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Glasmachers, Tobias; Krause, Oswin

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Convergence Analysis of the Hessian Estimation Evolution Strategy

Tobias Glasmachers
Institute for Neural Computation, Ruhr-University Bochum, Germany
tobias.glasmachers@ini.rub.de

Oswin Krause
Department of Computer Science, University of Copenhagen, Denmark
oswin.krause@di.ku.dk

Abstract

The class of algorithms called Hessian Estimation Evolution Strategies (HE-ESs) update the covariance matrix of their sampling distribution by directly estimating the curvature of the objective function. The approach is practically efficient, as attested by respectable performance on the BBOB testbed, even on rather irregular functions.

In this paper we formally prove two strong guarantees for the (1+4)-HE-ES, a minimal elitist member of the family: stability of the covariance matrix update, and as a consequence, linear convergence on all convex quadratic problems at a rate that is independent of the problem instance.

1 Introduction

The theoretical analysis of state-of-the-art variable metric Evolution Strategies (ESs) is a long-standing open problem in evolutionary computation. While simple step-size adaptive ESs without Covariance Matrix Adaptation (CMA) have been analyzed with good success [Jägersküpper 2006, Akimoto et al. 2018, Morinaga and Akimoto 2019], we are still lacking appropriate tools for rigorously proving stability and convergence of variable metric methods like CMA-ES [Hansen and Ostermeier 2001].

Most theoretical work on the rigorous analysis of evolution strategies focuses on simple ESs without CMA. Notable early work in this area was conducted by Jägersküpper [2006], who proved linear convergence of the (1+1)-ES with 1/5 success rule on convex quadratic functions with a progress rate of $O\left(\frac{1}{d\kappa(H)}\right)$, which translates into the runtime growing linearly with problem dimension $d$ and the problem difficulty. Here, problem difficulty is measured by the conditioning $\kappa(H)$ (quotient of largest and smallest eigenvalue) of the Hessian $H$ of a quadratic objective function. Akimoto et al. [2018] proved a similar result restricted to the sphere function but providing explicit runtime bounds with drift theory methods [Doerr et al. 2011]. That result was the basis of the much stronger result of Morinaga and Akimoto [2019], which establishes linear convergence of the (1+1)-ES on a large (non-parametric) class of problems, namely on $L$-smooth strongly convex functions.
The analysis of modern variable-metric ESs like CMA-ES and its many variants is significantly less developed. In particular, no (linear) convergence guarantees exist, mostly for the lack of proofs of stability of the CMA update. One significant approach to the problem is the Information Geometric Optimization (IGO) framework (Ollivier et al., 2017). It allows to interpret the so-called rank-\(\mu\) update of CMA-ES as a stochastic natural gradient step (Akimoto et al., 2010). This means that stability and convergence can be established provided the learning rate is small enough. However, the learning rates used in practice do not fulfill this condition, and hence establishing stability remains an open problem.

For non-evolutionary variable-metric methods the situation is mixed. For example, to the best of our knowledge, there does not exist an analysis showing that the classic Nelder-Mead simplex algorithm converges to the minimum of a convex quadratic function at a rate that is independent of the conditioning number. Restricted results exist in low dimensions (Lagarias et al., 2012). On the other hand, Powell’s NEWUOA method (Powell, 2008) can jump straight into the optimum once it has obtained enough samples to estimate the coefficients of the quadratic function exactly. The variable metric random pursuit algorithm of Stich et al. (2016) is of particular interest in our context, since it is conceptually close to evolutionary computation methods and at the same time provides a provably stable update that allows the covariance matrix to converge to the inverse Hessian.

In this paper we prove the stability of an alternative CMA mechanism, namely the recently proposed Hessian Estimation Evolution Strategy (HE-ES). To this end we introduce a minimal elitist variant of HE-ES and prove monotone convergence of its covariance matrix to a multiple of the inverse Hessian of a convex quadratic objective function. Informally speaking, we mean by stability that the covariance matrix does not drift arbitrarily far away from the inverse Hessian. Our result is stronger, since we prove that the covariance matrix converges monotonically to a multiple of the inverse Hessian. As a consequence we are able to transfer existing results on the convergence of simple ESs on the sphere function to HE-ES. This way we obtain a strong guarantee, namely linear convergence of our HE-ES variant at a rate that is independent of the conditioning number of the problem at hand.

The paper is organized as follows. We first introduce HE-ES and define the (1+4)-HE-ES as a minimal elitist variant. This algorithm is the main subject of our subsequent study. The next step is to show the stability and the convergence of the HE-ES covariance matrix update to the inverse Hessian of a quadratic objective function. We finally leverage the analysis of Morinaga and Akimoto (2019) to show linear convergence of (1+4)-HE-ES at a rate that is independent of the problem difficulty \(\kappa(H)\).

# 2 Hessian Estimation Evolution Strategies

The Hessian Estimation Evolution Strategy (HE-ES) is a recently proposed variable metric evolution strategy (Glasmachers and Krause, 2020). Its main characteristic is its mechanism for adapting the sampling covariance matrix. In this section we first present the original algorithm and then introduce a novel elitist variant.

## 2.1 The HE-ES Algorithm

HE-ES is a modern evolution strategy. It features non-elitist selection, global weighted recombination, cumulative step-size adaptation, and a special mechanism for covariance matrix adaptation.
Most of these mechanisms coincide with the design of standard CMA-ES \cite{Hansen2001}. In the following presentation we focus on the non-standard aspects of the algorithm, following \cite{Glasmachers2020}.

In each iteration, HE-ES draws a number of mirrored samples of the form $x_i^- = m - \sigma \cdot A b_i$ and $x_i^+ = m + \sigma \cdot A b_i$, where $\sigma > 0$ is the global step size and $A$ is a Cholesky factor of the covariance matrix $C = A^T A$. For brevity we write $x_i^\pm$, with $\pm$ representing either $+ \text{ or } -$. The vectors $b_i$ are drawn from the multi-variate Gaussian distribution $\mathcal{N}(0, I)$. Furthermore, the vectors $b_i$ are orthogonal, i.e., they fulfill $b_i^T b_j = 0$ for $i \neq j$. We also consider the normalized directions $\frac{b_i}{\|b_i\|}$ in the following.

The three points $x_i^-, m, x_i^+$ are arranged on a line, and restricted to each such line, the function values in these points give rise to the quadratic model

$$q_i(t) = c + g_i t + \frac{h_i}{2} t^2 \approx f \left( m + t \cdot A \frac{b_i}{\|b_i\|} \right)$$

of the objective function. Fitting its coefficients to the function values yields the offset $c = f(m)$, the gradient $g_i = \frac{f(x_i^+) - f(x_i^-)}{2\|b_i\|}$, and the Hessian $h_i = \frac{f(x_i^+) + f(x_i^-) - 2f(m)}{\sigma^2 \|b_i\|^2}$. The coefficients $h_i$ measure the curvature of the graphs of the quadratic models $q_i$. They are of particular interest in the following.

