Information geometric optimization (IGO, [OAAH11]) is a general framework for stochastic optimization problems aiming at limiting the influence of arbitrary parametrization choices. The initial problem is transformed into the optimization of a smooth function on a Riemannian manifold (following [AN07]), defining a parametrization-invariant first order differential equation. However, in practice, it is necessary to discretize time, and then, parametrization invariance holds only at first order in the step size.

We define the Geodesic IGO update (GIGO), which uses the Riemannian manifold structure to obtain an update entirely independent from the parametrization of the manifold. We test it with classical objective functions.

Thanks to Noether’s theorem from classical mechanics, we find an efficient way to write a first order differential equation satisfied by the geodesics of the statistical manifold of Gaussian distributions, and thus to compute the corresponding GIGO update. We then compare GIGO, pure rank-µ CMA-ES [Han11] and xNES [GSY+10] (two previous algorithms that can be recovered by the IGO framework), and show that while the GIGO and xNES updates coincide when the mean is fixed, they are different in general, contrary to previous intuition. We then define a new algorithm (Blockwise GIGO) that recovers the xNES update from abstract principles.
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### Introduction

Consider an objective function \( f: X \rightarrow \mathbb{R} \) to be minimized. We suppose we have absolutely no knowledge about \( f \): the only thing we can do is ask for its value at any point \( x \in X \) (black-box optimization), and that the evaluation of \( f \) is a costly operation. We are going to study algorithms that can be described in the IGO framework (see [OAAH11]).

A possible way to optimize such a function is the following:
We choose \((P_\theta)_{\theta \in \Theta}\) a family of probability distributions on \(X\), and an initial probability distribution \(P_{\theta_0}\). Now, we replace \(f\) by \(F: \Theta \rightarrow \mathbb{R}\) (for example \(F(\theta) = E_{x \sim P_\theta}[f(x)]\)), and we optimize \(F\) with a gradient descent:

\[
\frac{d\theta^t}{dt} = -\nabla_\theta E_{x \sim P_\theta}[f(x)].
\] (1)

However, because of the gradient, this equation depends entirely on the parametrization we chose for \(\Theta\), which is disturbing; we do not want to have two different updates because we chose different numbers to represent the objects we are working with. That is why invariance is a design principle behind IGO. More precisely, we want invariance with respect to monotone transformations of \(f\), and invariance under reparametrization of \(\theta\).

IGO provides a differential equation on \(\theta\) with the desired properties, but because of the discretization of time needed to obtain an explicit algorithm, we lose invariance under reparametrization of \(\theta\): two IGO algorithms for the same problem, but with different parametrizations, coincide only at first order in the step size. A possible solution to this problem is Geodesic IGO (GIGO), introduced here\(^2\), the initial direction of the update at each step of the algorithm remains the same as in IGO, but instead of moving straight for the chosen parametrization, we use the structure of Riemannian manifold of our family of probability distributions (see [AN07]) by following its geodesics.

Finding the geodesics of a Riemannian manifold is not always easy, but Noether’s theorem will allow us to obtain quantities that are preserved along the geodesics. In the case of Gaussian distributions, it is possible to find enough invariants to obtain a first order differential equation satisfied by the geodesics, which makes their computation easier.

Although the geodesic IGO algorithm is not strictly speaking parametrization invariant when no closed form for the geodesics is known, it is possible to compute them at arbitrary precision without increasing the numbers of objective function calls.

The first two sections are preliminaries: in Section 1, we recall the IGO algorithm, introduced in [OAAH11], and in Section 2, after a reminder about Riemannian geometry, we state Noether’s theorem, which will be our main tool to compute the GIGO update for Gaussian distributions.

In Section 3, we consider Gaussian distributions with covariance matrix proportional to the identity matrix: this space is isometric to the hyperbolic space, and the geodesics of the latter are known.

In Section 4.1, we consider the general Gaussian case, and we use Noether’s theorem to obtain two different sets of equations to compute the GIGO update. The equations were already known, see [Eri87], [CO91] and [ITW11], but the connection with Noether’s theorem has not been mentioned. We then give the explicit solution for these equations, from [CO91].

In Section 5, we recall quickly the xNES and CMA updates and we introduce a slight modification of the IGO algorithm to incorporate the direction-

---

1This is not the definition we want formally for \(\Theta\): the theoretical context is the context of differentiable manifolds. The importance of working in a manifold appears when changing the parametrization or when using a local parametrization. See [AN07].

2See also IGO-ML, in [OAAH11], for example.
dependent learning rates used in CMA-ES and xNES. We then compare these different algorithms, prove that xNES is not GIGO in general and we finally introduce a new family of algorithms extending GIGO and recovering xNES from abstract principles.

Finally, Section 3 presents numerical experiments, which suggest that when using GIGO with Gaussian distributions the step size must be chosen carefully.

To simplify notation, we will use \( \mathbb{R}^n \) instead of a general manifold as much as possible, but the latter is the “right” formal context.

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1 Definitions: IGO, GIGO

In this section, we recall what the IGO framework is, and we define the geodesic IGO update. Consider again Equation 1:

\[
\frac{d\theta^t}{dt} = -\nabla_{\theta} E_{x \sim P_\theta}[f(x)].
\]

Its main problems are that

- The gradient depends on the parametrization of our space of probability distributions (see 1.3 for an example).
- The equation is not invariant under monotone transformations of \( f \). For example, the optimization for \( 10f \) moves ten times faster than the optimization for \( f \).

In this section, we recall how IGO deals with this (see [OAAH11] for a better presentation).

1.1 Invariance under reparametrization of \( \theta \): Fisher metric

In order to achieve invariance under reparametrization of \( \theta \), it is possible to turn our family of probability distributions into a Riemannian manifold (it is the main topic of information geometry, see [AN07]), and therefore, there is a canonical gradient (called the natural gradient).

**Definition 1.** Let \( P, Q \) be two probability distributions on \( X \). The Kullback–Leibler divergence of \( Q \) from \( P \) is defined by:

\[
\text{KL}(Q||P) = \int_X \ln\left(\frac{Q(x)}{P(x)}\right)dQ(x).
\]

By definition, it does not depend on the parametrization. It is not symmetrical, but if for all \( x \), the application \( \theta \mapsto P_\theta(x) \) is \( C^2 \), then a second-order expansion yields:
KL\((P_{\theta + d\theta} \| P_{\theta})\) = \(\frac{1}{2} \sum_{i,j} I_{ij}(\theta) d\theta_i d\theta_j + o(d\theta^2)\), \hspace{1cm} (3)

where

\[
I_{ij}(\theta) = \int_X \frac{\partial \ln P_\theta(x)}{\partial \theta_i} \frac{\partial \ln P_\theta(x)}{\partial \theta_j} dP_\theta(x) = -\int_X \frac{\partial^2 \ln P_\theta(x)}{\partial \theta_i \partial \theta_j} dP_\theta(x). \hspace{1cm} (4)
\]

This is enough to endow the family \((P_\theta)_{\theta \in \Theta}\) with a Riemannian manifold structure.\(^3\) The matrix \(I(\theta)\) is called “Fisher information matrix”, the metric it defines is called the “Fisher metric”.

Given a metric, it is possible to define a gradient attached to this metric: the key property of the gradient is that for any smooth function \(f\)

\[
f(x + h) = f(x) + \sum_i h_i \frac{\partial f}{\partial x_i} + o(\|h\|) = f(x) + \langle h, \nabla f(x) \rangle + o(\|h\|), \hspace{1cm} (5)
\]

where \(\langle x, y \rangle = x^T I y\) is the dot product in metric \(I\). Therefore, in order to keep the property of Equation (5), we must have \(\nabla f = I^{-1} \frac{\partial f}{\partial \theta}\).

We have therefore the following gradient (called “natural gradient”, see [AN07]):

\[
\tilde{\nabla}_\theta = I^{-1}(\theta) \frac{\partial f}{\partial \theta}, \hspace{1cm} (6)
\]

and since the Kullback–Leibler divergence does not depend on the parametrization, neither does the natural gradient.

Later in this paper, we will study families of Gaussian distributions. The following proposition gives the Fisher metric for these families.

**Proposition 2.** Let \((P_\theta)_{\theta \in \Theta}\) be a family of normal probability distributions: \(P_\theta = N(\mu(\theta), \Sigma(\theta))\). If \(\mu\) and \(\Sigma\) are \(C^1\), the Fisher metric is given by:

\[
I_{ij}(\theta) = \left( \frac{\partial \mu^T}{\partial \theta_i} \Sigma^{-1} \frac{\partial \mu}{\partial \theta_j} + \frac{1}{2} \text{tr} \left( \Sigma^{-1} \frac{\partial \Sigma}{\partial \theta_i} \Sigma^{-1} \frac{\partial \Sigma}{\partial \theta_j} \right) \right). \hspace{1cm} (7)
\]

**Proof.** This is a non-trivial calculation. See [PF86] for more details.

As we will often be working with Gaussian distributions, we introduce the following notation:

**Notation 3.** \(\mathcal{G}_d\) is the manifold of Gaussian distributions in dimension \(d\), equipped with the Fisher metric.

\(\mathcal{G}_{d_{1}}\) is the manifold of Gaussian distributions in dimension \(d\), with covariance matrix proportional to identity in the canonical basis of \(\mathbb{R}^d\), equipped with the Fisher metric.
1.2 IGO flow, IGO algorithm

In IGO \cite{OAAH11}, invariance with respect to monotone transformations is achieved by replacing $f$ by the following transform: we set
\[ q(x) = P_{x' \sim P_{\theta}}(f(x') \leq f(x)), \] (8)
a non-increasing function $w: [0; 1] \rightarrow \mathbb{R}$ is chosen (the selection scheme), and finally
\[ W_\theta^f(x) = w(q(x)) \] By performing a gradient descent on $E_{x \sim P_{\theta}}[W_\theta^f(x)]$, we obtain the “IGO flow”:
\[ \frac{d\theta^t}{dt} = \tilde{\nabla}_\theta \int_X W_{\theta^t}^f(x)P_\theta(dx) = \int_X W_{\theta^t}^f(x)\tilde{\nabla}_\theta \ln P_\theta(x)P_{\theta^t}(dx). \] (9)

For practical implementation, the integral in (9) has to be approximated. For the integral itself, the Monte-Carlo method is used: $N$ values $(x_1, ..., x_N)$ are sampled from the distribution $P_{\theta^t}$, and the integral becomes
\[ \frac{1}{N} \sum_{i=1}^N W_{\theta^t}^f(x_i)\tilde{\nabla}_\theta \ln P_\theta(x_i) \] (10)
and we approximate $\frac{1}{N} W_{\theta^t}^f(x_i) = \frac{1}{N} w(q(x_i))$ by $\tilde{w}_i = \frac{1}{N} w(\frac{\text{rk}(x_i)+1}{2N})$, where $\text{rk}(x_i) = |\{j, f(x_j) < f(x_i)\}|$.

We now have an algorithm that can be used in practice if the Fisher information matrix is known.

Definition 4. The IGO update associated with parametrisation $\theta$, sample size $N$, step size $\delta t$ and selection scheme $w$ is given by the following update rule:
\[ \theta^{t+\delta t} = \theta^t + \delta t I^{-1}(\theta^t) \sum_{i=1}^N \tilde{w}_i \frac{\partial \ln P_\theta(x_i)}{\partial \theta}. \] (11)

We call IGO speed the vector $I^{-1}(\theta^t) \sum_{i=1}^N \tilde{w}_i \frac{\partial \ln P_\theta(x_i)}{\partial \theta}$.

1.3 Geodesic IGO

Although the IGO flow associated with a family of probability distributions is intrinsic (it only depends on the family itself, not the parametrization we choose for it), the IGO update is not. However, two different IGO updates are “close” when $\delta t \to 0$: the difference between two steps of IGO that differ only by the parametrization is a $O(\delta t^2)$.

Intuitively, the reason for this difference is that two IGO algorithms start at the same point, and follow “straight lines” with the same initial speed, but the definition of “straight lines” changes with the parametrization.

For instance, in the case of Gaussian distributions, let us consider two different IGO updates with Gaussian distributions in dimension 1, the first one with

\[ \text{This definition has to be slightly changed if the probability of a tie is not zero. See } \text{OAAH11} \text{ for more details.} \]

\[ \text{It can be proved (see } \text{OAAH11} \text{) that } \lim_{N \to \infty} N\tilde{w}_i = W_{\theta^t}(x_i). \text{ Here again, we are assuming there are no ties.} \]

\[ \text{One could start directly with the } \tilde{w}_i \text{ rather than } w, \text{ as we will do later.} \]
parametrization \((\mu, \sigma)\), and the second one with parametrization \((\mu, c := \sigma^2)\). We suppose the IGO speed for the first algorithm is \((\dot{\mu}, \dot{\sigma})\). The corresponding IGO speed in the second parametrization is given by the identity \(\dot{c} = 2\sigma \dot{\sigma}\). Therefore, the first algorithm gives the standard deviation \(c_{\text{new}, 1} = c_{\text{old}} + \delta t \dot{\sigma}\), and the variance \(c_{\text{new}, 1} = (c_{\text{new}, 1})^2 = c_{\text{old}} + 2\delta t \sigma \dot{\sigma} + \delta t^2 \dot{\sigma}^2 = c_{\text{new}, 2} + \delta t^2 \dot{\sigma}^2\).

The geodesics of a Riemannian manifold are the generalization of the notion of straight line: they are curves that locally minimize length. The notion will be explained precisely in Section 2, but let us define the geodesic IGO algorithm, which follows the geodesics of the manifold instead of following the straight lines for an arbitrary parametrization.

**Definition 5 (GIGO).** The geodesic IGO update (GIGO) associated with sample size \(N\), step size \(\delta t\) and selection scheme \(w\) is given by the following update rule:

\[
\theta^{t+\delta t} = \exp_{\theta^t}(Y \delta t)
\]

where

\[
Y = I^{-1}(\theta^t) \sum_{i=1}^{N} \hat{w}_i \frac{\partial \ln P_\theta(x_i)}{\partial \theta}
\]

is the IGO speed and \(\exp_{\theta^t}\) is the exponential of the Riemannian manifold \(\Theta\). Namely, \(\exp_{\theta^t}(Y \delta t)\) is the endpoint of the geodesic of \(\Theta\) starting at \(\theta^t\), with initial speed \(Y\), after a time \(\delta t\). By definition, this update does not depend on the parametrization \(\theta\).

