\nabla_\nu l_a) \\
+ \quad & (\nabla^\lambda l_c)(\nabla^\mu l_c)(\nabla^\nu l_b)(\nabla_\lambda\nabla_\mu\nabla_\nu l_a)
\end{aligned}
$$

where we use η to raise indices. To reduce clutter, we adapt the string notation of Penrose (1971). Then, in expectation over (l_c, l_b, l_a) drawn i.i.d.:

Above, each node corresponds to a loss function (here, red for l_c, green for l_b, blue for l_a), differentiated d times for a degree-d node (for instance, l_b is differentiated thrice in the first diagram and twice in the second). **Thin "edges"** mark contractions by η. **Fuzzy "ties"** denote independence relationships by connecting identical loss functions (here, l_c with l_c): nodes not connected by a path of fuzzy ties are independent. The colors are redundant with the fuzzy ties and used only so that we may concisely refer to a specific node in prose. Crucially, for a fixed, i.i.d. distribution over (l_c, l_b, l_a), **the topology of a diagram determines its expected value**. For instance, $\mathbb{E}$ $= \mathbb{E}$

because both are trees with two leaves tied. Thus follows the simplification on the second line above. As shown with braces, we may convert back to explicit tensor expressions, invoking independence between untied nodes to factor the expression. However, as we will see, the diagrammatic form of a tensor expression offers us physical intuition and guides us toward constructing unbiased estimators of the statistics they represent.

The recipes for writing down test (or train) losses of SGD (or GD and other variants) are straight-forward in the diagram notation because they reduce the problem of evaluating the previous dynamical expressions to the problem of counting isomorphic graphs. An appendix provides details and proofs for a variety of instances. For now, we illustrate how to compute the test loss of vanilla SGD.

3.2. Recipe for the Test Loss of Vanilla SGD

The diagrams relevant to order $(-\eta)^d$ of this Taylor expansion are trees with d thin edges, none of which connect fuzzily-tied nodes, and such that the rightmost node is not fuzzily tied. We regard a diagram as a partial order (by reading the thin edges as Hasse diagram) equipped with a partition of nodes (induced by the fuzzy ties). If a diagram's nodes partition into P sets of size $(d_p : 0 \le p < P)$, then the Taylor coefficient on that diagram's isomorphism class is

$$\frac{(-\eta)^d}{d!}\binom{T}{P}\binom{d}{d_0,\cdots,d_{P-1}}\cdot K_{D\to[d+1]} \in \Theta\left((\eta T)^d T^{P-d-1}\right) \quad (7)$$

where $K_{D\to[d+1]}$ counts the total orders that extend the partial order of D and in which each of the P parts appears as a contiguous segment. For example, at order $(-\eta)^3\binom{T}{3}$ there are two isomorphism classes respectively with 4 and 2 total orderings, respectively; at order $(-\eta)^3\binom{T}{2}$ there are three classes respectively with 2, 2, and 3 orderings; at order $(-\eta)^3\binom{T}{1}$ there is only one class and it has 1 ordering (see Table 1). Intuitively, we regard ηT as measuring the
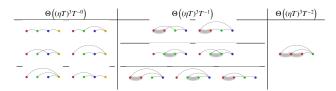

Table 1. Degree-3 scattering diagrams for test loss of vanilla SGD. **Left:** $(d, P) = (3, 3)$. Diagrams for ODE behavior. **Center:** $(d, P) = (3, 2)$. 1st order deviation of SGD away from ODE. **Right:** $(d, P) = (3, 1)$. 2nd order deviation of SGD from ODE with appearance of non-Gaussian statistics.

total **physical time** of the optimization process, and $1/T$ as measuring the **coarseness** of time discretization. More precisely, we have a double-series in $(\eta T)^d T^{P-d-1}$, where d counts thin edges and $d + 1 - P$ counts fuzzy ties; the $P = d + 1$ terms give us an ODE (hence noiseless) approximation to SGD, while $P \le d$ terms give us the effect of time-discretization and hence noise on SGD test loss. For Gaussian gradients, $= 3$ $- 2$

in expectation, but above, we make no such assumption. Indeed:

Theorem 1. *Up to an error term whose Taylor series in η*

vanishes, the test loss of vanilla SGD is given by a sum of diagrams with coefficients given in equation (7).

