A geometric interpretation of stochastic gradient descent using diffusion metrics

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Abstract. Stochastic gradient descent (SGD) is a key ingredient in the training of deep neural networks and yet its geometrical significance appears elusive. We study a deterministic model in which the trajectories of our dynamical systems are described via geodesics of a family of metrics arising from the diffusion matrix. These metrics encode information about the highly non-isotropic gradient noise in SGD. We establish a parallel with General Relativity models, where the role of the electromagnetic field is played by the gradient of the loss function. We compute an example of a two layer network.

Keywords: Deep Networks · Stochastic Gradient Descent · General Relativity.

1 Introduction

In this paper, we interpret the diffusion matrix for SGD (see [4]), as a metric for the parameters’ space; thus we provide a deterministic equation (10) that we compare, near the equilibrium points, to the stochastic gradient descent (1). We start with the definition of the diffusion matrix $D(x)$ and then we write it in the form (3), that shows clearly how $D(x)$ captures in an essential way the anisotropy of the dynamical system ruling the SGD. In other words, in which way $D(x)$ is one of key factors in the difference between the steady state solutions of SGD from those of ordinary GD (see comparison in [4]). Using the diffusion matrix, we then define a family of metrics on the parameters’ space, that we call diffusion metrics. We then take euristically Einstein equation describing the geodesic on a Riemannian manifold, for the motion of a particle subject to gravity and electromagnetic field and we replace the electromagnetic field contribution by the forcing term represented by the ordinary gradient, the gravity taken into account by the diffusion metric itself. After some mild hypotheses on the network, we obtain that the geodesics with respect to this equation, correspond precisely to the evolution of a dynamical system, which not subject to euclidean
gradient descent, but to relativistic gradient descent (RGD) with respect to the family of diffusion metrics.

In the end we obtain the equation \[10\] which is along the same vein as in \[3\], that is, natural gradient descent, but whose significance is much deeper in the context of SGD, since it stems from the anisotropy of the loss with respect to the various parameters, which encodes the difference in the dynamics between GD and SGD. We also compare our result with the ones in \[4\] and show they are perfectly compatible.

2 Continuous-time SGD and Diffusion matrix

Stochastic gradient descent performs an update of the weights \(x\) of a neural network, replacing the ordinary gradient of the loss function \(f = \sum_{i=1}^{N} f_i\) with \(\nabla_B f\):

\[
dx = -\nabla_B f dt, \quad \nabla_B f = \frac{1}{|B|} \sum_{i \in B} \nabla f_i
\]

(1)

where \(dx\) represents the continuous version of the weight update at step \(j\): \(x_{j+1} = x_j - \eta \nabla_B f(x_j)\), with the learning rate \(\eta\) incorporated into the expression of \(\nabla_B f\) and \(B\) is the mini-batch. In the expression of the loss function \(f = \sum_{i=1}^{N} f_i\), \(f_i\) is the loss relative to the \(i\)-th element in our dataset \(\Sigma\) of size \(|\Sigma| = N\).

We assume that weights belong to a compact subset \(\Omega \subset \mathbb{R}^d\) and that the \(f_i\)'s satisfy suitable regularity conditions (see \[4\] Sec. 2 for more details).

We define the diffusion matrix as the product of the size of the mini-batch \(|B|\) and the variance of \(\nabla_B f\), viewed as a random variable, \(\phi : \Sigma \rightarrow \mathbb{R}^d\), \(\phi(z_i) = \nabla f_i\):

\[
D(x) = \mathbb{E}[(\phi - \mathbb{E}[\phi])(\phi - \mathbb{E}[\phi])^t]
\]

(2)

Notice that \(D(x)\) is \(d \times d\) matrix independent from the mini-batch size; it only depends on the weights \(x\) and loss function \(f\) and the dataset \(\Sigma\). With a direct calculation one shows that:

\[
D = \frac{1}{N} \sum_k (\nabla f_k)(\nabla f_k)^t - (\nabla f)(\nabla f)^t = \frac{1}{N^2}((\partial r \hat{f}, \partial s \hat{f}))
\]