Notice that while the GIGO update is compatible with the IGO flow (in the sense that when \(\delta t \to 0\) and \(N \to \infty\), a parameter \(\theta^t\) updated according to the GIGO algorithm is a solution of Equation 9 the equation defining the IGO flow), it not necessarily an IGO update. More precisely, the GIGO update is an IGO update if and only the geodesics of \(\Theta\) are straight lines for some parametrization.

The main problem with this update is that in general, obtaining equations for the geodesics is a difficult problem. In the next section, we will state Noether’s Theorem, which will be our main tool to compute the GIGO update for Gaussian distributions.

### 2 Riemannian geometry, Noether’s Theorem

#### 2.1 Riemannian geometry

The goal of this section is to state Noether’s theorem. We will not prove anything here, see [AVW89] for the proofs, [Bou07] or [JLJ98] for a more detailed presentation. Noether’s theorem states that if a system has symmetries, then, there are invariants attached to this symmetries. Firstly, we need some definitions.

---

1. In particular, given two points \(a\) and \(b\) on the Riemannian manifold \(M\), the shortest path from \(a\) to \(b\) is always a geodesic. The converse is not true, though.

2. By Beltrami’s theorem, this is equivalent to \(\Theta\) having constant curvature.
Definition 6 (Motion in a Lagrangian system). Let $M$ be a differentiable manifold, $TM$ the set of tangent vectors on $M$, and $\mathcal{L} : TM \to \mathbb{R}$ a differentiable function (called the Lagrangian function). A “motion in the lagrangian system $(M, \mathcal{L})$ from $x$ to $y$” is map $\gamma : [t_0, t_1] \to M$ such that:

- $\gamma(t_0) = x$
- $\gamma(t_1) = y$
- $\gamma$ is a local extremum of the functional:

$$\Phi(\gamma) = \int_{t_0}^{t_1} \mathcal{L}(\gamma(t), \dot{\gamma}(t)) dt,$$

among all curves $c : [t_0, t_1] \to M$ such that $c(t_0) = x$, and $c(t_1) = y$.

For example, when $(M, g)$ is a Riemannian manifold, the length of a curve $\gamma$ between $\gamma(t_0)$ and $\gamma(t_1)$ is:

$$\int_{t_0}^{t_1} \sqrt{g(\dot{\gamma}(t), \dot{\gamma}(t))} dt.$$

The curves that follow the shortest path between two points $x, y \in M$ are therefore the minima $\gamma$ of the functional such that $\gamma(t_0) = x$ and $\gamma(t_1) = y$, and the corresponding Lagrangian function is $(q, v) \mapsto \sqrt{g(v, v)}$. The solution to the problem of finding a parametrized curve with a shortest length is not unique: any curve following the shortest trajectory will have minimum length. For example, if $\gamma_1 : [a, b] \to M$ is a curve of shortest path, so is $\gamma_2 : t \mapsto \gamma_1(t^2)$: these two curves define the same trajectory in $M$, but they do not travel along this trajectory at the same speed. This leads us to the following definition:

Definition 7 (Geodesics). Let $I$ be an interval of $\mathbb{R}$, $(M, g)$ be a Riemannian manifold. A curve $\gamma : I \to M$ is called a geodesic if for all $t_0, t_1 \in I$, $\gamma|_{[t_0, t_1]}$ is a motion in the Lagrangian system $(M, \mathcal{L})$ from $\gamma(t_0)$ to $\gamma(t_1)$, where

$$\mathcal{L}(\gamma) = \int_{t_0}^{t_1} (g(\dot{\gamma}(t), \dot{\gamma}(t))) dt.$$

It can be shown (see [Bou07]) that geodesics are curves that locally minimize length, with constant velocity, which solves the previous uniqueness problem. More precisely, given a starting point and a starting speed, the geodesic is unique. This motivates the definition of the exponential of a Riemannian manifold.

Definition 8. Let $(M, g)$ be a Riemannian manifold. We call exponential of $M$ the application:

$$\exp : TM \to M$$

$$(x, v) \mapsto \exp_x(v),$$

such that for any $x \in M$, if $\gamma$ is the geodesic of $M$ satisfying $\gamma(0) = x$ and $\gamma'(0) = v$, then $\exp_x(v) = \gamma(1)$.

9A tangent vector is identified by the point at which it is tangent, and a vector in the tangent space.

10In general, it could depend on $t$.

11In the sense that $\frac{dg(\gamma(t), \dot{\gamma}(t))}{dt} = 0$. 

8
In order to find an extremal of a functional, the most commonly used result is called the “Euler–Lagrange equations” (see [AVW89] for example). Using them, it is possible to show that the geodesics of a Riemannian manifold follow the “geodesic equations”:

\[ \ddot{x}^k + \Gamma^k_{ij} \dot{x}^i \dot{x}^j = 0, \]  

(17)

where

\[ \Gamma^k_{ij} = \frac{1}{2} g^{lk} \left( \frac{\partial g_{jl}}{\partial q^i} + \frac{\partial g_{li}}{\partial q^j} - \frac{\partial g_{ij}}{\partial q^l} \right) \]  

(18)

are called “Christoffel symbols” of the metric \( g \). However, these coefficients are tedious (and sometimes difficult) to compute, and (17) is a second order differential equation. Noether’s theorem will give us a first order equation to compute the geodesics.

2.2 Noether’s Theorem

**Definition 9.** Let \( h: M \rightarrow M \) a diffeomorphism. We say that the Lagrangian system \((M, \mathcal{L})\) admits the symmetry \( h \) if for any \((q, v) \in TM\),

\[ \mathcal{L}(h(q), dh(v)) = \mathcal{L}(q, v), \]  

(19)

where \( dh \) is the differential of \( h \).

If \( M \) is obvious, we will sometimes say that \( \mathcal{L} \) is invariant under \( h \).

An example will be given in the proof of Theorem [18].

We can now state Noether’s theorem (see for example [AVW89]).

**Theorem 10 (Noether’s Theorem).** If the Lagrangian system \((M, \mathcal{L})\) admits the one-parameter group of symmetries \( h^s: M \rightarrow M, s \in \mathbb{R} \), then the following quantity remains constant during the motions in the system \((M, \mathcal{L})\). Namely,

\[ I(\gamma(t), \dot{\gamma}(t)) = \frac{\partial \mathcal{L}}{\partial v} \left( \frac{dh^s(\gamma(t))}{ds} \right)_{s=0} \]  

(20)

does not depend on \( t \) if \( \gamma \) is a motion in \((M, \mathcal{L})\).

Now, we are going to apply this theorem to our problem: computing the geodesics of Riemannian manifolds of Gaussian distributions.

3 GIGO in \( \tilde{\mathbb{G}}_d \)

We do not know of a closed form for the geodesics of \( \mathbb{G}_d \). However, the situation is better if we force the covariance matrix to be either diagonal or proportional to the identity matrix. In the former case, the manifold we are considering is \((\mathbb{G}_1)^d\), and in the latter case, it is \( \tilde{\mathbb{G}}_d \). The geodesics of \((\mathbb{G}_1)^d\) are given by

**Proposition 11.** Let \( M \) be a Riemannian manifold, let \( d \in \mathbb{N} \), let \( \Phi \) be the Riemannian exponential of \( M^d \), and let \( \phi \) be the Riemannian exponential of \( M \). We have:

\[ \Phi(x_1, ..., x_n)((v_1, ..., v_n)) = (\phi_{x_1}(v_1), ..., \phi_{x_n}(v_n)) \]  

(21)

In particular, knowing the geodesics of \( \mathbb{G}_1 \) is enough to compute the geodesics of \((\mathbb{G}_1)^d\).
This is true because a block of the product metric does not depend on variables of the other blocks.

Consequently, a GIGO update with a diagonal covariance matrix with the sample $(x_i)$ is equivalent to $d$ separate 1-dimensional GIGO updates using the same samples. Moreover, $\mathcal{G}_1 \cong \mathcal{G}_d$, the geodesics of which are given below.

We will show that $\mathcal{G}_d$ and the “hyperbolic space”, of which the geodesics are known, are isometric.

### 3.1 Preliminaries: Poincaré half-plane, hyperbolic space

In dimension 2, the hyperbolic space is called “hyperbolic plane”, or Poincaré half-plane. We recall its definition:

**Definition 12** (Poincaré half-plane). We call “Poincaré half-plane” the Riemannian manifold

$$\mathcal{H} = \{ (x, y) \in \mathbb{R}^2, \ y > 0 \},$$

with the metric $ds^2 = \frac{dx^2 + dy^2}{y^2}$.

We also recall the expression of its geodesics (see for example [GHL04]):

**Proposition 13** (Geodesics of the Poincaré half-plane). The geodesics of the Poincaré half-plane are exactly the:

$$t \mapsto (\text{Re}(z(t)), \text{Im}(z(t))),$$

where

$$z(t) = \frac{aie^{vt} + b}{cie^{vt} + d},$$

(22) with $ad - bc = 1$, and $v > 0$.

The geodesics are half-circles perpendicular to the line $y = 0$, and vertical lines.

![Figure 1: Geodesics of the Poincaré half-plane](image)

The generalization to higher dimension is the following:

**Definition 14** (Hyperbolic space). We call “hyperbolic space of dimension $n$” the Riemannian manifold

$$\mathcal{H}_n = \{ (x_1, ..., x_{n-1}, y) \in \mathbb{R}^n, \ y > 0 \},$$

with the metric $ds^2 = \frac{dx_1^2 + ... + dx_{n-1}^2 + dy^2}{y^2}$. 

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Its geodesics stay in a plane containing the direction $y$ and the initial speed. The induced metric on this plane is the metric of the Poincaré half-plane. The geodesics are therefore given by the following proposition:

**Proposition 15 (Geodesics of the hyperbolic space).** If $\gamma: t \mapsto (x_1(t), \ldots, x_{n-1}(t), y(t)) = (x(t), y(t))$ is a geodesic of $\mathcal{H}_n$, then, there exists $a, b, c, d \in \mathbb{R}$ such that $ad - bc = 1$ and $v > 0$ such that

$$x(t) = x(0) + \frac{v}{\|\dot{x}\|} \tilde{x}(t), \quad y(t) = \text{Im}(\gamma_C(t)), \quad \text{with} \quad \tilde{x}(t) = \text{Re}(\gamma_C(t))$$

and

$$\gamma_C(t) := \frac{aie^{vt} + b}{cie^{vt} + d}. \quad (23)$$

### 3.2 Computing the GIGO update in $\tilde{G}_d$

If we want to implement the GIGO algorithm in $\tilde{G}_d$, we need to compute the natural gradient in $\tilde{G}_d$, and to be able to compute the Riemannian exponential of $\tilde{G}_d$.

Using Proposition 2, we can compute the metric of $\tilde{G}_d$ in the parametrization $(\mu, \sigma) \mapsto N(\mu, \sigma^2 I)$. We find:

$$\begin{pmatrix}
\frac{1}{\sigma^2} & 0 & \ldots & 0 \\
0 & \ddots & \ddots & \vdots \\
\vdots & \ddots & \frac{1}{\sigma^2} & 0 \\
0 & \ldots & 0 & \frac{2d}{\sigma^2}
\end{pmatrix}. \quad (24)$$

Since this matrix is diagonal, it is easy to invert, and we immediately have the natural gradient, and, consequently, the IGO speed.

**Proposition 16.** In $\tilde{G}_d$, the IGO speed $Y$ is given by:

$$Y_\mu = \sum_i \hat{w}_i (x_i - \mu), \quad (25)$$

$$Y_\sigma = \sum_i \hat{w}_i \left( \frac{(x_i - \mu)^T(x_i - \mu)}{2d\sigma} - \frac{\sigma}{2} \right). \quad (26)$$

**Proof.** We recall the IGO speed is defined by $Y = I^{-1}(\theta^t) \sum_{i=1}^N \hat{w}_i \frac{\partial \ln P_{\theta}(x_i)}{\partial \theta}$. Since $P_{\mu,\sigma}(x) = (2\pi\sigma^2)^{-d/2} \exp\left(\frac{-(x-x_\mu)^T(x-x_\mu)}{2\sigma^2}\right)$, we have

$$\frac{\partial \ln P_{\mu,\sigma}(x)}{\partial \mu} = x - \mu,$$

$$\frac{\partial \ln P_{\mu,\sigma}(x)}{\partial \sigma} = -\frac{d}{\sigma} + \frac{(x-\mu)^T(x-\mu)}{\sigma^3}. \quad \text{The result follows.}$$

The metric defined by Equation 24 is not exactly the metric of the hyperbolic space, but with the substitution $\mu \leftarrow \frac{\mu}{\sqrt{2d}}$, the metric becomes $\frac{2d}{\sigma^2} I$, which is proportional to the metric of the hyperbolic space, and therefore defines the same geodesics.

---

12A possible way is to prove this is to use Noether’s theorem: the Lagrangian for the geodesics is invariant under all translations along the $x_i$. 

11
**Theorem 17 (Geodesics of $\tilde{G}_d$).** If $\gamma: t \mapsto N(\mu(t), \sigma(t)^2 I)$ is a geodesic of $\tilde{G}_d$, then, there exists $a, b, c, d \in \mathbb{R}$ such that $ad - bc = 1$ and $v > 0$ such that

$$\mu(t) = \mu(0) + \sqrt{2d} \frac{\dot{\mu}}{\|\dot{\mu}\|} \hat{r}(t), \quad \sigma(t) = \text{Im}(\gamma_C(t)), \quad \text{with} \quad \hat{r}(t) = \text{Re}(\gamma_C(t)) \quad \text{and}$$

$$\gamma_C(t) := \frac{ae^{vt} + b}{c e^{vt} + d}.$$  

(27)

Now, in order to implement the corresponding GIGO algorithm, we only need to be able to find the coefficients $a, b, c, d, v$ corresponding to an initial position $(\mu_0, \sigma_0)$, and an initial speed $(\dot{\mu}_0, \dot{\sigma}_0)$. It is a tedious but easy computation, the result of which is given in Proposition 34.

The pseudocode of GIGO in $\tilde{G}_d$ is also given in the Appendix: it is obtained by concatenating Algorithms 1 and 7.

4 **GIGO in $G_d$**

4.1 **Obtaining a first order differential equation for the geodesics of $G_d$**

In the case where both the covariance matrix and the mean can vary freely, the equations of the geodesics have been computed in [CO91] and [Eri87]. However, these articles start with the equations of the geodesics obtained with the Christoffel symbols, then partially integrate them, obtaining equations (38) and (39) of Theorem 19. These equations are in fact a consequence of Noether’s theorem, and can be found directly.