The intuition behind this construction is as follows: Each $h_i$ is a finite difference estimate of a diagonal coefficient of the Hessian matrix $H$. This is strictly true if $b_i$ is parallel to an axis of the coordinate system. Otherwise, $h_i$ contains exactly the same type of information, but not referring to an axis and a corresponding diagonal entry, but to an arbitrary direction $b_i$. Therefore, estimating the modes $q_i$ and $h_i$ in particular allows HE-ES to obtain curvature information about the problem, and more specifically, information about the Hessian of a quadratic objective function.

The goal of HE-ES is to adapt its sampling covariance matrix $C$ towards a multiple of the inverse of the Hessian $H$ of a convex quadratic objective function

$$f(x) = \frac{1}{2}(x - x^*)^T H(x - x^*) + f^*$$

(1)

with global optimum $x^*$, optimal value $f^*$, and strictly positive definite symmetric Hessian $H$. Its covariance matrix update therefore updates $C$ in direction $b_i$ (measured by $\frac{b_i^T}{\|b_i\|} C \frac{b_i}{\|b_i\|}$) towards a multiple of $H^{-1}$ (measured by $\alpha \cdot \frac{b_i^T}{\|b_i\|} H^{-1} \frac{b_i}{\|b_i\|}$). This corresponds to learning a good shape of the multi-variate normal distribution, while we leave learning of its position to the mean update, and learning of its global scale to the step size update. In other words, adapting to the (arbitrary) scaling factor $\alpha > 0$ is left to step size update, which usually operates at a faster time scale (larger learning rate) than covariance matrix adaptation.

Since the scaling factor $\alpha$ is arbitrary, a meaningful update can only change different components of $C$ relative to each other. Say, if

$$h_i \cdot \frac{b_i^T}{\|b_i\|} C \frac{b_i}{\|b_i\|} \gg h_j \cdot \frac{b_j^T}{\|b_j\|} C \frac{b_j}{\|b_j\|},$$

(2)

then the variance in direction $b_i$ should be reduced while the variance in direction $b_j$ should be increased. This way, HE-ES keeps the scale of its sampling distribution (measured by $\det(C)$)
fixed. If we fully trust the data and the model, i.e., when minimizing a noise-free quadratic function, then equalizing left-hand-side and right-hand-side of inequality (2) is the optimal (greedy) update step.

**Algorithm 1:** Hessian Estimation Evolution Strategy (HE-ES)

1: **input** \( m^{(0)} \in \mathbb{R}^d, \sigma^{(0)} > 0, A^{(0)} \in \mathbb{R}^{d \times d} \)
2: **parameters** \( \tilde{\lambda} \in \mathbb{N}, c_s, d_s, w \in \mathbb{R}^{2\tilde{\lambda}} \)
3: \( B \leftarrow \lfloor \tilde{\lambda}/d \rfloor \)
4: \( p_s^{(0)} \leftarrow 0 \in \mathbb{R}^d \)
5: \( g_s^{(0)} \leftarrow 0 \)
6: \( t \leftarrow 0 \)
7: **repeat**
8: **for** \( j \in \{1, \ldots, B\} \) **do**
9: \( b_{ij}, \ldots, b_{dj} \leftarrow \text{sampleOrthogonal}() \)
10: \( x_{ij} \leftarrow m^{(t)} - \sigma^{(t)} \cdot A^{(t)} b_{ij} \) for \( i + (j - 1)B \leq \tilde{\lambda} \)
11: \( x_{ij}^+ \leftarrow m^{(t)} + \sigma^{(t)} \cdot A^{(t)} b_{ij} \) for \( i + (j - 1)B \leq \tilde{\lambda} \) # mirrored sampling
12: \( A^{(t+1)} \leftarrow A^{(t)} \cdot \text{computeG}(\{b_{ij}\}, f(m), \{f(x_{ij}^+)\}, \sigma) \) # matrix adaptation
13: \( w^\pm_{ij} \leftarrow w_{\rank(f(x_{ij}^+))} \)
14: \( m^{(t+1)} \leftarrow \sum_{ij} w_{ij}^+ \cdot x_{ij}^+ \) # mean update
15: \( g_s^{(t+1)} \leftarrow (1 - c_s)^2 \cdot g_s^{(t)} + c_s \cdot (2 - c_s) \)
16: \( p_s^{(t+1)} \leftarrow (1 - c_s) \cdot p_s^{(t)} + \sqrt{c_s \cdot (2 - c_s) \cdot \mu_{\text{mirrored}}^{\text{mean}}} \cdot \sum_{ij} (w_{ij}^+ - w_{ij}^-) \cdot b_{ij} \)
17: \( \sigma^{(t+1)} \leftarrow \sigma^{(t)} \cdot \exp \left( \frac{c_s}{d_s} \cdot \left[ \frac{\|p_{ij}^{(t+1)}\|}{\chi_d^2} - \sqrt{g_s^{(t+1)}} \right] \right) \) # CSA
18: \( t \leftarrow t + 1 \)
19: **until** stopping criterion is met

**Algorithm 2:** sampleOrthogonal

1: **input** dimension \( d \)
2: \( z_1, \ldots, z_d \sim \mathcal{N}(0, I) \)
3: \( n_1, \ldots, n_d \leftarrow \|z_1\|, \ldots, \|z_d\| \)
4: apply the Gram-Schmidt procedure to \( z_1, \ldots, z_d \)
5: return \( y_i = n_i \cdot z_i, \quad i = 1, \ldots, d \)

Algorithm 1 provides an overview of the resulting HE-ES algorithm. It is designed to be conceptually close to CMA-ES, using multi-variate Gaussian samples and cumulative step-size adaptation (CSA, Hansen and Ostermeier 2001). One difference is the use of orthogonal mirrored samples (see algorithm 2). If there are more directions than dimensions (the population size \( \lambda \) exceeds \( 2d \)) then multiple independent blocks of orthogonal samples are used. The core update mechanism discussed above is realized in algorithm 3 applied to the Cholesky factor \( A \) of the covariance matrix \( C = A^T A \). Since practical objective functions are hardly exactly quadratic, the algorithm dampens update steps with a learning rate and limits the impact of non-positive curvature estimates (\( h_i \leq 0 \)). A further notable property of HE-ES is its correction for mirrored samples.
Algorithm 3: computeG

1: input $b_{ij}$, $f(m)$, $f(x_{ij}^\pm)$, $\sigma$
2: parameters $\kappa$, $\eta_A$
3: $h_{ij} \leftarrow \frac{f(x_{ij}^+) + f(x_{ij}^-) - 2f(m)}{\sigma^2 \|b_{ij}\|^2}$  # estimate curvature along $b_{ij}$
4: if $\max(\{h_{ij}\}) \leq 0$ then return I
5: $c \leftarrow \max(\{h_{ij}\})/\kappa$
6: $h_{ij} \leftarrow \max(h_{ij}, c)$  # truncate to trust region
7: $q_{ij} \leftarrow \log(h_{ij})$
8: $q_{ij} \leftarrow q_{ij} - \frac{1}{\kappa} \cdot \sum_{ij} q_{ij}$  # subtract mean → ensure unit determinant
9: $q_{ij} \leftarrow q_{ij} \cdot \frac{-\eta_A}{2}$  # learning rate and inverse square root (exponent $-1/2$)
10: $q_{i,B} \leftarrow 0 \quad \forall i \in \{dB - \tilde{\lambda}, \ldots, 0\}$  # neutral update in the unused directions
11: return $\frac{1}{2} \sum_{ij} \frac{\exp(q_{ij})}{\|b_{ij}\|^2} \cdot b_{ij}b_{ij}^T$

sampling in CSA, which removes a bias that is otherwise present in the method (Glasmachers and Krause, 2020). We do not discuss these additional mechanisms in detail, since they do not play a role in the subsequent analysis.