(3)

where:

\[
\hat{f} = (f_1 - f_2, f_1 - f_3, \ldots, f_{N-1} - f_N) \in \mathbb{R}^{N(N-1)/2}
\]
and \((\cdot, \cdot)\) is the euclidean scalar product. In fact:

\[
D_{rs} = \frac{1}{N} \sum_{k=1}^{N} \partial_r f_k \partial_s f_k - \frac{1}{N^2} \sum_{i,j=1}^{N} \partial_r f_i \partial_s f_j
\]

\[
= \frac{1}{N^2} \left[ N(\partial_r f_1 \partial_s f_1 + \cdots + \partial_r f_N \partial_s f_N) + 
- (\partial_r f_1 \partial_s f_1 + \partial_r f_1 \partial_s f_2 + \cdots + \partial_r f_N \partial_s f_N) \right] = 
= \frac{1}{N^2} [(N-1)\partial_r f_1 \partial_s f_1 - \partial_r f_1 \partial_s f_2 - \cdots - \partial_r f_1 \partial_s f_N + 
- \partial_r f_2 \partial_s f_1 + (N-1)\partial_r f_2 \partial_s f_2 - \cdots - \partial_r f_2 \partial_s f_N + \cdots 
- \partial_r f_N \partial_s f_1 - \partial_r f_N \partial_s f_2 + \cdots + (N-1)\partial_r f_N \partial_s f_N]
\]

which gives (almost immediately):

\[
D_{rs} = \frac{1}{N^2} \left[ (\partial_r f_1 - \partial_r f_2)(\partial_s f_1 - \partial_s f_2) + (\partial_r f_1 - \partial_r f_3)(\partial_s f_1 - \partial_s f_3) + \cdots 
+ (\partial_r f_1 - \partial_r f_N)(\partial_s f_1 - \partial_s f_N) + (\partial_r f_2 - \partial_r f_3)(\partial_s f_2 - \partial_s f_3) + \cdots 
+ (\partial_r f_{N-1} - \partial_r f_N)(\partial_s f_{N-1} - \partial_s f_N) \right] = \frac{1}{N^2} \langle (\partial_r \hat{f}, \partial_s \hat{f}) \rangle
\]

The diffusion matrix measures effectively the anisotropy of our data: \(D = 0\) if and only if \(\partial_r (f_i) = \partial_r (f_j)\) for all \(r = 1, \ldots, d\) and \(i, j = 1, \ldots, N\). In other words the diffusion matrix measures how the loss of each datum depends, at first order, on the weights in different way with respect to the loss of each of the other data. So, it tells us how much we should expect the SGD dynamics to differ from the GD one.

Notice that the expression (3) gives us immediately a bound on the rank of \(D\), namely \(\text{rk}(D) \leq N - 1\).

### Table 1.

| Architecture       | \(d = |\text{Weights}|\) | \(N = |\text{Data}|, \text{CIFAR}\) | \(N = |\text{Data}|, \text{SVHN}\) |
|--------------------|-----------------|--------------------------|--------------------------|
| ResNet             | 1.7M            | 60K                      | 600K                     |
| Wide ResNet        | 11M             | 60K                      | 600K                     |
| DenseNet (k=12)    | 1M              | 60K                      | 600K                     |
| DenseNet (k=24)    | 27.2M           | 60K                      | 600K                     |

This table suggests that in many algorithms currently available, the diffusion matrix has low rank, hence it is singular; this just by comparing the size \(d\) of \(D\) and its rank which bound by \(N\). This fact turns out to be very important in the construction of the diffusion metrics, that we will see below.
3 Diffusion metrics and General Relativity

The evolution of a dynamical system in general relativity takes place along the geodesics according to the metric imposed on the Minkowski space by the presence of gravitational masses. The equation for such geodesics, once Einstein equation is solved, is:

$$\frac{d^2 x^\mu}{dt^2} + \Gamma^\mu_{\rho\sigma} \frac{dx^\rho}{dt} \frac{dx^\sigma}{dt} = \frac{q}{m} F^\mu_{\nu} \frac{dx^\nu}{dt}$$  \hspace{1cm} (4)

where $\Gamma^\mu_{\rho\sigma}$ are the Christoffel symbols for the Levi-Civita connection:

$$\Gamma^w_{uv} = \frac{1}{2} g^{wj} (\partial_u g_{vz} - \partial_z g_{uv} + \partial_v g_{uz})$$  \hspace{1cm} (5)

and $\frac{q}{m} F^\mu_{\nu} \frac{dx^\nu}{dt}$ is a term regarding an external force, e.g. one coming from an electromagnetic field.

If we take time derivative of the differential equation ruling the ordinary (i.e. non stochastic) gradient descent:

$$\frac{d^2 x^\mu}{dt^2} = -\frac{d}{dt} \partial_\mu f$$

and we compare with (4), it is clear that $-\frac{d}{dt} \partial_\mu f$ effectively replaces the force term $(q/m) F^\mu_{\nu} \frac{dx^\nu}{dt}$. Hence, the geodesic equation (4) models the ordinary GD equation, if we take a constant metric and we replace the force term with the gradient of the loss; furthermore this corresponds to the condition $D = 0$ in SGD dynamics equation (1).