**Theorem 18.** Let $\gamma : t \mapsto N(\mu_t, \Sigma_t)$ be a geodesic of $G_d$. Then, the following quantities do not depend on $t$:

$$J_{\mu} = \Sigma_t^{-1} \dot{\mu}_t, \quad (28)$$

$$J_{\Sigma} = \Sigma_t^{-1} (\dot{\mu}_t \mu_t^T + \Sigma_t). \quad (29)$$

**Proof.** It is a direct application of Noether’s theorem, with suitable groups of diffeomorphisms. By Proposition 2, the Lagrangian associated with the geodesics of $G_d$ is

$$\mathcal{L}(\mu, \Sigma, \dot{\mu}, \dot{\Sigma}) = \dot{\mu}^T \Sigma^{-1} \dot{\mu} + \frac{1}{2} \text{tr}(\dot{\Sigma} \Sigma^{-1} \dot{\Sigma} \Sigma^{-1}). \quad (30)$$

Its derivative is

$$\frac{\partial \mathcal{L}}{\partial \theta} = \left[(h, \dot{H}) \mapsto 2\dot{\mu}^T \Sigma^{-1} h + \text{tr}(H \Sigma^{-1} \dot{\Sigma} \Sigma^{-1})\right]. \quad (31)$$

Let us show that this Lagrangian is invariant under affine changes of basis (thus illustrating Definition 9).

The general form of an affine change of basis is $\phi_{\mu_0, A} : (\mu, \Sigma) \mapsto (A \mu + \mu_0, A \Sigma A^T)$, with $\mu_0 \in \mathbb{R}^d$ and $A \in \text{GL}_d(\mathbb{R})$.

We have

13 Proposition 34 and the pseudocode in the Appendix allow the metric to be slightly modified, see Section 5.2.
\[ L(\phi_{\mu_0}, A(\mu, \Sigma), d\phi_{\mu_0}, A(\mu, \Sigma)) = \dot{A}^T (A \Sigma A^T)^{-1} \dot{A} + \frac{1}{2} \text{tr} \left( A \dot{\Sigma} A^T (A \Sigma A^T)^{-1} A \dot{\Sigma} A^T (A \Sigma A^T)^{-1} \right), \]

(32)

and since \( \dot{A} = A \dot{\mu} \) and \( \dot{A} \Sigma A^T = A \dot{\Sigma} A^T \), we find easily that

\[ L(\phi_{\mu_0}, A(\mu, \Sigma), d\phi_{\mu_0}, A(\mu, \Sigma)) = L(\mu, \Sigma, \dot{\mu}, \dot{\Sigma}), \]

(33)

or in other words: \( L \) is invariant under \( \phi_{\mu_0}, A \) for any \( \mu_0 \in \mathbb{R}^d, A \in \text{GL}_d(\mathbb{R}) \).

In order to use Noether’s theorem, we also need one-parameter groups of transformations. We choose the following:

1. Translations of the mean vector. For any \( i \in [1, d] \), let \( h_{s_i} : (\mu, \Sigma) \mapsto (\mu + se_i, \Sigma) \), where \( e_i \) is the \( i \)-th basis vector. We have \( \frac{dh_{s_i}}{ds}|_{s=0} = (e_i, 0) \), so by Noether’s theorem,

\[ \frac{\partial L}{\partial \dot{\theta}}(e_i, 0) = 2\dot{\mu}^T \Sigma^{-1} e_i = 2e_i^T \Sigma^{-1} \dot{\mu} \]

remains constant for all \( i \). The fact that \( J_{\mu} \) is an invariant immediately follows.

2. Linear base changes. For any \( i, j \in [1, d] \), let \( h_{s_{ij}} : (\mu, \Sigma) \mapsto (\exp(sE_{ij}) \mu, \exp(sE_{ij}) \Sigma \exp(sE_{ji})) \), where \( E_{ij} \) is the matrix with a 1 at position \((i, j)\), and zeros elsewhere. We have \( \frac{dh_{s_{ij}}}{ds}|_{s=0} = (E_{ij} \mu, E_{ij} \Sigma + \Sigma E_{ji}) \). So by Noether’s theorem, we then obtain the following invariants:

\[ J_{ij} := \frac{\partial L}{\partial \theta}(E_{ij} \mu, E_{ij} \Sigma + \Sigma E_{ji}) \]

(34)

\[ = 2\dot{\mu}^T \Sigma^{-1} E_{ij} \mu + \text{tr}((E_{ij} \Sigma + \Sigma E_{ji}) \Sigma^{-1} \dot{\Sigma} \Sigma^{-1}) \]

(35)

\[ = 2(\Sigma^{-1} \dot{\mu})^T E_{ij} \mu + \text{tr}(E_{ij} \dot{\Sigma} \Sigma^{-1}) + \text{tr}(E_{ji} \Sigma^{-1} \dot{\Sigma}) \]

(36)

\[ = 2(\dot{J}_{\mu} \mu^T)_{ij} + 2(\Sigma^{-1} \dot{\Sigma})_{ij}, \]

(37)

and the coefficients of \( J_{\Sigma} \) in (29) are the \((J_{ij}/2)\).

This leads us to first order equations satisfied by the geodesics mentionned in [Eri87, CO91] and [ITW11].

**Theorem 19** (GIGO-\( \Sigma \)). \( t \mapsto N(\mu_t, \Sigma_t) \) is a geodesic of \( \mathbb{G}_d \) if and only if \( \mu : t \mapsto \mu_t \) and \( \Sigma : t \mapsto \Sigma_t \) satisfy the equations

\[ \dot{\mu}_t = \Sigma_t J_{\mu} \]

(38)

\[ \dot{\Sigma}_t = \Sigma_t (J_{\Sigma} - J_{\Sigma} \mu_t \mu_t^T) = \Sigma_t J_{\Sigma} - \dot{\mu}_t \mu_t^T, \]

(39)

where

\[ J_{\mu} = \Sigma_0^{-1} \dot{\mu}_0, \]

and

\[ J_{\Sigma} = \Sigma_0^{-1} \left( \dot{\mu}_0 \mu_0^T + \Sigma_0 \right). \]
Proof. It is an immediate consequence of Proposition \[18\].

These equations can be solved analytically (see [CO91]), but usually, that is not the case, and they have to be solved numerically, for example with the Euler method (the corresponding algorithm, which we call GIGO-$\Sigma$, is described in the Appendix). The goal of the remainder of the subsection is to show that having to use the Euler method is fine.

To avoid confusion, we will call the step size of the GIGO algorithm ($\delta t$ in Proposition \[5\]) “GIGO step size”, and the step size of the Euler method (inside a step of the GIGO algorithm) “Euler step size”.

Having to solve our equations numerically brings two problems:

The first one is a theoretical problem: the main reason to study GIGO is its invariance under reparametrization of $\theta$, and we lose this invariance property when we use the Euler method. However, GIGO can get arbitrarily close to invariance by decreasing the Euler step size. In other words, the difference between two different IGO algorithms is $O(\delta t^2)$, and the difference between two different implementations of the GIGO algorithm is $O(h^2)$, where $h$ is the Euler step size, and it is easier to reduce the latter. Still, without a closed form for the geodesics of $\mathbb{G}_d$, the GIGO update is rather expensive to compute, but it can be argued that most of the computation time will still be the computation of the objective function $f$.

The second problem is purely numerical: we cannot guarantee that the co-variance matrix remains positive definite along the Euler method. Here, apart from finding a closed form for the geodesics, we have two solutions.

We can enforce this \textit{a posteriori}: if the covariance matrix we find is not positive definite after a GIGO step, we repeat the failed GIGO step with a reduced Euler step size (in our implementation, we divided it by 4, see Algorithm \[2\] in the Appendix.).

The other solution is to obtain differential equations on a square root of the covariance matrix.$^{14}$

Theorem 20 (GIGO-A). If $\mu : t \mapsto \mu_t$ and $A : t \mapsto A_t$ satisfy the equations

\[
\dot{\mu}_t = A_tA_t^T J_{\mu},
\]

\[
\dot{A}_t = \frac{1}{2}(J_{\Sigma} - J_{\mu}\mu_t^T)A_t,
\]

where

\[
J_{\mu} = (A_0^{-1})^T A_0^{-1} \mu_0,
\]

and

\[
J_{\Sigma} = (A_0^{-1})^T A_0^{-1}(\mu_0\mu_0^T + \dot{\mu}_0 A_0^T + A_0\dot{A}_0^T),
\]

then, $t \mapsto \mathcal{N}(\mu_t, A_tA_t^T)$ is a geodesic of $\mathbb{G}_d$.

Proof. This is a simple rewriting of Theorem \[19\] if we write $\Sigma := AA^T$, we find that $J_{\mu}$ and $J_{\Sigma}$ are the same as in Theorem \[19\] and we have

\[
\dot{\mu} = \Sigma J_{\mu},
\]

$^{14}$any matrix $A$ such that $\Sigma = AA^T$. 

14
and
\[ \dot{\Sigma} = (AA^T + AA^T) = \frac{1}{2}(J\dot{\Sigma} - J\mu^T)^T AA^T + \frac{1}{2} AA^T (J\dot{\Sigma} - J\mu^T) \]

\[ = \frac{1}{2}(J\dot{\Sigma} - J\mu^T)^T \Sigma + \frac{1}{2} \Sigma(J\dot{\Sigma} - J\mu^T) = \frac{1}{2} \Sigma(J\dot{\Sigma} - J\mu^T) + \frac{1}{2} [\Sigma(J\dot{\Sigma} - J\mu^T)]^T. \]

By Theorem 19, \( \Sigma(J\dot{\Sigma} - J\mu^T) \) is symmetric (since \( \dot{\Sigma} \) has to be symmetric). Therefore, we have \( \dot{\Sigma} = \Sigma(J\dot{\Sigma} - J\mu^T) \), and the result follows.

Notice that Theorem 20 gives an equivalence, whereas Theorem 19 does not. The reason is that the square root of a symmetric positive definite matrix is not unique. Still, it is canonical, see discussion in Section 5.1.1.

As for Theorem 19, we can solve Equations 40 and 41 numerically, and we obtain another algorithm (Algorithm 4 in the Appendix, we will call it GIGO-A), with a behavior similar to the previous one (with equations 38 and 39). For both of them, numerical problems can arise when the covariance matrix is almost singular.

We have not managed to find any example where one of these two algorithms converged to the minimum of the objective function whereas the other did not, and their behavior is almost the same.

More interestingly, the performances of these two algorithms are also the same as the performances of the exact GIGO algorithm, using the equations of Section 4.2.

Notice that even though GIGO-A directly maintains a square root of the covariance matrix, which makes sampling new points easier\(^\text{15}\) both GIGO-\(\Sigma\) and GIGO-A still have to invert the covariance matrix (or its square root) at each step, which is as costly as the decomposition, so one of these algorithms is roughly as expensive to compute as the other.

4.2 Explicit form of the geodesics of \( \mathbb{G}_d \)

We now give the exact geodesics of \( \mathbb{G}_d \): the following results are a rewriting of Theorem 3.1 and its first corollary in [CO91].

**Theorem 21.** Let \( (\dot{\mu}_0, \dot{\Sigma}_0) \in T_{\mathcal{N}(0,1)} \mathbb{G}_d. \) The geodesic of \( \mathbb{G}_d \) starting from \( \mathcal{N}(0,1) \) with initial speed \( (\dot{\mu}_0, \dot{\Sigma}_0) \) is given by:

\[ \exp_{\mathcal{N}(0,1)}(s\dot{\mu}_0, s\dot{\Sigma}_0) = \mathcal{N}\left(2R(s)\text{sh}(\frac{sG}{2})G^- \dot{\mu}_0, R(s)R(s)^T\right), \quad (42) \]

where \( \exp \) is the Riemannian exponential of \( \mathbb{G}_d \), \( G \) is any matrix satisfying

\[ G^2 = \dot{\Sigma}_0^2 + 2\dot{\mu}_0\dot{\mu}_0^T, \quad (43) \]

\[ R(s) = \left(\left(\text{ch}(\frac{sG}{2}) - \dot{\Sigma}_0 G^- \text{sh}(\frac{sG}{2})\right)^{-1}\right)^T \quad (44) \]

and \( G^- \) is a pseudo-inverse of \( G \)\(^\text{16}\)

\(^\text{15}\)To sample a point from \( \mathcal{N}(\mu, \Sigma) \), a square root of \( \Sigma \) is needed.

\(^\text{16}\)In [CO91], the existence of \( G \) (as a square root of \( \dot{\Sigma}_0^2 + 2\dot{\mu}_0\dot{\mu}_0^T \)) is proved. Notice that anyway, in the expansions of (42) and (44), only even powers of \( G \) appear.
And since for all $A \in GL_d(\mathbb{R})$, for all $\mu_0 \in \mathbb{R}^d$, the application
\[ \phi : \mathbb{G}_d \rightarrow \mathbb{G}_d \]
\[ \mathcal{N}(\mu, \Sigma) \mapsto \mathcal{N}(A\mu + \mu_0, A\Sigma AT) \]  
(45)
preserves the geodesics, we find the general expression for the geodesics of $\mathbb{G}_d$.

**Corollary 22.** Let $\mu_0 \in \mathbb{R}^d$, $A \in GL_d(\mathbb{R})$, and $(\dot{\mu}_0, \dot{\Sigma}_0) \in T_{\mathcal{N}(\mu_0, A_0 A_0^T)\mathbb{G}_d}$. The geodesic of $\mathbb{G}_d$ starting from $\mathcal{N}(\mu, \Sigma)$ with initial speed $(\dot{\mu}_0, \dot{\Sigma}_0)$ is given by:
\[
\exp_{\mathcal{N}(\mu_0, A_0 A_0^T)}(s\dot{\mu}_0, s\dot{\Sigma}_0) = \mathcal{N}(\mu_1, A_1 A_1^T),
\]
(46)
with
\[
\mu_1 = 2A_0 R(s) \text{sh}(\frac{s}{2}G)A_0^{-1}\dot{\mu}_0 + \mu_0,
\]
(47)
\[
A_1 = A_0 R(s),
\]
(48)
where $\exp$ is the Riemannian exponential of $\mathbb{G}_d$, $G$ is any matrix satisfying
\[
G^2 = A_0^{-1}(\dot{\Sigma}_0 \Sigma_0^{-1} \Sigma_0 + 2\dot{\mu}_0 \dot{\Sigma}_0^T)(A_0^{-1})^T,
\]
(49)
\[
R(s) = \left(\text{ch}(\frac{s}{2}) - A_0^{-1}\dot{\Sigma}_0 (A_0^{-1})^T \text{sh}(\frac{s}{2}G)\right)^{-1} \right)^T,
\]
(50)
and $G^{-}$ is a pseudo-inverse of $G$.