3.3. Renormalization

An important idea is that of renormalization, i.e. the summarization of myriad small-scale interactions into an effective large-scale theory. We can use this two ways: (**A**) to refine our computations if we know the hessian; (**B**) to refine our computations if we know the "effective propagator". Lorem ipsum dolor sit amet, consectetur adipiscing elit...

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3.4. Descent as Scattering

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space time with some diagrams	one diagram, many embeddings
interepoch shuffling	multiepoch vs gd

Figure 1. Lorem ipsum dolor sit amet, consectetur adipiscing elit...

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4. Consequences and Applications

4.1. Vanilla SGD

For single-epoch SGD with singleton batches, we sum all relevant diagrams through order 3; the coefficients $4, 2; 2, 2, 3; 1$ come from counting the elements of Table 1, and the other coefficients come from analogous tables.

This yields:

$$\mathcal{L}_{\text{test}}^{\text{SGD}}(T,\eta) \in$$

$$\bullet \;-\; \frac{\eta}{1!}\binom{T}{1}\left(\,\rule{0pt}{1em}\!\!\!\!\right)$$

$$+\; \frac{\eta^2}{1!1!}\binom{T}{2}\left(2\,\rule{0pt}{1em}\right) + \frac{\eta^2}{2!}\binom{T}{1}\left(\,\rule{0pt}{1em}\right)$$

$$-\; \frac{\eta^3}{1!1!1!}\binom{T}{3}\left(4\,\rule{0pt}{1em} + 2\,\rule{0pt}{1em}\right)$$

$$-\; \frac{\eta^3}{2!1!}\binom{T}{2}\left(2\,\rule{0pt}{1em} + 2\,\rule{0pt}{1em} + 3\,\rule{0pt}{1em}\right)$$

$$-\; \frac{\eta^3}{3!}\binom{T}{1}\left(\,\rule{0pt}{1em}\right) + o(\eta^3)[1]$$

By contrast, the generalization gap $\mathcal{L}_{\text{gen}}^{\text{SGD}} = \mathcal{L}_{\text{test}}^{\text{SGD}} - \mathcal{L}_{\text{train}}^{\text{SGD}}$ is suppressed by a factor $1/N$ ($N \le T$):

$$N \cdot \mathcal{L}_{\text{gen}}^{\text{SGD}}(T,\eta) \in$$

$$+\eta\binom{T}{1}\left(\,\rule{0pt}{1em} - \rule{0pt}{1em}\right) - \eta^2\binom{T}{2}\left(\,\rule{0pt}{1em} + \rule{0pt}{1em} - 2\,\rule{0pt}{1em}\right)$$

$$-\; \frac{\eta^2}{2!}\binom{T}{1}\left(\,\rule{0pt}{1em} - \rule{0pt}{1em}\right) + o(\eta^2)$$

The leading order term is $N \cdot \mathcal{L}_{\text{gen}}^{\text{SGD}}(T,\eta) \approx \eta T\left(\,\rule{0pt}{1em} - \rule{0pt}{1em}\right) = T \cdot \eta^{\lambda\mu} C_{\lambda\mu}$, where C is the covariance of gradients. We thus recover a main result of Roberts (2018). Lorem ipsum dolor sit amet, consectetur adipiscing elit...

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[1] We use little-$o(\eta^d)$ instead of big-$O(\eta^{d+1})$ to avoid specializing to analytic functions. Error terms depend on the loss landscape and on T. When gradients are uniformly bounded, the T dependence is at most linear.

small T: eta curve	test loss decrease near minimum
small T gen gap: actual vs predicted	nongaussian example

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4.2. Emulating Small Batches with Large Ones

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batch matching over one init

batch matching over multiple inits

scan over betas

summary over many models

Figure 3. Lorem ipsum dolor sit amet, consectetur adipiscing elit...

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4.3. Analyzing Second Order Methods

We demonstrate how our approach extends to more sophisticated optimizers by analyzing momentum and a hessian-based method.

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Now consider a hessian-based update parameterized by a scalar λ:

$$\theta \leftsquigarrow \theta - (\eta^{-1} + \lambda\nabla\nabla l_t(\theta))^{-1}\nabla l_t(\theta)$$

invhess

momentum

invhess

Figure 4. Lorem ipsum dolor sit amet, consectetur adipiscing elit...

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4.4. Epochs and Overfitting

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multiepoch vs sgd limit

multiepoch vs gd limit

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4.5. Myopic Model Selection

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rankings: actual vs predicted

architecture vs optimization ease

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4.6. Comparison to Continuous Time

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distinguishing landscape

ode vs sde vs sgd performance on landscape

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4.7. Thermodynamic Engine

We clarify Lorem ipsum dolor sit amet, consectetur adipiscing elit...