It was demonstrated by Glasmachers and Krause (2020) that HE-ES shows excellent performance on many problems, including some highly rugged and non-convex functions, which strongly violate the assumption of a quadratic model. However, for the sake of a tractable analysis, we restrict ourselves to objective functions of the form given in equation (1). In general, quadratic functions should not be optimized with HE-ES; for example, NEWUOA is a more suitable method for this type of problem. The relevance of the function class lies in the fact that in the late phase of convergence, every twice continuously differentiable objective function is well approximated by its second order Taylor polynomial around the optimum, which is of the form (1).

2.2 A Minimal Elitist HE-ES

In this section we design a minimal variant of the HE-ES family. For the sake of a tractable analysis, we aim at simplicity in the algorithm design, and at mechanisms that allow us to leverage existing analysis techniques, but without losing the main characteristics of a variable-metric ES, and of course without changing the covariance matrix adaptation principle. Several similarly reduced models exists for CMA-ES, for example the (1+1)-CMA-ES (Igel et al., 2007), natural evolution strategies (NES) (Wierstra et al., 2014), and the matrix-adaptation ES (MA-ES) of Beyer and Sendhoff (2017). HE-ES already implements most of the simplifying elements of MA-ES. Our main means of breaking down the algorithm therefore is to design an elitist variant.

For HE-ES, a naive (1+1) selection scheme is not meaningful, for two reasons: mirrored samples always come in pairs, and HE-ES always needs to sample at least two directions, so it can assess relative curvatures. Therefore, the minimal scheme proposed here is the (1+4)-HE-ES. In each generation, it draws two random orthogonal directions and generates four mirrored samples. To keep the algorithm as close as possible to the (1+1)-ES used by Akimoto et al. (2018) and Morinaga and Akimoto (2019), we will only consider one sample for updating $m(t)$ and $\sigma(t)$ and use a variant of the classic $1/5$-rule (Rechenberg, 1973; Kern et al., 2004). Thus the 3 additional samples drawn in each iteration are only used for updating $A(t)$. Removing line 8 (the covariance
Algorithm 4: (1+4)-HE-ES

1: **input** $m(0) \in \mathbb{R}^d$, $\sigma(0) > 0$, $A(0) \in \mathbb{R}^{d \times d}$, $c_\sigma > 1$
2: $t \leftarrow 0$
3: repeat
4: \hspace{1em} $b_1, \ldots, b_d \leftarrow \text{sampleOrthogonal}()$
5: \hspace{1em} $x^-_i \leftarrow m(t) - \sigma(t) \cdot A(t)b_i$ for $i \in \{1, 2\}$ # mirrored sampling
6: \hspace{1em} $x^+_i \leftarrow m(t) + \sigma(t) \cdot A(t)b_i$ for $i \in \{1, 2\}$ # evaluate the four offspring
7: \hspace{1em} $f^\pm_i \leftarrow f(m(t))$ # matrix adaptation
8: \hspace{1em} $A(t+1) \leftarrow A(t) \cdot \text{computeG}\{\{b_i\}, f(m(t)), \{f^\pm_i\}, \sigma(t)\}$
9: \hspace{1em} if $f^+_1 \leq f(m(t))$ then
10: \hspace{2em} $m(t+1) \leftarrow x^+_1$ # mean update using the first sample
11: \hspace{2em} $\sigma(t+1) \leftarrow \sigma(t) \cdot c_\sigma$ # increase step size (1/5 rule)
12: \hspace{1em} else
13: \hspace{2em} $\sigma(t+1) \leftarrow \sigma(t) \cdot c_\sigma^{-1/4}$ # decrease step size (1/5 rule)
14: \hspace{1em} $t \leftarrow t + 1$
15: until stopping criterion is met

matrix update) of Algorithm 4 and fixing $A(0) = I$ leads to what we refer to as the (1+1)-ES.

The resulting (1+4)-HE-ES is given in Algorithm 4. We find its adaptation behavior to be comparable to the full HE-ES on convex quadratic problems. Due to its minimal population size it cannot implement an increasing population (IPOP) scheme, which limits its performance on highly multi-modal problems. However, it otherwise successfully maintains the character of the full HE-ES algorithm.

In the subsequent analysis we focus on noise-free convex quadratic objective functions. In this situation Algorithm 3 is simplified as follows: the check for a negative definite Hessian in line 4 can be dropped. Equally well, the trust region mechanism in lines 5 and 6 is superfluous. Finally, we can afford a learning rate of $\eta_A = 1$. With $h_1$ and $h_2$ as defined in line 3, we find that the simplified algorithm returns the matrix

$$G = I + \left(4 \frac{\sqrt{h_1}}{h_2} - 1\right) \frac{b_1 b_1^T}{\|b_1\|^2} + \left(4 \frac{\sqrt{h_2}}{h_1} - 1\right) \frac{b_2 b_2^T}{\|b_2\|^2}, \quad (3)$$

where $I$ is the identity matrix. The update modifies the factor $A$ only in directions $b_1$ and $b_2$ and leaves the orthogonal subspace unchanged.

### 2.3 Relation to other Algorithms

There are a few approaches in the literature that adapt the covariance matrix based on Hessian information. Most closely related to our approach are variable-metric random pursuit algorithms by Stich et al. (2016). Here, a search-direction $b_1$ is sampled uniformly on a sphere with radius $\|b_1\| = \epsilon$ and the matrix is updated as:

$$C(t+1) = C(t) + \left(h_1 - \frac{b_1^T C(t) b_1}{\|b_1\|^2}\right) \frac{b_1 b_1^T}{\|b_1\|^2}.$$
It is easy to show that for this update holds

$$\frac{b_1^T C^{(t+1)} b_1}{\|b_1\|^2} = h_1,$$

i.e., the update learns the exact curvature of the problem in direction $b_i$, assuming that $\epsilon$ is small enough or the function is quadratic.

Another relevant algorithm is BOBYQA (Powell, 2009). Instead of using local curvature approximation, the algorithm keeps track of a set of $m$ points $x_i$, $i = 1, \ldots, m$ with function values $f(x_i)$. In each iteration, the algorithm estimates the Hessian $\hat{H}^{(t+1)} = (C^{(t+1)})^{-1}$ by minimizing

$$\min_{c, g, \hat{H}^{(t+1)}} \|\hat{H}^{(t+1)} - \hat{H}^{(t)}\|_F$$

s.t.

$$\frac{1}{2} x_i^T \hat{H}^{(t+1)} x_i + g^T x_i + c = f(x_i), \ i = 1, \ldots, m \quad (5)$$

Thus, it fits a quadratic function on the selected points under the condition that the approximation $\hat{H}$ of the Hessian is as similar as possible to the one used in the previous iteration. Given a set of $m = (n + 1)(n + 2)/2$ points on a quadratic function, the algorithm is capable of learning the exact Hessian.