It should be noted that the final values for mean and covariance do not depend on the choice of $G^2$. The reason for this is that $\text{ch}(G)$ is a Taylor series in $G^2$, and so are $\text{sh}(G)G^{-}$ and $G^{-}\text{sh}(G)$.

For our practical implementation, we actually used these Taylor series instead of the expression of the corollary.

5 Comparing GIGO, xNES and pure rank-$\mu$ CMA-ES

5.1 Definitions

In this section, we recall the xNES and pure rank-$\mu$ CMA-ES, and we describe them in the IGO framework, thus allowing a reasonable comparison with the GIGO algorithms.

5.1.1 xNES

We recall a restriction\(^\text{17}\) of the xNES algorithm, introduced in [GSY+10].

\(^{17}\)As a square root of $A_0^{-1}(\dot{\Sigma}_0 \Sigma_0^{-1} \Sigma_0 + 2\dot{\mu}_0 \dot{\Sigma}_0^T)(A_0^{-1})^T$.

\(^{18}\)This restriction is sufficient to describe the numerical experiments in [GSY+10], the article which introduced xNES.
Definition 23 (xNES algorithm). The xNES algorithm with sample size $N$, weights $w_i$, and learning rates $\eta_\mu$ and $\eta_\Sigma$ updates the parameters $\mu \in \mathbb{R}^d$, $A \in M_d(\mathbb{R})$ with the following rule: At each step, $N$ points $x_1, \ldots, x_N$ are sampled from the distribution $\mathcal{N}(\mu, AA^T)$. Without loss of generality, we assume $f(x_1) < \ldots < f(x_N)$. The parameter is updated according to:

$$
\mu \leftarrow \mu + \eta_\mu AG_\mu,
$$

$$
A \leftarrow A \exp(\eta_\Sigma GM/2),
$$

where, setting $z_i = A^{-1}(x_i - \mu)$:

$$
G_\mu = \sum_{i=1}^{N} w_i z_i,
$$

$$
G_M = \sum_{i=1}^{N} w_i (z_i z_i^T - I).
$$

The more general version decomposes the matrix $A$ as $\sigma B$, where $\det B = 1$, and uses two different learning rates for $\sigma$ and for $B$. We gave the version where these two learning rates are equal. This restriction of the xNES algorithm can be described in the IGO framework, provided all the learning rates are equal (most of the elements of the proof can be found in [GSY+10] or in [OAAH11]):

Proposition 24 (xNES as IGO). The xNES algorithm with sample size $N$, weights $w_i$, and learning rates $\eta_\mu = \eta_\Sigma = \delta t$ coincides with the IGO algorithm with sample size $N$, weights $w_i$, step size $\delta t$, and in which, given the current position $(\mu_t, A_t)$, the set of Gaussians is parametrized by

$$
\phi_{\mu_t, A_t} : (\delta, M) \mapsto \mathcal{N} \left( \mu_t + A_t \delta, A_t \exp \left( \frac{1}{2} M \right) \left( A_t \exp \left( \frac{1}{2} M \right)^T \right) \right),
$$

with $\delta \in \mathbb{R}^m$ and $M \in \text{Sym}(\mathbb{R}^m)$.

The parameters maintained by the algorithm are $(\mu, A)$, and the $x_i$ are sampled from $\mathcal{N}(\mu, AA^T)$.

Proof. Let us compute the IGO update in the parametrization $\phi_{\mu_t, A_t}$; we have $\delta t = 0$, $M t = 0$, and by using Proposition 2, we can see that for this parametrization, the Fisher information matrix at $(0, 0)$ is the identity matrix. The IGO update is therefore,

$$
(\delta, M)^{t+\delta t} = (\delta, M)^{t} + \delta t Y_\delta(\delta, M) + \delta t Y_M(\delta, M) = \delta t Y_\delta(\delta, M) + \delta t Y_M(\delta, M),
$$

where

$$
Y_\delta(\delta, M) = \sum_{i=1}^{N} w_i \nabla_\delta \ln(p(x_i|\delta, M))
$$

In particular, for the default parameters in [GSY+10], these two learning rates are equal.

The proposition below essentially states that xNES is a natural gradient update.
\[ Y_M(\delta, M) = \sum_{i=1}^{N} w_i \nabla_M \ln(p(x_i|\delta, M)) \].

Since
\[ \ln P_{\delta,M}(x) = -\frac{d}{2} \ln(2\pi) - \frac{1}{2} \ln(\det A) - \frac{1}{2} \| \exp(-\frac{1}{2} M)A^{-1}(x - \mu - A\delta) \|^2, \]
a straightforward computation yields
\[ Y_\delta(\delta, M) = \sum_{i=1}^{N} w_i z_i = G_\mu, \]
and
\[ Y_M(\delta, M) = \frac{1}{2} \sum_{i=1}^{N} w_i (z_i z_i^T - I) = G_M. \]

Therefore, the IGO update is:
\[
\begin{align*}
\delta(t + \delta t) &= \delta(t) + \delta t G_\mu, \\
M(t + \delta t) &= M(t) + \delta t G_M,
\end{align*}
\]
or, in terms of mean and covariance matrix:
\[
\begin{align*}
\mu(t + \delta t) &= \mu(t) + \delta t A(t) G_\mu \\
A(t + \delta t) &= A(t) \exp(\delta t G_M/2),
\end{align*}
\]
or
\[ \Sigma(t + \delta t) = A(t) \exp(\delta t G_M) A(t)^T. \]

This is the xNES update.  

\[ \square \]

**Using a square root of the covariance matrix**

Firstly, we recall that the IGO framework (on $G_d$, for example) emphasizes the Riemannian manifold structure on $G_d$. All the algorithms studied here (including GIGO, which is not strictly speaking an IGO algorithm) define a trajectory in $G_d$ (a new point for each step), and to go from a point $\theta$ to the next one ($\theta'$), we follow some curve $\gamma : [0, \delta t] \to G_d$, with $\gamma(0) = \theta$, $\gamma(\delta t) = \theta'$, and $\dot{\gamma}(0)$ given by the natural gradient ($\dot{\gamma}(0) = \sum_{i=1}^{N} \hat{w}_i \nabla_{\theta} P_\theta(x_i) \in T_\theta G_d$).

To be compatible with this point of view, an algorithm giving an update rule for a square root of the covariance matrix $A$ has to satisfy the following condition: For a given initial speed, the covariance matrix $\Sigma(t+\delta t)$ after one step must depend only on $\Sigma(t)$, and not on the square root $A'$ chosen for $\Sigma(t)$. 

The xNES algorithm does satisfy this condition: consider two xNES algorithms, with the same learning rates, respectively at ($\mu, A'_1$) and ($\mu, A'_2$), with

\[ ^{21} \text{Using } \text{tr}(M) = \log(\det(\exp(M))) \]
Algorithm 2.1

We have shown that what we will call the "xNES trajectory" is well-defined. Using the definitions of Section 5.3, we have just shown that what we will call

\[ A_1^T(A_1^T)^T = A_2^T(A_2^T)^T \] (i.e.: they define the same \( \Sigma' \)), we can use the same samples \( x_i \) to compute the natural gradient update\(^{22}\) then we will have \( \Sigma_{i+dt} = \Sigma_{i+dt}^\prime \).

Using the definitions of Section 5.3, we have just shown that what we will call the "xNES trajectory" is well-defined.

It is also important to notice that, in order to be well defined, a natural gradient algorithm updating a square root of the covariance matrix has to specify more conditions than simply following the natural gradient.

The reason for this is that the natural gradient is a vector tangent to \( G_d \): it lives in a space of dimension \( d(d+3)/2 \) (the dimension of \( G_d \)) whereas the vector \( (\mu, A) \) lives in a space of dimension \( d(d+1) \), which is too large: we will have no uniqueness for the solutions of the equations expressed with \( A \) (this is why Theorem 20 is simply an implication, whereas Theorem 19 is an equivalence).

More precisely, let us consider \( A \) in \( GL_d(\mathbb{R}) \), and \( v_A, v_A' \) two infinitesimal updates of \( A \). Since \( \Sigma = AA^T \), the infinitesimal update of \( \Sigma \) corresponding to \( v_A \) (resp. \( v_A' \)) is \( \Sigma v_A = Av_A^T + v_A A^T \) (resp. \( \Sigma v_A' = Av_A'^T + v_A' A^T \)).

It is now easy to see that \( v_A \) and \( v_A' \) define the same direction for \( \Sigma \) (i.e. \( \Sigma v_A = \Sigma v_A' \)) if and only if \( AM^T + MA^T = 0 \), where \( M = v_A - v_A' \). This is equivalent to \( A^{-1}M \) antisymmetric.

For any \( A \in M_d(\mathbb{R}) \), let us denote by \( T_A \) the space of the matrices \( M \) such that \( A^{-1}M \) is antisymmetric, or in other words \( T_A := \{ u \in M_d(\mathbb{R}), Au^T + uA^T = 0 \} \). Having a subspace \( S_A \) in direct sum with \( T_A \) for all \( A \) is sufficient (but not necessary) to have a well-defined update rule. Namely, consider the (linear) application

\[
\phi_A : M_d(\mathbb{R}) \rightarrow S_d(\mathbb{R})
\]

sending an infinitesimal update of \( A \) to the corresponding update of \( \Sigma \). It is not bijective, but as we have seen before, \( \text{Ker} \phi_A = T_A \), and therefore, if we have, for some \( U_A \),

\[
M_d(\mathbb{R}) = U_A \oplus T_A,
\]

then \( \phi_A|_{U_a} \) is an isomorphism. Let \( v_\Sigma \) be an infinitesimal update of \( \Sigma \). We choose the following update of \( A \) corresponding to \( v_\Sigma \):

\[
v_A := (\phi_A|_{U_a})^{-1}(v_\Sigma).
\]

Any \( U_A \) such that \( U_A \oplus T_A = M_d(\mathbb{R}) \) is a reasonable choice to pick \( v_A \) for a given \( v_\Sigma \). The choice \( S_A = \{ u \in M_d(\mathbb{R}), Au^T + uA^T = 0 \} \) has an interesting additional property: it is the orthogonal of \( T_A \) for the norm

\[
\|v_A\|_2^2 := \text{Tr}(v_A^T \Sigma^{-1} v_A) = \text{Tr}((A^{-1} v_A)^T A^{-1} v_A). \]

\(^{22}\) We are talking about the \( x_i \) of Definition 23 which are sampled from \( \mathcal{N}(\mu, AA^T) \), not the \( z_i \), which are sampled from \( \mathcal{N}(0, I) \), and are actually used to compute the \( x_i \) by \( x_i = \mu + Az_i \). Notice that consequently, the “sampled points” will not be the same for the two algorithms if they use the same random number generator with the same seed. However, \( \theta \) will have the same probability distribution for both algorithms.

\(^{23}\) To prove this, remark that \( T_A = \{ M \in M_d(\mathbb{R}), A^{-1}M \text{ antisymmetric} \} \) and \( S_A = \{ M \in \)

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and consequently, it can be defined without referring to the parametrization, which makes it a canonical choice.

Let us now show that this is the choice made by xNES and GIGO-A (which are well-defined algorithms updating a square root of the covariance matrix).

Proposition 25. Let $A \in M_n(\mathbb{R})$. The $v_A$ given by the xNES and GIGO-A algorithms lies in $S_A = \{ u \in M_d(\mathbb{R}), A u^T - u A^T = 0 \} = S_A$.

Proof. For xNES, let us write $\dot{\gamma}(0) = (v_\mu, v_\Sigma)$, and $v_A := \frac{1}{2} AG$. We have $A^{-1} v_A = \frac{1}{2} G_M$, and therefore, forcing $M$ (and $G_M$) to be symmetric in xNES is equivalent to $A^{-1} v_A = (A^{-1} v_A)^T$, which can be rewritten as $A v_A^T = v_A A^T$. For GIGO-A, Equation 39 shows that $\Sigma_t(J \Sigma - J \mu \mu^T)_{t}$ is symmetric, and with this fact in mind, Equation 41 shows that we have $A v_A^T = v_A A^T$ ($v_A$ is $\dot{A}_t$).

5.1.2 Pure rank-$\mu$ CMA-ES

We now recall the pure rank-$\mu$ CMA-ES algorithm. The general CMA-ES algorithm is described in [Han11].

Definition 26 (pure rank-$\mu$ CMA-ES algorithm). The pure rank-$\mu$ CMA-ES algorithm with sample size $N$, weights $w_i$, and learning rates $\eta_\mu$ and $\eta_\Sigma$ is defined by the following update rule: At each step, $N$ points $x_1, ..., x_N$ are sampled from the distribution $N(\mu, \Sigma)$. Without loss of generality, we assume $f(x_1) < ... < f(x_N)$. The parameter is updated according to:

$$
\mu \leftarrow \mu + \eta_\mu \sum_{i=1}^{N} w_i(x_i - \mu), \\
\Sigma \leftarrow \Sigma + \eta_\Sigma \sum_{i=1}^{N} w_i((x_i - \mu)(x_i - \mu)^T - \Sigma).
$$

The pure rank-$\mu$ CMA-ES can also be described in the IGO framework, see for example [ANOK10].

Proposition 27 (pure rank-$\mu$ CMA-ES as IGO). The pure rank-$\mu$ CMA-ES algorithm with sample size $N$, weights $w_i$, and learning rates $\eta_\mu = \eta_\Sigma = \delta t$ coincides with the IGO algorithm with sample size $N$, weights $w_i$, step size $\delta t$, and the parametrization $(\mu, \Sigma)$.

5.2 Twisting the metric

As we can see, the IGO framework does not allow to recover the learning rates for xNES and pure rank-$\mu$ CMA-ES, which is a problem, since usually, the covariance learning rate is set much smaller than the mean learning rate (see either [GSY+10] or [Han11]).