...sunt in culpa qui officia deserunt mollit anim id est laborum. We constructed a counter-intuitive loss landscape

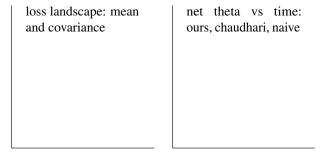| loss landscape: mean and covariance	net theta vs time: ours, chaudhari, naive

Figure 8. Lorem ipsum dolor sit amet, consectetur adipiscing elit...

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wherein, for arbitrarily small learning rates, SGD cycles counterclockwise around a circle of minima. Our mechanism differs from that discovered by Chaudhari & Soatto (2018) discuss the thermodynamic significance of both

5. Conclusion

We presented a novel diagrammatic tool for analyzing gradient-based descent. By presenting a new regularizing term, we showed that **large-batch GD can be made to emulate small-batch SGD**, thus completing a project suggested by Roberts (2018). This is significant because, while small batch sizes can lead to better generalization (Bottou, 1991), modern infrastructure increasingly rewards large batch sizes (Goyal et al., 2018). We showed also that in multi-epoch SGD, inter-epoch shuffling induces only a 3rd order effect on test loss. Intuitively, we proved that **the hessian matters asymptotically more than shuffling order**.

The diagram method is also a rich source of intuitions and physical analogies. For example, it offers a clearer understanding of the empirically verified limit cycles found in Chaudhari. As our physical analogy emphasizes the un-derlying metric, it reconciles competing views of whether sharp or flat minima generalize. Further exploration of this bridge to particle physics, especially within the framework of renormalization theory, pose a promising direction for future research.

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A. Derivation of Diagram Rules

5.2. Dyson Series for Iterative Optimizers

If a density ρ governs a point θ in weight space, then after a sequence of updates $\theta \mapsto \theta - \eta^{\mu\nu}\nabla_\mu l(\theta)$ on losses ($l_t : 0 \leq t < T$), the following density (up to an error term whose Taylor series vanishes; all perturbative results will implicitly carry such terms) will govern the new point:

$$\exp\left(+\eta^{\mu\nu}\nabla_\mu l_{T-1}(\theta)\nabla_\nu\right)\cdots\exp\left(+\eta^{\mu\nu}\nabla_\mu l_0(\theta)\nabla_\nu\right)\rho \quad (8)$$

or $\prod \exp\left(+\eta\nabla l\nabla\right)\rho$ for short. The exponent above is a linear operator that acts on a space of sufficiently smooth maps; in particular, the ∇_ν does not act on the $\nabla_\mu l(\theta)$ with which it pairs. Integrating by parts, we write the expectation over initial values after T steps of a function s of weight space (e.g. s may be test or train loss) as:

$$\int_\theta \rho(\theta)\left(\prod_{0\leq t\leq T}\exp\left(-\eta^{\mu\nu}\nabla_\mu l(\theta)\nabla_\nu\right)s\right)(\theta) \quad (9)$$

Since the exponentials above might not commute, we may not compose the product of exponentials into an exponential of a sum. We instead compute an expansion in powers of η. Setting the initialization $\rho(\theta) = \delta(\theta - \theta_0)$ to be deterministic, and labeling as θ_t the weight after t steps, we find:

$$s(\theta_T) = \sum_{0\leq d<\infty} (-\eta)^d \sum_{\substack{(d_t:0\leq t<T)\\ \sum_t d_t=d}}\left(\prod_{0\leq t<T}\frac{(\nabla l_t(\theta)\nabla)^{d_t}}{d_t!}\right)s(\theta_0) \quad (10)$$

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B. Tutorial on Diagram Rules

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C. Derivations of Perturbative Results

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D. Diagram Rules vs Direct Perturbation

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F. Autonomous ODE Fitting

We fit a . These have the benefit In particular:

$$y\prime(t) = a \rightarrow \qquad\qquad y(t) = y(0) + at \tag{11}$$

$$y\prime(t) = by + a \rightarrow \quad y(t) = (y(0) - (a/b)) \exp(bt) + (a/b) \tag{12}$$

$$y\prime(t) = cy^2 + by + a \rightarrow \tag{13}$$

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E. The η-Series' Domain of Convergence

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