In contrast to our proposed method, both mentioned algorithms do not constrain the covariance matrix or the Hessian matrix to be positive definite. While Stich et al. (2016) handle the case that an update can lead to a non-zero eigenvalue, they still assume that the correct estimate of the curvature is positive. Thus, a negative curvature of the underlying function can lead to a break-down of the method. In contrast, BOBYQA allows for negative curvature and instead of sampling from a normal distribution, a trust-region problem is solved.

3 Stability and Convergence of the Covariance Matrix

In the following we consider the (1+4)-HE-ES as introduced in the previous section. Our aim is to show the stability and the monotonic convergence of its covariance matrix to a multiple of the inverse Hessian of a convex quadratic function.

We use the following notation. Let $m \in \mathbb{R}^d$, $\sigma > 0$, and $A \in \text{SL}^\pm(d, \mathbb{R})$ denote the parameters of the current sampling distribution $N(m, \sigma^2 C)$ with $C = A^T A$. Here $\text{SL}^\pm(d, \mathbb{R})$ denotes the group of $d \times d$ matrices with determinant $\pm 1$, which is closely related to the special linear group $\text{SL}(d, \mathbb{R})$. We obtain $\det(C) = 1$, hence the covariance matrix $C \in \text{SL}(d, \mathbb{R})$ is an element of the special linear group. In the following, we assume $d \geq 2$.

In order to clarify the goals of this section we start by defining stability and convergence of the covariance matrix.

**Definition 1.** Consider the space of positive definite symmetric $d \times d$ matrices, equipped with a pre-metric $\delta$ (a symmetric, non-negative function fulfilling $\delta(x, x) = 0$). Let $(C_t)_{t \in \mathbb{N}}$ be a sequence of matrices, and let $R$ denote a reference matrix. We define the scale-invariant distance $\delta_R(C) = \min_{s > 0} \delta(s \cdot C, R)$ of $C$ from $R$. 
1. We call the sequence \((C_t)_{t \in \mathbb{N}}\) stable up to scaling if there exist constants \(t_0\) and \(\varepsilon > 0\) such that \(\delta_R(C_t) < \varepsilon\) for all \(t > t_0\).

2. We say that \((C_t)_{t \in \mathbb{N}}\) converges to \(R\) up to scaling if \(\lim_{t \to \infty} \delta_R(C_t) = 0\).

3. We call the convergence monotonic if \(t \mapsto \delta_R(C_t)\) is a monotonically decreasing sequence.

It is obvious that (monotonic) convergence up to scaling implies stability up to scaling for all \(\varepsilon > 0\). In the following, the reference matrix is always the inverse Hessian \(H^{-1}\).

### 3.1 Invariance Properties

In this section we formally establish the invariance properties of HE-ES. The analysis is not specific to a particular variant and hence applies also to the (1+4)-HE-ES. We start by showing that the HE-ES is invariant to affine transformations of the search space.

**Lemma 2.** Let \(g(x) = Mx + b\) be an invertible affine transformation. Consider the state trajectory

\[
\left( m^{(t)}, \sigma^{(t)}, A^{(t)} \right)_{t \in \mathbb{N}}
\]

of HE-ES or (1+4)-HE-ES applied to the objective function \(f\), and alternatively the state trajectory

\[
\left( \tilde{m}^{(t)}, \tilde{\sigma}^{(t)}, \tilde{A}^{(t)} \right)_{t \in \mathbb{N}}
\]

of the same algorithm with initial state

\[
\left( \tilde{m}^{(0)}, \tilde{\sigma}^{(0)}, \tilde{A}^{(0)} \right) = \left( g(m^{(0)}), \sigma^{(0)}, MA^{(0)} \right)
\]

applied to the objective function \(\tilde{f}(x) = f(g^{-1}(x))\). Assume further, that both algorithms use the same sequence of random vectors \(\left( b^{(t)}_{1,1}, \ldots, b^{(t)}_{B,d} \right)_{t \in \mathbb{N}}\). Then it holds that

\[
\left( \tilde{m}^{(t)}, \tilde{\sigma}^{(t)}, \tilde{A}^{(t)} \right) = \left( g(m^{(t)}), \sigma^{(t)}, MA^{(t)} \right)
\]

for all \(t \in \mathbb{N}\).

**Proof.** The straightforward proof is inductive. The base case \(t = 0\) holds by assumption, see equation (8). Assume that the assertion in equation (9) holds for some value of \(t\). In iteration \(t\) the HE-ES and (1+4)-HE-ES applied to \(\tilde{f}\) generate the offspring

\[
\tilde{x}^\pm_i = \tilde{m}^{(t)} \pm \tilde{\sigma}^{(t)} \cdot \tilde{A}^{(t)} b_i^{(t)}
\]

\[
= g(m^{(t)}) \pm \sigma^{(t)} \cdot MA^{(t)} b_i^{(t)}
\]

\[
= g \left( m^{(t)} \pm \sigma^{(t)} \cdot A^{(t)} b_i^{(t)} \right)
\]

\[
= g(x_i^\pm) .
\]
This identity immediately implies
\[ \tilde{f}(\tilde{x}_i^\pm) = f\left(g^{-1}(\tilde{x}_i^\pm)\right) = f\left(g^{-1}\left(g(x_i^\pm)\right)\right) = f(x_i^\pm), \] (11)
as well as
\[ \tilde{f}(\tilde{m}(t)) = f(m(t)), \]
with the same logic. Therefore the procedure computeG is called by both algorithms with the exact same parameters and we hence obtain the same matrix $G$ for the original and for the transformed problem. We conclude
\[ \tilde{A}^{(t+1)} = \tilde{A}^{(t)} G = M A^{(t)} G = M A^{(t+1)}. \]
Due to equation \ref{eq:11} it holds that $m^{(t+1)} = m^{(t)} \iff \tilde{m}^{(t+1)} = \tilde{m}^{(t)}$. If the means change then they are replaced with the point $\tilde{x}_i^+$ for (1+4)-ES, and with convex combinations $\sum_i w_i x_i^\pm$ and $\sum_i w_i \tilde{x}_i^\pm$ for the original non-elitist HE-ES. Obviously, the first case is a special case of the second one. Hence it holds that
\[ \tilde{m}(t+1) = \sum_i w_i \tilde{x}_i^+ = \sum_i w_i g(x_i^+) = g(m^{t+1}) \]
according to equation \ref{eq:10}. Equation \ref{eq:11} also guarantees that the step sizes are multiplied with the same factor $\delta$, since both CSA and the $1/5$-rule are rank-based methods. We obtain
\[ \tilde{\sigma}^{(t+1)} = \delta \cdot \tilde{\sigma}^{(t)} = \delta \cdot \sigma^{(t)} = \sigma^{(t+1)}. \]
We have shown that all three components of the tuples in equation \ref{eq:9} coincide for $t + 1$. \hfill \square

Affine invariance is an important property for handling non-separable ill-conditioned problems. HE-ES shares this invariance property with CMA-ES.