A way to recover these learning rates is to incorporate them directly into the metric (see also Blockwise GIGO, in Section 5.5). More precisely:

$$
\text{Tr}(M^T N) = \sum_{i,j=1}^{d} m_{ij} n_{ij} = \sum_{i=1}^{d} m_{ii} n_{ii} + \sum_{1 \leq i < j \leq d} m_{ij}(n_{ij} + n_{ji}) = 0, \quad (54)
$$

Md(\mathbb{R}), A^{-1}M \text{ symmetric},$ and that if $M$ is symmetric and $N$ is antisymmetric, then
Definition 28 (Twisted Fisher metric). Let $\eta_\mu, \eta_\Sigma \in \mathbb{R}$, and let $(P_\theta)_{\theta \in \Theta}$ be a family of normal probability distributions: $P_\theta = \mathcal{N}(\mu(\theta), \Sigma(\theta))$, with $\mu$ and $\Sigma$ $C^1$. We call “$(\eta_\mu, \eta_\Sigma)$-twisted Fisher metric” the metric defined by:

$$I_{i,j}(\eta_\mu, \eta_\Sigma)(\theta) = \frac{1}{\eta_\mu} \frac{\partial \mu^T}{\partial \theta_i} \Sigma^{-1} \frac{\partial \mu}{\partial \theta_j} + \frac{1}{\eta_\Sigma} \frac{1}{2} \text{tr} \left( \Sigma^{-1} \frac{\partial \Sigma}{\partial \theta_i} \Sigma^{-1} \frac{\partial \Sigma}{\partial \theta_j} \right).$$  \hspace{1cm} (55)

All the remainder of this section is simply a rewriting of the work in Section 1 with the twisted Fisher metric instead of the regular Fisher metric.

This approach seems to be somewhat arbitrary. Arguably, the mean and the covariance play a “different role” in the definition of a Gaussian (only the covariance can affect diversity, for example), but we lack a resasonable intrinsic characterization that would make this choice of twisting more natural. Moreover, this construction can be slightly generalized (see Appendix).

Still, we can define the corresponding Riemannian manifolds:

Notation 29. We denote by $G_d(\eta_\mu, \eta_\Sigma)$ (resp. $\tilde{G}_d(\eta_\mu, \eta_\Sigma)$) the manifold of Gaussian distributions (resp. Gaussian distributions with covariance matrix proportional to the identity) in dimension $d$, equipped with the $(\eta_\mu, \eta_\Sigma)$-twisted Fisher metric.

And the IGO flow and the IGO algorithms can be modified to take into account the twisting of the metric: the $(\eta_\mu, \eta_\Sigma)$-twisted IGO flow reads

$$\frac{d \theta^t}{dt} = I(\eta_\mu, \eta_\Sigma)^{-1}(\theta) \int_X W^f(\theta) \nabla \ln P_\theta(x) P_\theta(dx)$$  \hspace{1cm} (56)

This leads us to the twisted IGO algorithms.

Definition 30. The $(\eta_\mu, \eta_\Sigma)$-twisted IGO algorithm associated with parametri- sation $\theta$, sample size $N$, step size $\delta t$ and selection scheme $w$ is given by the following update rule:

$$\theta^{t+\delta t} = \theta^t + \delta t I(\eta_\mu, \eta_\Sigma)^{-1}(\theta^t) \sum_{i=1}^N \hat{w}_i \frac{\partial \ln P_\theta(x_i)}{\partial \theta}.$$  \hspace{1cm} (57)

Definition 31. The $(\eta_\mu, \eta_\Sigma)$-twisted geodesic IGO algorithm associated with sample size $N$, step size $\delta t$ and selection scheme $w$ is given by the following update rule:

$$\theta^{t+\delta t} = \exp_{\theta^t}(Y \delta t)$$  \hspace{1cm} (58)

where

$$Y = I(\eta_\mu, \eta_\Sigma)^{-1}(\theta^t) \sum_{i=1}^N \hat{w}_i \frac{\partial \ln P_\theta(x_i)}{\partial \theta}.$$  \hspace{1cm} (59)

By definition, the twisted geodesic IGO algorithm does not depend on the parametrisation$^{25}$.

$^{24}$The only difference with (9) is that $I^{-1}(\theta)$ has been replaced by $I(\eta_\mu, \eta_\Sigma)^{-1}(\theta)$.

$^{25}$Given that are working in $G_d(\eta_\mu, \eta_\Sigma)$, which is a “less canonical” manifold than $G_d$. 

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We can also notice that there is some redundancy between $\delta t$, $\eta$, and $\eta_\Sigma$: the only values actually appearing in the equations are $\delta t \eta_\mu$ and $\delta t \eta_\Sigma$. More formally:

**Proposition 32** (Obvious remark). Let $k, d, N \in \mathbb{N}$, $\eta_\mu, \eta_\Sigma, \delta t, \lambda_1, \lambda_2 \in \mathbb{R}$, and $w : [0; 1] \to \mathbb{R}$.

The $(\eta_\mu, \eta_\Sigma)$-twisted IGO algorithm with sample size $N$, step size $\delta t$, and selection scheme $w$ coincides with the $(\lambda_1 \eta_\mu, \lambda_2 \eta_\Sigma)$-twisted IGO algorithm with sample size $N$, step size $\lambda_2 \delta t$, and selection scheme $\frac{1}{\lambda_1 \lambda_2} w$. The same is true for geodesic IGO.

5.3 Algorithms after twisting

We now give all the algorithms mentioned earlier, but with the twisted Fisher metric. Except for Proposition 34, which is a simple calculation, the proofs of the following statements are an easy rewriting of their non-twisted counterparts: one can return to the non-twisted metric (up to a $\eta_\Sigma$ factor) by changing $\mu$ to $\sqrt{\frac{\mu}{\eta_\Sigma}} \mu$.

**Theorem 33.** If $\gamma : t \mapsto N(\mu(t), \sigma(t)^2 I)$ is a geodesic of $\tilde{G}_d(\eta_\mu, \eta_\sigma)$, then, there exists $a, b, c, d \in \mathbb{R}$ such that $ad - bc = 1$ and $v > 0$ such that

$$
\mu(t) = \mu(0) + \sqrt{\frac{2\eta_\mu}{\eta_\sigma}} \frac{v_0}{\|v_0\|} \tilde{r}(t), \quad \sigma(t) = \text{Im}(\gamma_C(t)), \quad \text{with } \tilde{r}(t) = \text{Re}(\gamma_C(t))
$$

where

$$
\eta = \eta(t) := aie^{\kappa t} + b,
$$

with

$$
\kappa := \frac{\sqrt{a^2 + b^2}}{c e^{\kappa t} + d}.
$$

**Proposition 34.** Let $n \in \mathbb{N}$, $v_\mu \in \mathbb{R}^n$, $v_\sigma$, $\eta_\mu$, $\eta_\sigma$, $\sigma_0 \in \mathbb{R}$, with $\sigma_0 > 0$.

Let $v_\tau := \|v_\mu\|$, $\lambda = \sqrt{\frac{2\eta_\mu}{\eta_\sigma}} v := \sqrt{\frac{\mu_0^2 + \sigma_0^2}{\sigma_0^2}}$, $M_0 := \frac{1}{\lambda} \frac{v_\mu}{v_\sigma}$, and $S_0 := \frac{v_\mu}{v_\sigma \sigma_0}$.

Let $\gamma_C(t) := \sigma_0 \frac{d e^{\kappa t} - c}{c e^{\kappa t} + d}$.

Then

$$
\gamma : t \mapsto N\left(\mu_0 + \lambda \frac{v_\mu}{\|v_\mu\|} \text{Re}(\gamma_C(t)), \text{Im}(\gamma_C(t))\right)
$$

is a geodesic of $\tilde{G}_n(\eta_\mu, \eta_\sigma)$ satisfying $\gamma(0) = (\mu_0, \sigma_0)$, and $\dot{\gamma}(0) = (v_\mu, v_\sigma)$.

**Theorem 35.** Let $\gamma : t \mapsto N(\mu(t), \Sigma(t))$ be a geodesic of $G_d(\eta_\mu, \eta_\Sigma)$. Then, the following quantities are invariant:

$$
J_\mu = \frac{1}{\eta_\mu} \Sigma^{-1}_t \dot{\mu}_t,
$$

$$
J_\Sigma = \Sigma^{-1}_t \left(\frac{1}{\eta_\mu} \dot{\mu}_t \mu_t^T + \frac{1}{\eta_\Sigma} \dot{\Sigma}_t\right).
$$

**Theorem 36.** If $\mu : t \mapsto \mu_t$ and $\Sigma : t \mapsto \Sigma_t$ satisfy the equations

$$
\dot{\mu}_t = \eta_\mu \Sigma_t J_\mu
$$

and

$$
\dot{\Sigma}_t = \eta_\Sigma \Sigma_t (J_\Sigma - J_\mu \mu_t^T) = \eta_\Sigma \Sigma_t J_\Sigma - \frac{\eta_\Sigma}{\eta_\mu} \dot{\mu}_t \mu_t^T,
$$

then...
where
\[ J_\mu = \frac{1}{\eta_\mu} \Sigma_0^{-1} \mu_0, \]
and
\[ J_\Sigma = \Sigma_0^{-1} \left( \frac{1}{\eta_\mu} \mu_0 \mu_0^T + \frac{1}{\eta_\Sigma} \dot{\Sigma}_0 \right). \]
then, \( t \mapsto \mathcal{N}(\mu_t, \Sigma_t) \) is a geodesic of \( \mathbb{G}_d(\eta_\mu, \eta_\Sigma) \).

**Theorem 37.** If \( \mu : t \mapsto \mu_t \) and \( A : t \mapsto A_t \) satisfy the equations
\[
\dot{\mu} = \eta_\mu A_t \dot{A}_t^T J_\mu, \\
\dot{A}_t = \frac{\eta_\Sigma}{2} (J_\Sigma - J_t \mu_t^T) T A_t,
\]
where
\[ J_\mu = \frac{1}{\eta_\mu} (A_0^{-1})^T A_0^{-1} \mu_0 \]
and
\[ J_\Sigma = (A_0^{-1})^T A_0^{-1} \left( \frac{1}{\eta_\mu} \mu_0 \mu_0^T + \frac{1}{\eta_\Sigma} \dot{A}_0 A_0^T + \frac{1}{\eta_\Sigma} A_0 \dot{A}_0^T \right), \]
then, \( t \mapsto \mathcal{N}(\mu_t, A_t A_t^T) \) is a geodesic of \( \mathbb{G}_d(\eta_\mu, \eta_\Sigma) \).

Notice that the equations found by twisting the metric are exactly the equations without twisting, except that we have “forced” the learning rates \( \eta_\mu, \eta_\Sigma \) to appear by multiplying the increments of \( \mu \) and \( \Sigma \) by \( \eta_\mu \) and \( \eta_\Sigma \).

**Proposition 38 (xNES as IGO).** The xNES algorithm with sample size \( N \), weights \( w_i \), and learning rates \( \eta_\mu = \eta_\Sigma \) coincides with the \( \eta_\mu, \eta_\Sigma \)-twisted IGO algorithm with sample size \( N \), weights \( w_i \), step size \( \delta t \), and in which, given the current position \( (\mu_t, A_t) \), the set of Gaussians is parametrized by
\[
(\delta, M) \mapsto \mathcal{N}\left(\mu_t + A_t \delta, A_t \exp(\frac{1}{2} M) \left(A_t \exp(\frac{1}{2} M) \right)^T\right),
\]
with \( \delta \in \mathbb{R}^m \) and \( M \in \text{Sym}(\mathbb{R}^m) \).

The parameters maintained by the algorithm are \( (\mu, A) \), and the \( x_i \) are sampled from \( \mathcal{N}(\mu, AA^T) \).

**Proposition 39 (pure rank-\( \mu \) CMA-ES as IGO).** The pure rank-\( \mu \) CMA-ES algorithm with sample size \( N \), weights \( w_i \), and learning rates \( \eta_\mu = \eta_\Sigma \) coincides with the \( \eta_\mu, \eta_\Sigma \)-twisted IGO algorithm with sample size \( N \), weights \( w_i \), step size \( \delta t \), and the parametrization \((\mu, \Sigma)\).

**Theorem 40.** Let \( \eta_\mu, \eta_\Sigma \in \mathbb{R}, \mu_0 \in \mathbb{R}^d, A_0 \in \text{GL}_d(\mathbb{R}), \) and \( (\mu_0, \Sigma_0) \in T_{\mathcal{N}(\mu_0, A_0 A_0^T)} \mathbb{G}_d \). Let
\[
h : \mathbb{G}_d \to \mathbb{G}_d, \\
\mathcal{N}(\mu, \Sigma) \mapsto \mathcal{N}(\sqrt{\frac{\eta_\mu}{\eta_\Sigma}} \mu, \Sigma),
\]
We denote by \( \phi \) (resp. \( \psi \)) the Riemannian exponential of \( \mathbb{G}_d \) (resp. \( \mathbb{G}_d(\eta_\mu, \eta_\Sigma) \)) at \( \mathcal{N}(\sqrt{\frac{\eta_\mu}{\eta_\Sigma}} \mu_0, A_0 A_0^T) \) (resp. \( \mathcal{N}(\mu_0, A_0 A_0^T) \)). We have:
\[
\psi(\mu_0, \Sigma_0) = h \circ \phi(\sqrt{\frac{\eta_\Sigma}{\eta_\mu}} \mu_0, \dot{\Sigma}_0)
\]
5.4 Trajectories of different IGO steps

As we have seen, two different IGO algorithms (or an IGO algorithm and the GIGO algorithm) coincide at first order in $\delta t$ when $\delta t \to 0$. In this section, we study the differences between pure rank-$\mu$ CMA-ES, xNES, and GIGO by looking at the second order in $\delta t$, and in particular, we show that xNES and GIGO do not coincide in the general case.

We view the updates done by one step of the algorithms as paths on the manifold $\mathbb{G}_d$, from $(\mu(t), \Sigma(t))$ to $(\mu(t + \delta t), \Sigma(t + \delta t))$, where $\delta t$ is the time step of our algorithms, seen as IGO algorithms. More formally:

**Definition 41.**

1. We call GIGO update trajectory the application $T_{\text{GIGO}}: (\mu, \Sigma, v_\mu, v_\Sigma) \mapsto \left( \delta t \mapsto \exp_{N(\mu, AA^T)}(\delta t\eta_\mu v_\mu, \delta t\eta_\Sigma v_\Sigma) \right)$.