This suggests heuristically to define a metric, depending on the diffusion matrix, which becomes constant when $D = 0$. As a side remark, notice that since $D$ is singular in many important practical applications (see Table 1), it is not reasonable to use it to define the metric itself. On the other hand, since $D$ measures the anisotropy of the weight space, it is reasonable to employ it to perturb the euclidean metric. So the stochastic nature of the dynamical system ruled by the SGD is replaced by a perturbation of the dynamics for the ordinary gradient descent. As an analogy, the presence of (small) masses in space, in the weak field approximation (see [2]) of general relativity, generate gravity, hence a (small) deformation of the euclidean metric.

At each point $x \in \Omega$, we define a metric called diffusion metric as

$$g(x) = \text{id} + \mathcal{E}(x) D(x)$$  \hspace{1cm} (6)

with $\mathcal{E}(x) < 1/M_x$, where $M_x = \max \{ \lambda \}$ with $\lambda$ eigenvalues of $D(x)$. This ensures that $g$ is non singular at each point. So we are defining a family of metrics depending on the real parameter $\mathcal{E}$.

We expect this model to approximate the Fokker Planck solution when $\beta^{-1}$ is very small (see [4] for the notation and more details).
Notice that our heuristic hypothesis on $E$ allows us to make the so called *weak field approximation* (see [2]):

$$g^{-1} = \text{id} - ED(x)$$

Hence, we have the following expression for the Christoffel’s symbols (in this approximation we discard $O(E^2)$):

$$\Gamma^w_{uv} = \frac{1}{2} \sum_z (\delta_{wz} - E d_{wz}) \mathcal{E} (\partial_u d_{vz} - \partial_z d_{uv} + \partial_v d_{uw}) = \frac{\mathcal{E}}{2} (\partial_u d_{vw} - \partial_w d_{uv} + \partial_v d_{uw})$$

(7)

where $d_{ij}$ are the coefficients of $D$, and $\delta_{wz}$ is the Kronecker delta.

Let us now compute the Christoffel’s symbols and then substitute them into the geodesic equation (4).

$$\Gamma^k_{ij} = \frac{\mathcal{E} N^2}{2} \left[ \langle \partial_i \partial_j \hat{f}, \partial_k \hat{f} \rangle \frac{dx^i}{dt} \frac{dx^j}{dt} + \langle \partial_j \partial_k \hat{f}, \partial_i \hat{f} \rangle \frac{dx^j}{dt} \frac{dx^k}{dt} + \langle \partial_k \partial_i \hat{f}, \partial_j \hat{f} \rangle \frac{dx^k}{dt} \frac{dx^i}{dt} \right] = \frac{\mathcal{E} N^2}{2} \langle \partial_i \partial_j \hat{f}, \partial_k \hat{f} \rangle.$$

Let us substitute in (4) (writing the sum now):

$$d^2 x^k \frac{dt^2}{dt^2} + \frac{\mathcal{E} N^2}{2} \sum_{i,j} \langle \partial_i \partial_j \hat{f}, \partial_k \hat{f} \rangle \frac{dx^i}{dt} \frac{dx^j}{dt} = \frac{d}{dt} \partial_k \hat{f}$$

(8)

Let us concentrate on the expression:

$$\frac{\mathcal{E} N^2}{4} \sum_{i,j} \langle \partial_i \partial_j \hat{f}, \partial_k \hat{f} \rangle \frac{dx^i}{dt} \frac{dx^j}{dt} = \frac{\mathcal{E} N^2}{4} \sum_{i,j} \langle \partial_i \partial_j \hat{f}, \partial_k \hat{f} \rangle \frac{dx^i}{dt} \frac{dx^j}{dt} = \frac{\mathcal{E} N^2}{4} \sum_{i,j} \langle \partial_i \partial_j \hat{f}, \partial_k \hat{f} \rangle \frac{dx^i}{dt} \frac{dx^j}{dt} =$$

$$= \frac{\mathcal{E} N^2}{4} \sum_{i,j} \langle \partial_i \partial_j \hat{f}, \partial_k \hat{f} \rangle \frac{dx^i}{dt} \frac{dx^j}{dt} = \frac{\mathcal{E} N^2}{4} \sum_{i,j} \langle \partial_i \partial_j \hat{f}, \partial_k \hat{f} \rangle \frac{dx^i}{dt} \frac{dx^j}{dt} =$$