Next we turn to invariance to transformations of objective function values. A significant difference between HE-ES and CMA-ES is that the former is not invariant to monotonically increasing transformations of fitness values, while the latter is: let $h : \mathbb{R} \to \mathbb{R}$ be a strictly monotonically increasing function, then CMA-ES minimizes $h \circ f$ the same way as $f$. HE-ES has the same property only for affine transformations $h(t) = at + b$, $a > 0$. It can be argued that in many situations a first order Taylor approximation (which is affine) of the transformation is good enough, but it is understood that this argument has limitations. Affine invariance of function values is formalized by the following lemma.

**Lemma 3.** Consider the state trajectory
\[ \left( m^{(t)}, \sigma^{(t)}, A^{(t)} \right)_{t \in \mathbb{N}} \] (12)
of HE-ES or (1+4)-HE-ES applied to the objective function $f$, and alternatively the state trajectory
\[ \left( \tilde{m}^{(t)}, \tilde{\sigma}^{(t)}, \tilde{A}^{(t)} \right)_{t \in \mathbb{N}} \] (13)
of the same algorithm with initial state
\[ \left( \tilde{m}^{(0)}, \tilde{\sigma}^{(0)}, \tilde{A}^{(0)} \right) = \left( m^{(0)}, \sigma^{(0)}, A^{(0)} \right) \] (14)
applied to the objective function $\tilde{f}(x) = a \cdot f(x) + b$, $a > 0$. Then it holds that
\[ \left( \tilde{m}^{(t)}, \tilde{\sigma}^{(t)}, \tilde{A}^{(t)} \right) = \left( m^{(t)}, \sigma^{(t)}, A^{(t)} \right) \] (15)
for all $t \in \mathbb{N}$. 

9
Proof. Due to $a > 0$ the transformation $h(t) = at + b$ is strictly monotonically increasing and hence preserves the order (ranking) of objective values. HE-ES and its variants are fully rank-based up to their covariance matrix update. Therefore most operations on $f$ and $h \circ f$ are exactly the same, even for general strictly monotonic transformations $h$. Procedure 3 needs a closer investigation. In the curvature estimates $h_{i,j}$ computed in line 3 the offset $b$ cancels out, while the factor $a$ enters linearly. It also enters linearly into the cutoff threshold $c$ computed in line 5, and hence in the truncation in line 6. It is then transformed into the summand $\log(a)$ for $g_{i,j}$ in line 7, which is removed in line 8 when subtracting the mean. We conclude that Procedure 3 is invariant to affine transformations of function values.

Affine invariance in effect means that it suffices to analyze HE-ES in an arbitrary coordinate system. For example, setting $g(x) = A^{-1}(x - m)$ we can transform the problem so that at the beginning of an iteration it holds that $m = 0$ and $A = C = I$. This reparameterization trick was first leveraged by Glasmachers et al. (2010) and used by Krause and Glasmachers (2015) and by Beyer and Sendhoff (2017). Alternatively we can transform the objective function into a simpler form, as discussed in the next section. In general we cannot achieve both at the same time.

3.2 Informal Discussion of the Covariance Matrix Update

Before we proceed with our analysis, we provide an intuition on the effect of the covariance matrix update of HE-ES. Consider a general convex quadratic objective function as given in equation (1), with symmetric and strictly positive definite Hessian $H$. In contrast, HE-ES actually achieves the above goal: its covariance matrix converges to the inverse Hessian, which is hence approximated to arbitrarily high precision. We note that in practice this difference does not matter, since a realistic black-box objective function is hardly exactly quadratic. This improved stability of the update, however, is what makes the subsequent matrix adaptation is to generate a sequence $(A(t))_{t \in \mathbb{N}}$ fulfilling

$$C(t) = (A(t))^T A(t) \xrightarrow{t \to \infty} I,$$

for all initial states $A(0)$. Due to random fluctuations and a non-vanishing learning rate, CMA-ES does not fully achieve this goal. Instead its covariance matrix keeps fluctuating around the inverse Hessian. In contrast, HE-ES actually achieves the above goal: its covariance matrix converges to the inverse Hessian, which is hence approximated to arbitrarily high precision. We note that in practice this difference does not matter, since a realistic black-box objective function is hardly exactly quadratic. This improved stability of the update, however, is what makes the subsequent analysis tractable.

Let $b_1, b_2 \sim \mathcal{N}(0, I)$ be the Gaussian random vectors sampled in the current generation of (1+4)-HE-ES, and define their normalized counterparts $u_i = b_i / \| b_i \|$. Note that by construction the directions are orthogonal: $b_1^T b_2 = 0 = u_1^T u_2$. We consider the four offspring

$$x_i^+ = m + \sigma \cdot Ab_i \quad \text{and} \quad x_i^- = m - \sigma \cdot Ab_i \quad \text{for} \quad i \in \{1, 2\}$$

forming two pairs of mirrored samples. From the corresponding function values we estimate the curvatures

$$h_i = \frac{f(x_i^+) + f(x_i^-) - 2f(m)}{\sigma^2 \cdot \| b_i \|^2} = u_i^T \bar{A}^T HAu_i. \quad (16)$$
We have seen above that thanks to affine invariance we can transform any convex quadratic objective function into the sphere function with Hessian $H = I$, without loss of generality. We stick to this choice from here on.

For another informal argument (which will be made precise below) we restrict the problem to the subspace $V$. In that subspace we use $u_1$ and $u_2$ as coordinate axes, so the components of the following two-dimensional vectors and matrices refer to that coordinate system. This immediately implies $u_1 = (1, 0)^T$ and $u_2 = (0, 1)^T$. We then deal with the $2 \times 2$ matrices

$$A = \begin{pmatrix} a_{11} & a_{21} \\ a_{12} & a_{22} \end{pmatrix} \quad \text{and} \quad G = \begin{pmatrix} \gamma_1 & 0 \\ 0 & \gamma_2 \end{pmatrix}.$$ 

It is due to the specific choice of the basis that the matrix $G$ is diagonal.

It then becomes apparent that at the core of the update the $(1+4)$-HE-ES alters the variance in the directions $u_1$ and $u_2$, disregarding the inherent structure of the covariance matrix (e.g., its eigenbasis). A related perspective is taken in methods for solving extremely large linear
Figure 1: Adaptation of an initially isotropic covariance matrix $C$ (illustrated as a circular iso-density curve) towards an ellipsoidal objective function (family of ellipsoidal level lines) in the two-dimensional subspace spanned by $u_1$ and $u_2$. The resulting covariance matrix $C'$ exhibits elliptic iso-density curves. The update changes $C$ into $C'$ along the directions $u_1$ and $u_2$. The different extents of the ellipses are illustrated by the dashed bounding boxes, which change from an initial square into a rectangle of equal area. The bounding box of the iso-density line of $C'$ is defined by the four (marked) intersections of the “coordinate axes” spanned by $u_1$ and $u_2$ with a level set of the objective function. It is clearly visible that the update does not learn the problem structure in a single step. Still, the resulting iso-density curve is closer to the level sets than the original iso-density curve. If $u_1$ and $u_2$ happen to be principal axes of the level set ellipsoids, then the adaptation is completed in a single step.
systems, where the problem can often be simplified through preconditioning [Van der Vorst 2003 Chapter 13]. Changing $A$ into $A' = A \cdot G$ can be understood as a measure for improving the conditioning of the problem, which is the same as decreasing the spread of the eigenvalues of $C$. The effect on $C' = G \cdot C \cdot G$ is two-sided preconditioning with the same matrix $G$. A diagonal preconditioner $G$ is among the simplest choices. In our analysis it arises naturally through the very definition of the $(1+4)$-HE-ES.