   (exp is the exponential of the Riemannian manifold $\mathbb{G}_d(\eta_\mu, \eta_\Sigma)$)

2. We call xNES update trajectory the application $T_{\text{xNES}}: (\mu, \Sigma, v_\mu, v_\Sigma) \mapsto \left( \delta t \mapsto N(\mu + \delta t\eta_\mu v_\mu, AA^T + \delta t\eta_\Sigma v_\Sigma) \right)$, with $AA^T = \Sigma$. The application above does not depend on the choice of a square root $A$.

3. We call CMA update trajectory the application $T_{\text{CMA}}: (\mu, \Sigma, v_\mu, v_\Sigma) \mapsto \left( \delta t \mapsto N(\mu + \delta t\eta_\mu v_\mu, AA^T + \delta t\eta_\Sigma v_\Sigma) \right)$.

These applications map the set of tangent vectors to $\mathbb{G}_d(T\mathbb{G}_d)$ to the curves in $\mathbb{G}_d(\eta_\mu, \eta_\Sigma)$.

We will also use the following notation: $\mu_{\text{GIGO}} := \phi_\mu \circ T_{\text{GIGO}}$, $\mu_{\text{xNES}} := \phi_\mu \circ T_{\text{xNES}}$, $\mu_{\text{CMA}} := \phi_\mu \circ T_{\text{CMA}}$, $\Sigma_{\text{GIGO}} := \phi_\Sigma \circ T_{\text{GIGO}}$, $\Sigma_{\text{xNES}} := \phi_\Sigma \circ T_{\text{xNES}}$, and $\Sigma_{\text{CMA}} := \phi_\Sigma \circ T_{\text{CMA}}$, where $\phi_\mu$ (resp. $\phi_\Sigma$) extracts the $\mu$-component (resp. the $\Sigma$-component) of a curve.

For instance, $T_{\text{GIGO}}(\mu, \Sigma, v_\mu, v_\Sigma)(\delta t)$ gives the position (mean and covariance matrix) of the GIGO algorithm after a step of size $\delta t$, while $\mu_{\text{GIGO}}$ and $\Sigma_{\text{GIGO}}$ give respectively the mean component and the covariance component of this position.

This formulation ensures that the trajectories we are comparing had the same initial position and the same initial speed, which is the case provided the sampled values are the same.

Different IGO algorithms coincide at first order in $\delta t$. The following proposition gives the second order expansion of the trajectories of the algorithms.

**Proposition 42** (second derivatives of the trajectories). We have:

$$\mu_{\text{GIGO}}(\mu, \Sigma, v_\mu, v_\Sigma)'(0) = \eta_\mu \eta_\Sigma v_\Sigma \Sigma_0^{-1} v_\mu,$$

$$\mu_{\text{xNES}}(\mu, \Sigma, v_\mu, v_\Sigma)'(0) = \mu_{\text{CMA}}(\mu, \Sigma, v_\mu, v_\Sigma)'(0) = 0,$$

These “sampled values” are values directly sampled from $N(\mu, \Sigma)$, not from $N(0, I)$ and transformed.
\[
\Sigma_{\text{GIGO}}(\mu, \Sigma, v_\mu, v_\Sigma)'(0) = \eta^2 \Sigma v_\Sigma - \eta \eta v_\Sigma v_\mu^T,
\]
\[
\Sigma_{\text{xNES}}(\mu, \Sigma, v_\mu, v_\Sigma)'(0) = \eta^2 \Sigma v_\Sigma^{-1} v_\Sigma,
\]
\[
\Sigma_{\text{CMA}}(\mu, \Sigma, v_\mu, v_\Sigma)'(0) = 0.
\]

**Proof.** We can immediately see that the second derivatives of \(\mu_{\text{xNES}}, \mu_{\text{CMA}},\) and \(\Sigma_{\text{CMA}}\) are 0. Next, we have

\[
\Sigma_{\text{xNES}}(\mu, \Sigma, v_\mu, v_\Sigma)(t) = A \exp[t A^{-1} \eta \Sigma v_\Sigma (\Sigma^{-1} T)] A^T
\]
\[
= A A^T + t \eta \Sigma v_\Sigma + \frac{t^2}{2} \eta^2 \Sigma (A^{-1} T) A^{-1} v_\Sigma + o(t^2)
\]
\[
= \Sigma + t \eta \Sigma v_\Sigma + \frac{t^2}{2} \eta^2 \Sigma^{-1} v_\Sigma + o(t^2).
\]

The expression of \(\Sigma_{\text{xNES}}(\mu, \Sigma, v_\mu, v_\Sigma)'(0)\) follows.

Now, for GIGO, let us consider the geodesic starting at \((\mu_0, \Sigma_0)\) with initial speed \((\eta \mu, \eta \Sigma v_\Sigma)\). By writing \(J_\mu(0) = J_\mu(t)\), we find \(\dot{\mu}(t) = \Sigma(t) \Sigma_0^{-1} \dot{\mu}_0\). We then easily have \(\ddot{\mu}(0) = \Sigma_0 \Sigma_0^{-1} \dot{\mu}_0\). In other words

\[
\mu_{\text{GIGO}}(\mu, \Sigma, v_\mu, v_\Sigma)'(0) = \eta \mu \eta \Sigma v_\Sigma \Sigma_0^{-1} v_\mu.
\]

Finally, by using Theorem 19 and differentiating, we find

\[
\dot{\Sigma} = \eta \Sigma \dot{\Sigma}(J_\Sigma - J_\mu \mu^T) - \eta \Sigma J_\mu \dot{\mu}^T,
\]
\[
\dot{\Sigma}_0 = \eta \Sigma \dot{\Sigma}_0 \frac{1}{\eta \Sigma} \Sigma_0^{-1} \dot{\Sigma}_0 - \eta \Sigma \dot{\mu}_0 \dot{\mu}_0^T = \eta^2 \Sigma v_\Sigma \Sigma_0^{-1} v_\Sigma - \eta \Sigma \eta v_\mu v_\mu^T.
\]

In order to interpret these results, we will look at what happens in dimension 1.

In higher dimensions, we can suppose the algorithms exhibit a similar behavior, but an exact interpretation is more difficult for GIGO in \(\mathbb{G}_d\).

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27In higher dimensions, we can suppose the algorithms exhibit a similar behavior, but an exact interpretation is more difficult for GIGO in \(\mathbb{G}_d\).
• The geodesics of \( G_1 \) are half-circles (see Figure 2 below — we recall \( G_1 \) is the Poincaré half-plane). Consequently, if the mean is supposed to move (which always happens), then \( \sigma \to 0 \) when \( \delta t \to \infty \). For example, a step whose initial speed has no component on the standard deviation will always decrease it. See also Proposition 6.2 about the optimization of a linear function.

• For the same reason, for a given initial speed, the update of \( \mu \) always stays bounded as a function of \( \delta t \): it is not possible to make one step of the GIGO algorithm go further than a fixed point by increasing \( \delta t \). Still, the geodesic followed by GIGO changes at each step, so the mean of the overall algorithm is not bounded.

\[
\theta^t + \delta t
\]

Figure 2: One step of GIGO update

We now show that xNES follows the geodesics of \( G_d \) if the mean is fixed but that xNES and GIGO do not coincide otherwise.

Proposition 43 (xNES is not GIGO in the general case). Let \( \mu, v_\mu \in \mathbb{R}^d, A \in \text{GL}_d, v_\Sigma \in M_d \).

Then the GIGO and xNES updates starting at \( N(\mu, \Sigma) \) with initial speeds \( v_\mu \) and \( v_\Sigma \) follow the same trajectory if and only if the mean remains constant. In other words:

\[
T_{\text{GIGO}}(\mu, \Sigma, v_\mu, v_\Sigma) = T_{\text{xNES}}(\mu, \Sigma, v_\mu, v_\Sigma) \quad \text{if and only if} \quad v_\mu = 0.
\]

Proof. If \( v_\mu = 0 \), then we can compute the GIGO update by using Theorem 19 since \( J_\mu = 0, \hat{\mu} = 0, \) and \( \mu \) remains constant. Now, we have \( J_\Sigma = \Sigma^{-1} \hat{\Sigma} \): this is enough information to compute the update. Since this quantity is also preserved by the xNES algorithm (see for example the proof of Proposition 47), the two updates coincide.

If \( v_\mu \neq 0 \), then \( \Sigma_{\text{xNES}}(\mu, \Sigma, v_\mu, v_\Sigma)''(0) = \Sigma_{\text{GIGO}}(\mu, \Sigma, v_\mu, v_\Sigma)''(0) = \eta_\Sigma v_\mu v_\mu^T \neq 0 \), and in particular \( T_{\text{GIGO}}(\mu, \Sigma, v_\mu, v_\Sigma) \neq T_{\text{xNES}}(\mu, \Sigma, v_\mu, v_\Sigma) \).

5.5 Blockwise GIGO

Although xNES is not GIGO, it is possible to define a family of algorithms extending GIGO and including xNES, by decomposing our family of probability distributions as a product, and by following the restricted geodesics simultaneously.
Definition 44 (Splitting). Let \( \Theta \) be a Riemannian manifold. A splitting of \( \Theta \) is \( n \) manifolds \( \Theta_1, \ldots, \Theta_n \) and a diffeomorphism \( \Theta \cong \Theta_1 \times \cdots \times \Theta_n \). If for all \( x \in \Theta \), for all \( 1 \leq i < j \leq n \), we also have \( T_{i,x}M \perp T_{j,x}M \) as subspaces of \( T_xM \) (see Notation 45), then the splitting is said to be compatible with the Riemannian structure.

We now give some notation, and we define the blockwise GIGO update:

Notation 45. Let \( \Theta \) be a Riemannian manifold, \( \Theta_1, \ldots, \Theta_n \) a splitting of \( \Theta \), \( \theta = (\theta_1, \ldots, \theta_n) \in \Theta \), \( Y \in T_\theta \Theta \), and \( 1 \leq i \leq n \).

- We denote by \( \Theta_{\theta,i} \) the Riemannian manifold \( \{\theta_1\} \times \cdots \times \{\theta_{i-1}\} \times \Theta_i \times \{\theta_{i+1}\} \times \cdots \times \{\theta_n\} \), with the metric induced from \( \Theta \). There is a canonical isomorphism of vector spaces \( T_\theta \Theta = \bigoplus_{i=1}^n T_{\theta,i} \). Moreover, if the splitting is compatible, it is an isomorphism of Euclidean spaces.

- We denote by \( \Phi_{\theta,i} \) the exponential at \( \theta \) of the manifold \( \Theta_{\theta,i} \).

Definition 46 (Blockwise GIGO update). Let \( \Theta_1, \ldots, \Theta_n \) be a compatible splitting.

The blockwise GIGO algorithm in \( \Theta \) with splitting \( \Theta_1, \ldots, \Theta_n \) associated with sample size \( N \), step sizes \( \delta t_1, \ldots, \delta t_n \) and selection scheme \( w \) is given by the following update rule:

\[
\theta \leftarrow (\theta_1^{t+\delta t_1}, \ldots, \theta_n^{t+\delta t_n})
\]

where

\[
Y = I^{-1}(\theta^t) \sum_{i=1}^N \hat{w}_i \frac{\partial \ln P_\theta(x_i)}{\partial \theta},
\]

\[
\theta_i^{t+\delta t_i} = \Phi_{\theta,i}(\delta t_i Y_i),
\]

with \( Y_i \) the \( T_{\theta,i} \)-component of \( Y \). This update only depends on the splitting (and not on the parametrization inside each \( \Theta_i \)).

Since blockwise GIGO only depends on the splitting (since we make no other choice), it can be thought almost parameterization-invariant.

Notice that blockwise GIGO updates and twisted GIGO updates are two different things: firstly, blockwise GIGO can be defined on any manifold with a compatible splitting, whereas twisted GIGO (and twisted IGO) are only defined for Gaussians. But even in \( Gd(\eta_\mu, \eta_\Sigma) \), with the splitting \( (\mu, \Sigma) \), these two algorithms are different: for instance, if \( \eta_\mu = \eta_\Sigma \), and \( \delta t = 1 \) then the twisted GIGO is the regular GIGO algorithm, whereas blockwise GIGO is not (actually, we will prove that it is the xNES algorithm). The only thing blockwise GIGO and twisted GIGO have in common is that they are compatible with the \( (\eta_\mu, \eta_\Sigma) \)-twisted IGO flow.

We now have a new description of the xNES algorithm:

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28 If the Riemannian manifold is not ambiguous, we will simply write a compatible splitting.

29 If the splitting is not compatible, it is possible to define exactly the same algorithm, but it does not seem relevant.

30 Except the tunable parameters: sample size, step sizes, and selection scheme.

31 Maybe a more general form of twisted IGO could be defined.

32 As defined at the end of Section 1.3. A parameter \( \theta^t \) following these updates with \( \delta t \to 0 \) and \( N \to \infty \) is a solution of Equation 56.
Proposition 47 (xNES is a Blockwise GIGO algorithm). The Blockwise GIGO algorithm in $G_d$ with splitting $\Phi : N(\mu, \Sigma) \mapsto (\mu, \Sigma)$, sample size $N$, step sizes $\delta t_\mu, \delta t_\Sigma$ and selection scheme $w$ coincides with the xNES algorithm with sample size $N$, weights $w_i$, and learning rates $\eta_\mu = \delta t_\mu, \eta_\sigma = \delta t_\Sigma$.

Proof. Firstly, notice that the splitting $(\mu, \Sigma)$ is compatible, by Proposition 2.

Now, let us compute the Blockwise GIGO update: we have $G_d \sim R^d \times P_d$ where $P_d$ is the space of real positive definite matrices of dimension $d$. We have $\Theta_{\theta^t,1} = ([R^d \times \{\Sigma^t\}] \hookrightarrow G_d, \Theta_{\theta^t,2} = (\{\mu^t\} \times P_d) \hookrightarrow G_d$. The induced metric on $\Theta_{\theta^t,1}$ is the Euclidian metric, so we have

$$\mu \leftarrow \mu + \delta t_1 Y_\mu.$$ 

Since we have already shown (using the notation in Definition 23) that $Y_\mu = AG_\mu$ (in the proof of Proposition 24), we find

$$\mu \leftarrow \mu + \delta t_1 AG_\mu.$$ 

On $\Theta_{\theta^t,2}$, we have the following Lagrangian for the geodesics:

$$\mathcal{L}(\Sigma, \dot{\Sigma}) = \frac{1}{2} \text{tr}(\dot{\Sigma} \Sigma^{-1} \Sigma \Sigma^{-1}).$$

By applying Noether’s theorem, we find that

$$J_\Sigma = \Sigma^{-1} \dot{\Sigma}$$

is invariant along the geodesics of $\Theta_{\theta^t,2}$, so they are defined by the equation $\dot{\Sigma} = \Sigma J_\Sigma = \Sigma \Sigma^{-1} \Sigma_0$ (and therefore, any update preserving the invariant $J_\Sigma$ will satisfy this first-order differential equation and follow the geodesics of $\Theta_{\theta^t,2}$). The xNES update for the covariance matrix is given by $A(t) = A_0 \exp(tG_M/2)$. Therefore, we have $\dot{\Sigma}(t) = A_0 \exp(tG_M)A_0^T, \Sigma^{-1}(t) = (A_0^{-1})^T \Sigma \Sigma_0, \Sigma(t) = A_0 \exp(tG_M)G_M A_0^T, $ and finally $\Sigma^{-1}(t) \Sigma(t) = (A_0^{-1})^T G_M A_0^T = \Sigma^{-1}_0 \Sigma_0$. So xNES preserves $J_\Sigma$, and therefore, xNES follows the geodesics of $\Theta_{\theta^t,2}$.