Now we take the integral in $dt$ (we compute by parts twice):

$$\frac{\mathcal{E} N^2}{4} \int \sum_{i,j} \langle \partial_i \partial_j \hat{f}, \partial_k \hat{f} \rangle \frac{dx^i}{dt} \frac{dx^j}{dt} dt = \frac{\mathcal{E} N^2}{4} \sum_{i,j} \left[ \frac{dx^i}{dt} \partial_i \hat{f} \alpha - \int \frac{dx^i}{dt} \partial_i \hat{f} \alpha \right] dt =$$

$$= \frac{\mathcal{E} N^2}{4} \sum_{i,j} \left[ \frac{dx^i}{dt} \partial_i \hat{f} \alpha - \int \frac{dx^i}{dt} \partial_i \hat{f} \alpha \right] dt =$$

Notice that, in many practical applications we have:

$$\frac{d^2}{dt^2} \partial_k \hat{f} \alpha = 0$$

(9)

because $\partial_i \partial_j \partial_k \hat{f} = 0$.

Hence

$$\frac{\mathcal{E} N^2}{4} \int \sum_{i,j} \langle \partial_i \partial_j \hat{f}, \partial_k \hat{f} \rangle \frac{dx^i}{dt} \frac{dx^j}{dt} dt = \frac{\mathcal{E} N^2}{4} \sum_{i,j} \left[ \partial_i \hat{f} \alpha \frac{dx^i}{dt} \partial_k \hat{f} \alpha - \int \frac{dx^i}{dt} \partial_i \hat{f} \alpha \right] dt =$$

$$= \mathcal{E} \sum_{i,j} \langle \hat{f} \alpha \frac{dx^i}{dt} \partial_k \hat{f} \alpha - \int \frac{dx^i}{dt} \partial_i \hat{f} \alpha \rangle \partial_k \hat{f} \alpha$$
We now substitute the obtained expression into the eq. (8), taking the integral in \( dt \):

\[
\frac{dx^k}{dt} + \mathcal{E} \sum_\ell d_{k,\ell} \frac{dx^\ell}{dt} - \frac{\mathcal{E}}{N^2} \sum_\alpha \hat{f}_\alpha \frac{d\hat{f}_\alpha}{dt} = -\partial_k f
\]

We may assume \( \mathcal{E} \) very small, as motivated by Table 1, hence discard this term. Writing the equation into vector form, we have:

\[
\frac{dx}{dt} + \mathcal{E} D \frac{dx}{dt} = -\nabla f
\]

Since by the weak field approximation \((I + \mathcal{E} D)^{-1} \cong (I - \mathcal{E} D)\), we can write:

\[
\frac{dx}{dt} = -(I - \mathcal{E} D)\nabla f = -\nabla_D f
\]

where \( \nabla_D f \) is the gradient computed according to the diffusion metric \( \mathcal{E} \).

We can summarize our result as follows: the SGD equation (1) can be replaced, provided the approximations (9) holds, by the deterministic equation (10), where the dynamical system evolves with respect to the gradient computed according to the diffusion metric \( \mathcal{E} \).

We now want to compare our result (10) with [4] Sec. 1, in order to understand how the steady state solutions of (10) compare to the SGD steady state solutions described by (1).

In [4] the authors regard SGD as minimizing the function \( \Phi \) instead of our loss \( f \). Let us focus on eq. (8) in [4], where the relation between \( f \) and \( \Phi \) is discussed. In our case, we take \( \nabla \Phi = \nabla_D f \) so that eq. (10) becomes

\[
- \nabla f(x) + \tilde{D}(x)\nabla \Phi(x) = 0
\]

where \( \tilde{D}(x) = (I + \mathcal{E} D(x)) \) is the diffusion metric.

If the term \( D(x) \) in (8) in [4] is spelled out as our \( \tilde{D}(x) \), we can write such equation as:

\[
j(x) = -\nabla f(x) + \tilde{D}(x)\nabla \Phi(x) - \beta^{-1} \nabla \cdot \tilde{D}(x)
\]

Notice that according to our approximation \( \mathcal{E} \), \( \nabla \cdot \tilde{D}(x) = 0 \). Hence, eq. (12) (that is (8) in [4]) is perfectly compatible with our treatment and furthermore the assumption 4 in [4] is fully justified by the fact \( j(x) = 0 \).

4 Conclusions

The General Relativity model helps to provide with a deterministic approach to the evolution of the dynamical system described by SGD. The results are compatible with [4].
A Riemannian Geometry

We collect few well known facts of Riemannian geometry, inviting the reader to consult [9] for more details.