A commonly agreed upon measure of problem hardness and of the spread of the eigenvalues is the conditioning number, which is the quotient of largest divided by the smallest eigenvalue. In general, absolute values of eigenvalues are considered, however, for the covariance matrix $C$ all eigenvalues are positive. Taking this perspective, we would like to show that the conditioning number of $C' = (A')^T A' = GA^T AG = GCG$ is smaller than or equal to the conditioning number of $C$, and that it is strictly smaller most of the time. Sticking to our two-dimensional view established above we can solve the eigenequation analytically by finding the zeros of the characteristic polynomial. It holds that

$$C = A^T A = \begin{pmatrix} a_{11}^2 + a_{12}^2 & a_{11}a_{21} + a_{12}a_{22} \\ a_{11}a_{21} + a_{12}a_{22} & a_{21}^2 + a_{22}^2 \end{pmatrix} = \begin{pmatrix} c_{11} & c_{12} \\ c_{12} & c_{22} \end{pmatrix}$$

and equation [16] yields $h_i = c_{ii}$. The eigenvalues of $C$ are the zeros of its characteristic polynomial

$$p_C(\lambda) = \det(\lambda \cdot I - C)$$

$$= (\lambda - c_{11})(\lambda - c_{22}) - c_{12}^2$$

$$= \lambda^2 - (c_{11} + c_{22})\lambda + c_{11}c_{22} - c_{12}^2$$

$$= \lambda^2 - \text{tr}(C)\lambda + \det(C)$$ .

We obtain the (real) eigenvalues $\lambda_{1/2} = \frac{\text{tr}(C)}{2} \pm \sqrt{\frac{\text{tr}(C)^2}{4} - \det(C)}$ and the conditioning number

$$\kappa(C) = \frac{\frac{\text{tr}(C)}{2} + \sqrt{\frac{\text{tr}(C)^2}{4} - \det(C)}}{\frac{\text{tr}(C)}{2} - \sqrt{\frac{\text{tr}(C)^2}{4} - \det(C)}} = 1 + \frac{1 - 4\frac{\det(C)}{\text{tr}(C)^2}}{1 - \frac{\text{tr}(C)}{\text{tr}(C)^2}} \quad (18)$$

It holds that $\det(G) = 1$ by construction, which implies $\det(C') = \det(C)$. With this property it is easy to see from equation [18] that the conditioning number $\kappa$ is a strictly monotonically increasing function of $\text{tr}(C)$. In the following we will therefore consider the goal of minimizing $\text{tr}(C)$ while keeping $\det(C)$ fixed. The minimizer of $\text{tr}(C)$ is a multiple of the identity matrix, which is indeed our adaptation goal. Therefore, independent of the monotonic relation to the condition number in the two-dimensional case, minimizing the trace of $C$ is justified as a covariance matrix adaptation goal in its own right. For a general Hessian this goal translates into minimizing $\text{tr}(H \cdot C)$ while keeping $\det(C)$ fixed, which is equivalent to adapting $C$ towards a multiple of $H^{-1}$. This construction is compatible with Definition [1] using the trace to construct the pre-metric

$$\delta(A, B) = \text{tr} \left( \frac{A}{\sqrt{\det(A)}} \cdot \frac{B^{-1}}{\sqrt{\det(B^{-1})}} \right) - d.$$
The following lemma computes the change of the trace induced by a single update step.

**Lemma 4.** For a matrix $A \in \text{GL}(d, \mathbb{R})$ and two orthonormal vectors $u_1, u_2 \in \mathbb{R}^d$ (fulfilling $\|u_i\| = 1$ and $u_1^T u_2 = 0$) we define the following quantities:

\[
C = A^T A, \quad h_i = u_i^T C u_i, \quad \gamma_i = \left( \frac{h_1 h_2}{h_i^2} \right)^{1/4},
\]

\[
G = I + \sum_{i=1}^{2} (\gamma_i - 1) u_i u_i^T, \quad A' = AG, \quad C' = (A')^T A' = GCG.
\]

It holds that $\det(C') = \det(C) > 0$ and

\[
\text{tr}(C) - \text{tr}(C') = h_1 + h_2 - 2\sqrt{h_1 h_2} \geq 0.
\]

**Proof.** The proof is elementary. Our first note is that $C$ is strictly positive definite, which implies $h_i > 0$ and $\gamma_i > 0$. We choose vectors $u_1, \ldots, u_d$ so that $u_1, \ldots, u_d$ form an orthonormal basis of $\mathbb{R}^d$. We collect these vectors as columns in the orthogonal matrix $U$. We then represent the matrix $C$ as an array of coefficients in the above basis:

\[
U^T C U = \begin{pmatrix}
c_{11} & c_{21} & \cdots & c_{1d} \\
c_{12} & c_{22} & \cdots & c_{2d} \\
\vdots & \vdots & \ddots & \vdots \\
c_{1d} & c_{2d} & \cdots & c_{dd}
\end{pmatrix}.
\]

In this basis the matrix $G$ has a particularly simple form:

\[
U^T G U = \begin{pmatrix}
\gamma_1 & 0 & 0 & \cdots & 0 \\
0 & \gamma_2 & 0 & \cdots & 0 \\
0 & 0 & \gamma_3 & \cdots & 0 \\
0 & 0 & 0 & \cdots & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
0 & 0 & 0 & 0 & \gamma_d
\end{pmatrix}.
\]

From $\gamma_1 \gamma_2 = 1$ we obtain $\det(U^T G U) = \det(G) = 1$, which immediately implies the first claim $\det(C') = \det(C)$. We compute the product $C' = GCG$ in the basis $U$ as follows: $U^T C' U = U^T GCG U = (U^T G U)(U^T C U)(U^T G U)$. We obtain the components

\[
U^T C' U = \begin{pmatrix}
\gamma_1^2 c_{11} & \gamma_1 \gamma_2 c_{21} & \gamma_1 c_{31} & \gamma_1 c_{41} & \cdots & \gamma_1 c_{d1} \\
\gamma_1 \gamma_2 c_{12} & \gamma_2^2 c_{22} & \gamma_2 c_{32} & \gamma_2 c_{42} & \cdots & \gamma_2 c_{d2} \\
\gamma_1 c_{13} & \gamma_2 c_{23} & c_{33} & c_{34} & \cdots & c_{3d} \\
\gamma_1 c_{14} & \gamma_2 c_{24} & c_{34} & c_{44} & \cdots & c_{4d} \\
\vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\
\gamma_1 c_{1d} & \gamma_2 c_{2d} & c_{3d} & c_{4d} & \cdots & c_{dd}
\end{pmatrix}.
\]

It holds that $\text{tr}(U^T C U) = \text{tr}(C)$ and $\text{tr}(U^T C' U) = \text{tr}(C')$ due to invariance of the trace under changes of the coordinate system. Our target quantity $\text{tr}(C) - \text{tr}(C')$ is hence the difference of the sums of the diagonals of the above computed matrices $U^T C U$ and $U^T C' U$, which amounts to

\[
c_{11} + c_{22} - \gamma_1^2 c_{11} - \gamma_2^2 c_{22}.
\]
Using $c_{ii} = u_i^T C u_i = h_i$ we obtain $\gamma_i^2 c_{ii} = \sqrt{h_1 h_2}$ for $i \in \{1, 2\}$. This immediately yields $\text{tr}(C^t) - \text{tr}(C) = h_1 + h_2 - 2\sqrt{h_1 h_2}$. The right hand side is never negative because the arithmetic average of two positive numbers is never smaller than their geometric average.