Although blockwise GIGO is somewhat “less natural” than GIGO, it can be easier to compute for some splittings (as we have just seen), and in the case of the Gaussian distributions, the mean-covariance splitting seems natural.

Another advantage of blockwise GIGO is that it allows us to recover the learning rates without having to twist the metric, which felt like an ad-hoc solution. In particular, blockwise GIGO can be defined for families of probability distributions that are not Gaussian.

6 Numerical Experiments

We conclude this article with some numerical experiments to compare the behavior of GIGO, xNES and CMA-ES (we give the pseudocodes for these articles in the Appendix). We made two series of tests. The first one is a performance test, using classical benchmark functions, and the settings from [GSY+10].

33 Notice that we had already proven this in Proposition 43 since we are looking at the geodesics of $G_d$ with fixed mean.
goal of the second series of tests is to illustrate the computations in Section 5.4 by plotting the trajectories (standard deviation versus mean) of these three algorithms in dimension 1.

The source code is available at [https://www.lri.fr/~bensadon](https://www.lri.fr/~bensadon).

### 6.1 Benchmarking

For the first series of experiments, presented in Figure 3, we used the following parameters, taken from [GSY+10]:

- Varying dimension.
- Sample size: \([4 + 3 \log(d)]\)
- Weights: 
  \[
  w_i = \frac{\max(0, \log(\frac{n}{2} + 1) - \log(i)}{\sum_{j=1}^{N} \max(0, \log(\frac{n}{2} + 1) - \log(j))} - \frac{1}{N}
  \]
- IGO step size and learning rates: \(\delta t = 1, \eta_{\mu} = 1, \eta_{\Sigma} = \frac{3 + \log(d)}{d \sqrt{d}}\).
- Initial position: \(\theta^0 = N(x_0, I)\), where \(x_0\) is a random point of the circle with center 0, and radius 10.
- Euler method for GIGO: Number of steps: 100. We used the GIGO-A variant of the algorithm [34]

  - We chose not to use the exact expression of the geodesics for this benchmarking to show that having to use the Euler method is fine. However, we did run the tests, and the results are basically the same as GIGO-A.

We plot the median number of runs to achieve target fitness \((10^{-8})\). Each algorithm has been tested in dimension 2, 4, 8, 16, 32 and 64: a missing point means that all runs converged prematurely.

34No significant difference was noticed with GIGO-\(\Sigma\), or with the exact GIGO algorithm. The only advantage of having an explicit solution of the geodesic equations is that the update is quicker to compute.
Failed runs

In Figure 3, a point is plotted even if only one run was successful. Below is the list of the settings for which some runs converged prematurely.

- Only one run reached the optimum for the cigar-tablet function with CMA in dimension 8
- Seven runs (out of 24) reached the optimum for the Rosenbrock function with CMA in dimension 16
- About half the runs reached the optimum for the sphere function with CMA in dimension 4.

For the following settings, all runs converged prematurely.

- GIGO did not find the optimum of the Rosenbrock function in any dimension.
- CMA did not find the optimum of the Rosenbrock function in dimension 2, 4, 32 and 64.
- All the runs converged prematurely for the Cigar-tablet function in dimension 2 with CMA, for the Sphere function in dimension 2 for all algorithms, and for the Rosenbrock function in dimension 2 and 4 for all algorithms.

As the last item of the list above shows, all the algorithms converge prematurely in low dimension, probably because the covariance learning rate has been set too high (or because the sample size is too small). This is different from the results in [GSY+10].

This remark aside, as noted in [GSY+10], the xNES algorithm shows more robustness than CMA and GIGO: it is the only algorithm able to find the minimum of the Rosenbrock function in high dimensions. However, its convergence is consistently slower.

In terms of performance, when both of them work, CMA and GIGO are extremely close (GIGO is usually a bit better). An advantage of GIGO is that it is theoretically defined for any $\delta t$, $\eta_\Sigma$, whereas the covariance matrix maintained by CMA (not only pure rank-$\mu$ CMA) can stop being positive definite if $\eta_\Sigma \delta t > 1$. However, in that case, the GIGO algorithm is prone to premature convergence (remember Figure 2 and see Proposition 6.2 below), and learning rates that high are rarely used in practice.

---

35We recall that we use a simplified version of CMA (pure rank-$\mu$), that can be described in the IGO framework. It would be more accurate to call it “IGO in the parametrization ($\mu$, $\Sigma$)”.

30
From 2 to 64

\[ N = 4 + 3 \log(d) \]

\[ \frac{\max(0, \log(n^2 + 1) - \log(i))}{\sum_{j=1}^{d} \max(0, \log(n^2 + 1) - \log(j))} - \frac{1}{1} \]

\[(w_i)_{i \in [1, N]} \]

\[ \delta t = 1 \]

\[ \eta_{\mu} = 1 \]

\[ \frac{\sum_{i=1}^{d} x_i^2}{d} \sqrt{d} \]

\[ 3 + \log(d) \]

\[ \frac{3 + \log(d)}{d \sqrt{d}} \]

Euler step-size

\[ h = 0.01(100 \text{ steps}) \]

GIGO implementation

\[ \text{GIGO-A} \]

Sphere function

\[ x \mapsto \sum_{i=1}^{d} x_i^2 \]

\[ x \mapsto x_1^2 + \sum_{i=2}^{d-1} 10^4 x_i^2 + 10^8 x_d^2 \]

\[ x \mapsto \sum_{i=1}^{d-1} (100(x_i^2 - x_{i+1})^2 + (x_i - 1)^2) \]

Cigar-tablet

Dimension

Number of function calls to reach fitness $10^{-8}$. 

Figure 3: Median number of function calls to reach $10^{-8}$ fitness on 24 runs for: Sphere function, Cigar-tablet function and Rosenbrock function. Initial position $\theta^0 = N(x_0, I)$, with $x_0$ uniformly distributed on the circle of center 0 and radius 10. We recall that the “CMA-ES” algorithm here is using the so-called pure rank-$\mu$ CMA update.
6.2 Plotting trajectories in $G_1$

We want the second series of experiments to illustrate the remarks about the trajectories of the algorithms in Section 5.4, so we decided to take a large sample size to limit randomness, and we chose a fixed starting point for the same reason. We use the weights below because of the property of quantile improvement proved in [AO13]: the $1/4$-quantile will improve at each step. The parameters we used were the following:

- Sample size: $\lambda = 5000$
- Dimension 1 only.
- Weights: $w = 4, 1_{q\leq 1/4}$ ($w_i = 4, 1_{i\leq 1250}$)
- IGO step size and learning rates: $\eta_\mu = 1, \eta_\sigma = \frac{\frac{3}{5} + \log(d)}{\sqrt{d}} = 1.8$, varying $\delta t$.
- Initial position: $\theta^0 = N(10, 1)$
- Dots are placed at $t = 0, 1, 2 \ldots$ (except for the graph $\delta t = 1.5$, for which there is a dot for each step).

Figures 4 to 8 show the optimization of $x \mapsto x^2$, and Figures 9 to 11 show the optimization of $x \mapsto -x$.

Proposition 48. Let $d \in \mathbb{N}$, $k$, $\eta_\mu$, $\eta_\sigma \in \mathbb{R}_+^*$ let $w = k, 1_{q\leq q_0}$, and let

$$g : \mathbb{R}^d \to \mathbb{R}$$

$$x \mapsto -x_1$$

Let $\mu_n$ be the first coordinate of the mean, and let $\sigma_n^2$ be the variance (at step $n$) maintained by the $(\eta_\mu, \eta_\sigma)$-twisted geodesic IGO algorithm in $\tilde{G}_d$ associated with selection scheme $w$, sample size $\infty$, and step size $\delta t$, when optimizing $g$.

There exists $\delta t_{cr}$ such that:

- if $\delta t > \delta t_{cr}$, $(\sigma_n)$ converges to 0 with exponential speed, and $(\mu_n)$ converges.

\footnote{Notice that for $q_0 \geq 0.5$, the discussion is not relevant because in that case, even the IGO flow converges prematurely. Also compare with the critical $\delta t$ of smoothed cross entropy method, and IGO ML, in [OAAH11].}

\footnote{It has been proved in [OAAH11] that IGO algorithms are consistent with the IGO flow, i.e. they get closer and closer to the IGO flow as sample size tends to infinity. In other words

$$\lim_{N \to \infty} \sum_{i=1}^{N} w_i \frac{\partial \ln P_\theta(x_i)}{\partial \theta} = \nabla_\theta \int_X W_{\theta(x)} P_\theta(dx).$$

Sample size $\infty$ means we replace the IGO speed in the GIGO update by its limit for large $N$. In particular, it is not random.}
• if $\delta t = \delta t_{cr}$, $(\sigma_n)$ remains constant, and $(\mu_n)$ tends to $\infty$ with linear speed.

• if $0 < \delta t < \delta t_{cr}$, both $(\sigma_n)$ and $\mu_n$ tend to $\infty$ with exponential speed.

The proof and the expression of $\delta t_{cr}$ can be found in the Appendix.

In the case corresponding to $k = 4$, $n = 1$, $q_0 = 1/4$, $\eta_\mu = 1$, $\eta_\sigma = 1.8$, we find:

$$\delta t_{cr} \approx 0.84.$$  \hfill (72)
Figure 4: Trajectories of GIGO, CMA and xNES optimizing $x \mapsto x^2$ in dimension 1 with $\delta t = 0.01$, sample size 5000, weights $w_i = 4.1_{i \leq 1250}$ and learning rates $\eta_\mu = 1$, $\eta_\Sigma = 1.8$. One dot every 100 steps. All algorithms exhibit a similar behavior.

Figure 5: Trajectories of GIGO, CMA and xNES optimizing $x \mapsto x^2$ in dimension 1 with $\delta t = 0.1$, sample size 5000, weights $w_i = 4.1_{i \leq 1250}$ and learning rates $\eta_\mu = 1$, $\eta_\Sigma = 1.8$. One dot every 10 steps. All algorithms exhibit a similar behavior, differences start to appear. It cannot be seen on the graph, but the algorithm closest to zero after 400 steps is CMA ($\sim 1.10^{-16}$), followed by xNES ($\sim 6.10^{-16}$) and GIGO ($\sim 2.10^{-15}$).
Figure 6: Trajectories of GIGO, CMA and xNES optimizing $x \mapsto x^2$ in dimension 1 with $\delta t = 0.5$, sample size 5000, weights $w_i = 4.1_{i\leq 1250}$, and learning rates $\eta_\mu = 1$, $\eta_\Sigma = 1.8$. One dot every 2 steps. Stronger differences. Notice that after one step, the lowest mean is still GIGO ($\sim 8.5$, whereas xNES is around 8.75), but from the second step, GIGO has the highest mean because of the lower variance.

Figure 7: Trajectories of GIGO, CMA and xNES optimizing $x \mapsto x^2$ in dimension 1 with $\delta t = 1$, sample size 5000, weights $w_i = 4.1_{i\leq 1250}$, and learning rates $\eta_\mu = 1$, $\eta_\Sigma = 1.8$. One dot per step. The CMA-ES algorithm fails here, because at the fourth step, the covariance matrix is not positive definite anymore (It is easy to see that the CMA-ES update is always defined if $\delta t\eta_\Sigma < 1$, but this is not the case here). Also notice (see also Proposition 6.2) that at the first step, GIGO decreases the variance, whereas the $\sigma$-component of the IGO speed is positive.
Figure 8: Trajectories of GIGO, CMA and xNES optimizing $x \mapsto x^2$ in dimension 1 with $\delta t = 1.5$, sample size 5000, weights $w_i = 4.1_{i \leq 1250}$, and learning rates $\eta_\mu = 1$, $\eta_\Sigma = 1.8$. One dot per step. Same as $\delta t = 1$ for CMA, GIGO converges prematurely.

Figure 9: Trajectories of GIGO, CMA and xNES optimizing $x \mapsto -x$ in dimension 1 with $\delta t = 0.01$, sample size 5000, weights $w_i = 4.1_{i \leq 1250}$, and learning rates $\eta_\mu = 1$, $\eta_\Sigma = 1.8$. One dot every 100 steps. Almost the same for all algorithms.
Figure 10: Trajectories of GIGO, CMA and xNES optimizing \( x \to -x \) in dimension 1 with \( \delta t = 0.1 \), sample size 5000, weights \( w_i = 4.1_{i \leq 1250} \), and learning rates \( \eta_\mu = 1 \), \( \eta_\Sigma = 1.8 \). One dot every 10 steps. It is not obvious on the graph, but xNES is faster than CMA, which is faster than GIGO.

Figure 11: Trajectories of GIGO, CMA and xNES optimizing \( x \to -x \) in dimension 1 with \( \delta t = 1 \), sample size 5000, weights \( w_i = 4.1_{i \leq 1250} \), and learning rates \( \eta_\mu = 1 \), \( \eta_\Sigma = 1.8 \). One dot per step. GIGO converges, for the reasons discussed earlier.
Conclusion

We introduced the geodesic IGO algorithm and, we showed that in the case of Gaussian distributions, Noether’s theorem directly gives a first order equation satisfied by the geodesics. In terms of performance, the GIGO algorithm is similar to pure rank-µ CMA-ES, which is rather encouraging; it would be interesting to test GIGO on real problems. Moreover, GIGO is a reasonable and totally parametrization invariant algorithm, and as such, it should be studied for other families of probability distributions. Noether’s theorem could be a crucial tool for this.