In Riemannian geometry, we define a metric $g$ on a smooth manifold $M$, as a smooth assignment $p \mapsto g_p$, which gives, for each $p \in M$, a (non degenerate) scalar product on $T_p(M)$, the tangent space of $M$ at $p$. Usually, this scalar product is assumed to be positive definite, however, for general relativity, it is necessary to drop this assumption, so that we speak of a pseudometric, because our main example is the Minkowski metric. To ease the terminology, we say “metric”, to include also this more general setting.

Once a metric is given, we say that $M$ is a Riemannian manifold. In local coordinates, $x^1, \ldots, x^n$, we express the metric using 1-forms:

$$g = \sum_{i,j} g_{ij} \, dx^i \otimes dx^j.$$

where

$$g_{ij}|_p := g_p \left( \frac{\partial}{\partial x^i}|_p, \frac{\partial}{\partial x^j}|_p \right)$$

and

$$\left\{ \frac{\partial}{\partial x^1|_p}, \ldots, \frac{\partial}{\partial x^n|_p} \right\}$$

is a basis of the tangent space $T_p M$.

For example $\mathbb{R}^n$, identified with its tangent space at every point, has a canonical or standard metric given by:

$$g^\text{can}_p : T_p \mathbb{R}^n \times T_p \mathbb{R}^n \rightarrow \mathbb{R}, \quad \left( \sum_i a_i \frac{\partial}{\partial x^i}, \sum_j b_j \frac{\partial}{\partial x^j} \right) \mapsto \sum_i a_i b_i.$$

Here, $g^\text{can}_ij = \delta_{ij}$.

Usually, we drop the $\sum$ symbol, following Einstein convention.

An affine connection $\nabla$ on a smooth manifold $M$ is an bilinear map $(X, Y) \mapsto \nabla_X Y$ associating to a pair of vector fields $X, Y$ on $M$ another vector field $\nabla_X Y$, satisfying:

1. $\nabla f X Y = f \nabla_X Y$ for all functions $f$ on $M$;
2. $\nabla_X (f Y) = df(X)Y + f \nabla_X Y$.

Once this definition is given, it is possible to define $\nabla$ on tensors of every order.

On a Riemannian manifold we have a unique affine connection, the Levi-Civita connection $\nabla$, which is torsion free and preserves the metric, i.e. $\nabla g = 0$. In local coordinates the components of the connection are called the Christoffel symbols:

$$\nabla_{\frac{\partial}{\partial x^i}} \frac{\partial}{\partial x^j} = \Gamma^k_{ij} \frac{\partial}{\partial x^k}.$$
By the above mentioned uniqueness, the $\Gamma^k_{ij}$’s are expressed in terms of the metric components $g_{ij}$:

$$\Gamma^l_{jk} = \frac{1}{2}g^{lr}(\partial_k g_{rj} + \partial_j g_{rk} - \partial_r g_{jk})$$

where as usual $g^{ij}$ are the coefficients of the dual metric tensor, i.e. the entries of the inverse of the matrix ($g_{kl}$). The torsion freeness is equivalent to the symmetry

$$\Gamma^l_{jk} = \Gamma^l_{kj}.$$

In $\mathbb{R}^n$ the gradient of a scalar function $f$ is the vector field characterized by the property: $\text{grad}(f) \cdot v = D_v$ (we shall denote it with $\nabla(f)$ whenever no confusion arises). In other words, its scalar product (in the euclidean metric) with a tangent vector $v$ gives the directional derivative of $f$ along $v$. When $M$ is a Riemannian manifold with metric $g$, the gradient of a function $f$ on $M$ is defined in the same way, except that the scalar product is now given by $g$. So, in local coordinates, we have:

$$\nabla_g f = \frac{\partial f}{\partial x^i} g^{ij} \frac{\partial}{\partial x^j}$$

Notice that when $g_{ij} = \delta_{ij}$, we retrieve the usual definition in $\mathbb{R}^n$.

We end our short summary of the key concepts, with the notion of geodesic.

A geodesic $\gamma$ on a smooth manifold $M$ with an affine connection $\nabla$ is a curve defined by the following equation:

$$\nabla_{\dot{\gamma}} \dot{\gamma} = 0$$

Geometrically, this expresses the fact that the parallel transport, given by $\nabla$, along the curve $\gamma$ preserves any tangent vector to the curve. In local coordinates this becomes:

$$\frac{d^2 \gamma^\lambda}{dt^2} + \Gamma^\lambda_{\mu\nu} \frac{d \gamma^\mu}{dt} \frac{d \gamma^\nu}{dt} = 0 ,$$

Notice that when the metric is constant, we have the familiar equation:

$$\frac{d^2 \gamma^\lambda}{dt^2} = 0$$

that is, the geodesics are straight lines.

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