The lemma shows that the trace never increases due to a covariance matrix update, no matter how the offspring are sampled. This is a strong guarantee for the stability of the update. In contrast, the update of CMA-ES can move the covariance matrix arbitrarily far away from its target. Although large deviations happen with extremely small probability, the probabilistic nature of its stability as an unbounded Markov chain (Auger 2005) significantly complicates the analysis. With $(1+4)$-HE-ES we are in the comfortable situation of monotonic improvements, which is somewhat analogous to analyzing algorithms with elitist selection.

We have established that for $H = I$ the sequence $\text{tr}(C(t))$ is monotonically decreasing. With fixed determinant $\det(C(t)) = D$ it is bounded from below by $d\sqrt{D}$, hence it converges due to the monotone convergence theorem. In the general setting, using affine invariance, this translates into monotone decrease of the sequence $\text{tr}(C(t)H)$.

### 3.4 Convergence of the Covariance Matrix to the Inverse Hessian

It is left to show that the trace indeed converges to its lower bound, which implies convergence of $C(t)$ to a multiple of $H^{-1}$. We are finally in the position to guarantee this property.

**Theorem 5.** Let $A(t)$ denote the sequence of transformation matrices of $(1+4)$-HE-ES when optimizing a convex quadratic function with strictly positive definite symmetric Hessian $H$. We define the sequence of covariance matrices $C(t) := (A(t))^T A(t)$. Then with full probability it holds that

$$\lim_{t \to \infty} C(t) = \alpha \cdot H^{-1} \quad \text{with} \quad \alpha = d\sqrt{\det(C(0)) \cdot \det(H)} .$$

**Proof.** The proof is based on topological arguments and drift. For technical reasons and for ease of notation, and importantly without loss of generality, we restrict ourselves to the case $\det(C(t)) = 1$, $H = I$, and hence $\alpha = 1$.

Under the constraint $\det(C) = 1$ the function $\text{tr}(C)$ attains its minimum $\text{tr}(I) = d$ at the unique minimizer $C = I$. Consider a fixed covariance matrix $C$ and random vectors $u_1, u_2$. According to Lemma 4 the function

$$\Delta_C(u_1, u_2) = u_1^T C u_1 + u_2^T C u_2 - 2\sqrt{u_1^T C u_1 \cdot u_2^T C u_2} \geq 0$$

computes the single-step reduction of the trace when sampling in directions $u_1$ and $u_2$. The function is analytic in $C$ and in $u_i$, and for $C \neq I$ it is non-constant in $u_i$, hence it is zero only on a set of measure zero with respect to the random variables $u_1, u_2$. We conclude that in expectation over $u_1$ and $u_2$ it holds that

$$\mathbb{E}[\Delta_C] > 0 \quad \forall C \neq I .$$

In the next step we exploit the continuity of the function $C \mapsto \mathbb{E}[\Delta_C]$.

We fix a “quality” level $\rho = \text{tr}(C)$. In other words, for a given suboptimal level $\rho > d$ we consider an arbitrary covariance matrix $C$ fulfilling $\text{tr}(C) = \rho$ and $\det(C) = 1$. The set

$$\text{tr}^{-1}(\rho) = \{C \in \text{SL}(d, \mathbb{R}) \mid \text{tr}(C) = \rho\}$$
is compact: being the pre-image of a point under a continuous map it is closed, the eigenvalues of $C$ are upper bounded by $\rho$, and the space of eigenbases is the orthogonal group, which is compact. Therefore the expected progress $\mathbb{E}[\Delta C]$ attains its minimum and its maximum on this set. We denote them by

$$Q(\rho) = \min_{C \in \text{tr}^{-1}(\rho)} \mathbb{E}[\Delta C] \quad \text{and} \quad R(\rho) = \max_{C \in \text{tr}^{-1}(\rho)} \mathbb{E}[\Delta C].$$

We note three convenient properties:

- It holds that $Q(\rho) > 0 \iff \rho > d \iff R(\rho) > 0$.
- $Q$ and $R$ are monotonically increasing functions, and
- $Q$ and $R$ are continuous functions.

We aim to show that the sequence $\rho^{(t)} = \text{tr}(C^{(t)})$ converges to $d$ with full probability. To this end we pick a target level $\rho^* > d$, so we have to show that the sequence $\rho^{(t)}$ falls below $\rho^*$. This is achieved by applying an additive drift argument and using the monotonicity of $R$ and $Q$ as well as the monotonic decrease of $\rho^{(t)}$ (Lemma 4). By construction it holds that

$$\mathbb{E} \left[ \rho^{(t)} - \rho^{(t+1)} \right] \in \left[ Q(\rho^{(t)}), R(\rho^{(t)}) \right] \subset \left[ Q(\rho^*), R(\rho(0)) \right]. \quad (19)$$

Here, the monotonic reduction of $\rho^{(t)}$ together with the monotonicity of $Q$ and $R$ yield $t$-independent lower and upper bounds on the expected progress, as long as it holds that $\rho^{(t)} \geq \rho^*$. The existence of the two bounds allows us to apply a drift argument. We define the first hitting time $T(\rho^*) = \min\{ t \in \mathbb{N} \mid \rho(t) \leq \rho^* \}$ of reaching the target $\rho^*$. [Hajek 1982, theorem 2.3, equation 2.9] guarantees that the probability $\text{Pr}(T(\rho^*) > k)$ tends to zero as $k \to \infty$ (and it does so exponentially fast). Hence, the sequence $\rho^{(t)}$ eventually falls below $\rho^*$ with probability one. Since $\rho^* > d$ was arbitrary we conclude that $\rho^{(t)} \to d$ with full probability. This proves $C^{(t)} \to I$ in our case, and hence in general $C^{(t)} \to \alpha \cdot H^{-1}$ due to affine invariance. The form of the scaling factor $\alpha = \sqrt[4]{\det(C^{(0)}) \cdot \det(H)}$ results immediately from affine invariance and the need to fulfill $\det(HC^{(t)}) = \det(HC^{(0)}) = \det(H) \det(C^{(0)}) = \alpha$.

The above theorem establishes that the update of (1+4)-HE-ES is not only stable and improving the covariance matrix monotonically, but that it also achieves its goal of converging to a multiple of the inverse Hessian. To the best of our knowledge, this is the first theorem proving that the covariance matrix update of a variable-metric evolution strategy has this property. This stability of $C^{(t)}$ will allow us to derive a strong convergence speed result for $m^{(t)}$ in the next section.