We also showed that xNES and GIGO are not the same algorithm, and we defined Blockwise GIGO, a simple extension of the GIGO algorithm showing that xNES has a special status as it admits a definition which is “almost” parametrization-invariant.

---

38 Provided we can compute the solution of the equations of the geodesics.
39 Like Bernoulli distributions. However, in that case, the length of the geodesics is finite, and other problems arise.
Appendix

Proof of Proposition 6.2. Let us first consider the case \( k = 1 \).

When optimizing a linear function, the non-twisted IGO flow in \( \tilde{G}_d \) with the selection function \( w : q \mapsto 1_{q \leq q_0} \) is known [OAAH11], and in particular, we have:

\[
\mu_t = \mu_0 + \frac{\beta(q_0)}{\alpha(q_0)} \sigma_t,
\]

(73)

\[
\sigma_t = \sigma_0 \exp(\alpha(q_0)t),
\]

(74)

where, if we denote by \( N \) a random vector following a standard normal distribution, and \( F \) the cumulative distribution of a standard normal distribution,

\[
\alpha(q_0, d) = \frac{1}{2d} \int_{q_0}^{\infty} \frac{1}{u^2} \left( \int_{0}^{q_0} F^{-1}(u)^2 du - q_0 \right) du,
\]

(75)

and

\[
\beta(q_0) = \mathbb{E}(N^2 1_{N \leq F^{-1}(q_0)}).
\]

(76)

In particular, \( \alpha := \alpha(\frac{1}{4}, 1) \approx 0.107 \) and \( \beta := \beta(\frac{1}{4}) \approx -0.319 \).

With a minor modification of the proof in [OAAH11], we find that the \((\eta, \sigma)\)-twisted IGO flow is given by:

\[
\mu_t = \mu_0 + \frac{\beta(q_0)}{\alpha(q_0)} \sigma_0 \exp(\eta \mu \alpha(q_0)t),
\]

(77)

\[
\sigma_t = \sigma_0 \exp(\eta \sigma \alpha(q_0)t),
\]

(78)

Notice that Equation 77 shows that the assertions about the convergence of \((\sigma_n)\) immediately imply the assertions about the convergence of \((\mu_n)\).

Let us now consider a step of the GIGO algorithm: The twisted IGO speed is \( Y = (\eta \mu \beta \sigma_0, \eta \sigma \alpha \sigma_0) \), with \( \beta \sigma_0 > 0 \) (i.e. the variance should be increased).

Proposition 34 shows that the covariance at the end of the step is (using the same notation):

\[
\sigma(\delta t) = \sigma(0) \text{Im} \left( \frac{d e^{\nu \delta t} - c}{c e^{\nu \delta t} + d} \right) = \sigma(0) e^{\nu \delta t} (d^2 + c^2) =: \sigma(0) f(\delta t),
\]

(79)

and it is easy to see that \( f \) only depends on \( \delta t \) (and on \( q_0 \)). In other words, \( f(\delta t) \) will be the same at each step of the algorithm. The existence of \( \delta t_{cr} \) easily follows, and \( \delta t_{cr} \) is the positive solution of \( f(x) = 1 \).

After a quick computation, we find:

\[
\exp(\nu \delta t_{cr}) = \sqrt{1 + u^2} + 1
\]

(80)

where

\[
u := \sqrt{\frac{\eta_\mu \beta}{2 \eta \sigma \alpha}}
\]

(81)

\[40\text{This is where we need } q_0 < 0.5.\]

\[41\text{Also recall Figure 3 in Section 3.4.}\]
and
\[ v := \sqrt{\eta^2 \alpha^2 + \frac{\eta \mu \eta}{2n} \beta^2}. \] (82)

Finally, for \( w = k.1_{q \leq q_0} \), Proposition 32 shows that
\[ \delta t_{cr} = \frac{1}{k} \ln \left( \frac{\sqrt{1 + u^2} + 1}{\sqrt{1 + u^2} - 1} \right). \] (83)

\[ \square \]

**Generalization of the twisted Fisher metric**

The following definition is a more general way to introduce the twisted Fisher metric.

**Definition 49.** Let \( (\Theta, g) \) be a Riemannian manifold, \( (\Theta_1, g|_{\Theta_1}), \ldots, (\Theta_n, g|_{\Theta_n}) \) a splitting (as defined in Section 5.5) of \( \Theta \) compatible with the metric \( g \).

We call \( (\eta_1, \ldots, \eta_n) \)-twisted metric on \( (\Theta, g) \) for the splitting \( \Theta_1, \ldots, \Theta_n \) the metric \( g' \) on \( \Theta \) defined by \( g'|_{\Theta_i} = \frac{1}{\eta_i} g|_{\Theta_i} \) for \( 1 \leq i \leq n \).

**Proposition 50.** The \( (\eta_\mu, \eta_{\Sigma}) \)-twisted metric on \( \mathbb{G}_d \) with the Fisher metric for the splitting \( \mathcal{N}(\mu, \Sigma) \mapsto (\mu, \Sigma) \) coincides with the \( (\eta_\mu, \eta_{\Sigma}) \)-twisted Fisher metric from Definition 28.

**Proof.** It is easy to see that the \( (\eta_\mu, \eta_{\Sigma}) \)-twisted Fisher metric satisfies the condition in Definition 49. \( \square \)

**Pseudocodes**

For all algorithms

All studied algorithms have a common part, given here:

Variables: \( \mu, \Sigma \) (or \( A \) such that \( \Sigma = AA^T \)).

List of parameters: \( f: \mathbb{R}^d \to \mathbb{R}, \) step size \( \delta t, \) learning rates \( \eta_\mu, \eta_{\Sigma}, \) sample size \( \lambda, \) weights \( (w_i)_{i \in [1, \lambda]}, \) \( N \) number of steps for the Euler method, \( r \) Euler step size reduction factor (for GIGO-\( \Sigma \) only).

Notice that we always need a square root \( A \) of \( \Sigma \) to sample the \( x_i, \) but the decomposition \( \Sigma = AA^T \) is not unique. Two different decompositions will give two algorithms such that one is a modification of the other as a stochastic process: same law (the \( x_i \) are abstractly sampled from \( \mathcal{N}(\mu, \Sigma) \)), but different trajectories (for given \( z_i \), different choices for the square root will give different \( x_i, \) see also footnote 22 in Section 5.1.1). For GIGO-\( \Sigma, \) since we have to invert the covariance matrix, we used the Cholesky decomposition (\( A \) lower triangular). Usually, in CMA-ES, the square root of \( \Sigma (\Sigma = AA^T, A \) symmetric) is used.

\[ \text{42} \] We recall that the other implementation directly maintains a square root of \( \Sigma. \)
Algorithm 1 For all algorithms

\[ \mu \leftarrow \mu_0 \]

if The algorithm updates \( \Sigma \) directly then
\[ \Sigma \leftarrow \Sigma_0 \]
Find some \( A \) such that \( \Sigma = AA^T \)
else (The algorithm updates a square root \( A \) of \( \Sigma \))
\[ A \leftarrow A_0 \]
\[ \Sigma = AA^T \]
end if

while NOT (Termination criterion) do
for \( i = 1 \) to \( \lambda \) do
\[ z_i \sim \mathcal{N}(0, I) \]
\[ x_i = Az_i + \mu \]
end for
Compute the IGO initial speed (included in the algorithms below)
Update the mean and the covariance (the updates are Algorithms [2 to 6])
end while
Updates

When describing the different updates, $\mu$, $\Sigma$, $A$, the $x_i$ and the $z_i$ are those defined in Algorithm 1.

For Algorithm 2 (GIGO-$\Sigma$), when the covariance matrix after one step is not positive definite, we compute the update again, with a step size divided by $r$ for the Euler method.

Algorithm 2 GIGO Update, one step, updating the covariance matrix

1. Compute the IGO speed:
   \[
   v_\mu = A \sum_{i=1}^{\lambda} w_i z_i,
   \]
   \[
   v_\Sigma = A \sum_{i=1}^{\lambda} w_i (z_i z_i^T - I) A^T.
   \]

2. Compute the Noether invariants:
   \[
   J_\mu \leftarrow \Sigma^{-1} v_\mu,
   \]
   \[
   J_\Sigma \leftarrow \Sigma^{-1} (v_\mu^T \mu + v_\Sigma).
   \]

3. Solve numerically the equations of the geodesics:
   Unhappy $\leftarrow$ true
   $\mu_0 \leftarrow \mu$
   $\Sigma_0 \leftarrow \Sigma$
   $k = 0$
   while Unhappy do
     $\mu \leftarrow \mu_0$
     $\Sigma \leftarrow \Sigma_0$
     $h \leftarrow \delta t / (N r^k)$
     for $i = 1$ to $N r^k$ do
       $\mu \leftarrow \mu + h n_{\mu} \Sigma J_\mu$
       $\Sigma \leftarrow \Sigma + h n_{\Sigma} (J_\Sigma - J_\mu \mu^T)$
     end for
     if $\Sigma$ positive definite then
       Unhappy $\leftarrow$ false
     end if
     $k \leftarrow k + 1$
   end while
   return $\mu$, $\Sigma$

42 We have no reason to recommend any particular value of $r$, the only constraint is $r > 1.$
Algorithm 3 GIGO Update, one step, updating a square root of the covariance matrix

1. Compute the IGO speed:
   \[ v_\mu = A \sum_{i=1}^{\lambda} w_i z_i, \]
   \[ v_\Sigma = A \sum_{i=1}^{\lambda} w_i (z_i z_i^T - I) A^T. \]

2. Compute the Noether invariants:
   \[ J_\mu \leftarrow \Sigma^{-1} v_\mu, \]
   \[ J_\Sigma \leftarrow \Sigma^{-1} (v_\mu \mu + v_\Sigma). \]

3. Solve numerically the equations of the geodesics:
   \[ h \leftarrow \delta t/N \]
   \[ \text{for } i = 1 \text{ to } N \text{ do} \]
   \[ \mu \leftarrow \mu + h \eta_\mu A A^T J_\mu \]
   \[ A \leftarrow A + \frac{h}{2} \eta_\Sigma (J_\Sigma - J_\mu \mu^T) A \]
   \[ \text{end for} \]
   return \( \mu, A \)
Algorithm 4 Exact GIGO, one step. Not exactly our implementation, see the discussion after Corollary 22.

1. Compute the IGO speed:
   \[ v_\mu = A \sum_{i=1}^{\lambda} w_i z_i, \]
   \[ v_\Sigma = A \sum_{i=1}^{\lambda} w_i (z_i z_i^T - I) A^T. \]

2. Learning rates
   \[ \lambda \leftarrow \sqrt{\eta_\Sigma}, \]
   \[ \mu \leftarrow \lambda \mu, \]
   \[ v_\mu \leftarrow \eta_\mu \lambda v_\mu, \]
   \[ v_\Sigma \leftarrow \eta_\Sigma v_\Sigma. \]

3. Intermediate computations.
   \[ G^2 \leftarrow A^{-1} \left( v_\Sigma (A^{-1})^T A^{-1} + 2 v_\mu v_\mu^T \right) (A^{-1})^T \]
   \[ C_1 \leftarrow \text{ch} \left( \frac{G}{2} \right) \]
   \[ C_2 \leftarrow \text{sh} \left( \frac{G}{2} \right) G^{-1} \]
   \[ R \leftarrow \left( (C_1^{-1} v_\Sigma (A^{-1})^T C_2)^{-1} \right)^T \]

4. Actual update
   \[ \mu \leftarrow \mu + 2 A R C_2 A^{-1} v_\mu \]
   \[ A \leftarrow A R \]

5. Return to the “real” \( \mu \)
   \[ \mu \leftarrow \frac{\mu}{\lambda} \]
   \[ \text{return } \mu, A \]

Algorithm 5 xNES update, one step

1. Compute \( G_\mu \) and \( G_M \) (equivalent to the computation of the IGO speed):
   \[ G_\mu = \sum_{i=1}^{\lambda} w_i z_i \]
   \[ G_M = \sum_{i=1}^{\lambda} w_i (z_i z_i^T - I) \]

2. Actual update:
   \[ \mu \leftarrow \mu + \eta_\mu AG_\mu \]
   \[ A \leftarrow A + A \exp(\eta_\Sigma G_M / 2) \]

\[ \text{return } \mu, A \]
Algorithm 6 pure rank-$\mu$ CMA-ES update, one step

1. Computation of the IGO speed:

   \[ v_\mu = \sum_{i=1}^{\lambda} w_i (x_i - \mu) \]

   \[ v_\Sigma = \sum_{i=1}^{\lambda} w_i \left( (x_i - \mu)(x_i - \mu)^T - \Sigma \right) \]

2. Actual update:

   \[ \mu \leftarrow \mu + \eta_v v_\mu \]

   \[ \Sigma \leftarrow \Sigma + \eta_\Sigma v_\Sigma \]

   return \( \mu, \Sigma \)
Algorithm 7 GIGO in $\mathcal{G}_d$, one step

1. Compute the IGO speed:
\[
Y_\mu = \sum_{i=1}^{\lambda} w_i (x_i - \mu)
\]
\[
Y_\sigma = \sum_{i=1}^{\lambda} w_i \left( \frac{(x_i - \mu)^T (x_i - \mu)}{2d\sigma} - \frac{\sigma}{2} \right)
\]
2. Better parametrization:
\[
\lambda := \sqrt{\frac{2d\eta}{\mu}}
\]
\[
v_r := \frac{\eta}{\lambda} ||Y_\mu||
\]
\[
v_\sigma := \eta Y_\sigma
\]
3. Find $a, b, c, d, v$ corresponding to $\mu, \sigma, \dot{\mu}, \dot{\sigma}$:
\[
v = \sqrt{\frac{v_r^2 + v_\sigma^2}{\sigma^2}}
\]
\[
S_0 := \frac{v_r}{v_\sigma^2}
\]
\[
M_0 := \frac{\sigma}{v_\sigma^2}
\]
\[
C := \sqrt{S_0^2 + M_0^2} - S_0
\]
\[
D := \sqrt{S_0^2 + M_0^2 + S_0^2}
\]
\[
c := \sqrt{C}
\]
\[
d := \sqrt{D}
\]
4. Actual Update:
\[
z := \frac{\sigma d e^{i\omega t} - c}{c e^{i\omega t} + d}
\]
\[
\mu := \mu + \lambda \text{Re}(z) \frac{Y_\mu}{||Y_\mu||}
\]
\[
\sigma := \text{Im}(z)
\]
\textbf{return} $\mu, \sigma$
References

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