We would like to note that equation [19] can be understood as a variable drift condition [Doerr et al. 2011] for $\rho^{(t)}$. A more detailed drift analysis bears the potential to bound the time it takes for the covariance matrix to adapt to the problem at hand. However, the task of bounding $Q$ and $R$ is non-trivial. In practice we find that the covariance matrix converges at a linear rate, see figure 2.

4 Linear Convergence of HE-ES on Convex Quadratic Functions

In this section we establish that the (1+4)-HE-ES converges at a linear rate that is independent of the problem difficulty $\kappa(H)$. The proof builds on the stability of the covariance matrix update...
Figure 2: The plots show the time evolution of condition number $\kappa(C)$ (solid curve) and trace $\text{tr}(C)$ (dashed curve), both with their global minima of 1 and $d$ subtracted, on a logarithmic scale, for (1+4)-HE-ES on the left and (1+1)-CMA-ES on the right. For CMA-ES, the trace is computed on a suitably normalized multiple of the covariance matrix. The algorithms are run on the sphere function, but they are initialized with a covariance matrix resembling an optimization run of an ellipsoid function with conditioning number $10^6$ when starting from an isotropic search distribution. The curves are medians over 99 independent runs. In the right half of the left plot the covariance matrix is already adapted extremely close to the identity. It is clearly visible that in this late phase $\kappa(C)$ and $\text{tr}(C)$ both converge at a linear rate. In contrast, with the CMA-ES update the precision saturates at some non-optimal value.

established in the previous section, as well as on the analysis of the (1+1)-ES by Morinaga and Akimoto (2019). We adapt notations and definitions in the following to make the two analyses compatible.

Defining linear convergence of stochastic algorithms is not a straight-forward task. We define linear convergence in terms of the first hitting time:

**Definition 6.** Let $(X(t))_{t \in \mathbb{N}}$ a sequence of random variables with $\mathbb{E}[X(t)] \to X^*$ and let $\Psi(t) = \Psi(X(t))$ be a potential function with $\mathbb{E}[\Psi(t)] \to -\infty$. The first hitting time of the target $\delta$ is defined as

$$T_\Psi(\delta) = \min \{ t \in \mathbb{N} \mid \Psi(t) < \delta \}.$$  

We say that $X(t)$ converges $\Psi$-linearly to $X^*$, if there exists $Q$ such, that

$$\lim_{\epsilon \to 0} \mathbb{E} \left[ \frac{T_\Psi(\log \epsilon)}{-\log \epsilon} \right] \leq \log(Q).$$

The intuition of this definition is that $\Psi$ measures the logarithmic distance from the optimum, e.g. $\Psi(x) = \log \|x - x^*\|$. When considering a deterministic algorithm, i.e. $X(t)$ is a sequence of dirac-distributions, this choice of $\Psi$ makes our definition equivalent to $Q$-linear convergence.

The recent work of Akimoto et al. (2018) established linear convergence of the (1+1)-ES on the sphere function by means of drift analysis. The result was significantly extended by Morinaga and Akimoto (2019) to a large class of functions, including strongly convex $L$-smooth functions. As a special case it establishes linear convergence for all convex quadratic problems. Unsurprisingly this comes at the price of a worse convergence rate, a result that was first established by Jägersküpper (2006). This is because all of the above results refer to a simple ES without covariance matrix adaptation. Analyzing an ES with CMA has proven to be significantly more difficult than analyzing an ES without CMA on a potentially ill-conditioned convex quadratic function. The
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Figure 3: Visualization of the function-sequence described in Corollary 7. For a set of three points \( m^{(t)} \), three functions \( \tilde{f}^{(t)} \) are depicted (continuous, dotted, and dashed contour-lines). The functions \( \tilde{f}^{(t)} \) and \( \tilde{f}^{(t+1)} \) are chosen such that their function-values agree at point \( m^{(t+1)} \) and thus function-value decreases of a successful step (black-arrows) amount to the same progress as on the target function \( f \). Further note that contour-lines of same function-values between functions encompass the same area, which is proven in Lemma 8.

reason is that adapting the covariance matrix can turn the problem into any convex quadratic function, with unbounded conditioning number (or trace), while the condition number is bounded in case of an arbitrary but fixed convex quadratic problem and isotropic mutations. However, the stability of the update established in the previous section allows us to derive a strong convergence result even with an elaborate CMA mechanism in place.

The technically rather complicated proof in this section is based on a simple idea. Using invariance properties, the optimization problem faced by (1+4)-HE-ES can be transformed into a convex quadratic problem faced by the simple (1+1)-ES, independently in each iteration. This amounts to optimizing a dynamically changing sequence of convex quadratic objective function with the (1+1)-ES. The sequence of objective functions lies within a class that is covered by Morinaga and Akimoto (2019). We need to adapt that analysis only slightly, arguing that it does not only hold for a single function from a flexible class of functions, but uniformly for function classes with bounded conditioning of the Hessian. Then the analysis holds even for dynamically changing functions, as long as the sequence remains inside of the function class. The last part is a direct consequence of the stability of the HE-ES update.

We consider (1+4)-HE-ES optimizing the convex quadratic function \( (1) \) with unique minimum \( x^* \), optimal value \( f^* \), and strictly positive definite Hessian \( H \). The following corollary will allow us to rephrase the results of the previous section in terms that are more compatible with Morinaga and Akimoto (2019).
Corollary 7. Consider the state-trajectory \((m^{(t)}, \sigma^{(t)}, A^{(t)})_{t \in \mathbb{N}}\) of the \((1+4)\)-HE-ES applied to the convex quadratic function
\[
f(x) = \frac{1}{2} (x - x^*)^T H (x - x^*) + f^* .
\]
There exists a sequence of functions \(\tilde{f}^{(t)} = f \circ [g^{(t)}]^{-1}\) such that the state-trajectory is equivalent to the run of a \((1+1)\)-ES optimizing \(\tilde{f}^{(t)}\) in iteration \(t\) starting from \((m^{(0)}, \sigma^{(0)})\). The state-trajectory of the \((1+1)\)-ES is \((\tilde{m}^{(t)}, \tilde{\sigma}^{(t)})_{t \in \mathbb{N}}\) and for all \(t \in \mathbb{N}\) it holds that
\begin{enumerate}
  \item \(f(m^{(t)}) = \tilde{f}^{(t)}(\tilde{m}^{(t)})\)
  \item \(\tilde{\sigma}^{(t)} = \sigma^{(t)}\)
  \item \(f(m^{(t+1)}) = \tilde{f}^{(t)}(\tilde{m}^{(t+1)})\)
  \item \(\nabla^2 \tilde{f}^{(t)}(x) \xrightarrow{t \to \infty} \alpha I, \alpha > 0\)
\end{enumerate}

Proof. The proof is straight-forward. We define
\[
g^{(t)}(x) = [A^{(t)}]^{-1} (x - m^{(t)}) + \tilde{m}^{(t)} .
\]
With this choice, the first statement is fulfilled by construction. The second statement can be derived analogous to the proof of Lemma 2 equation (10) and the third statement can be obtained by noting that
\[
[g^{(t)}]^{-1}(\tilde{m}^{(t+1)}) = m^{(t)} + A^{(t)}(\tilde{m}^{(t+1)} - \tilde{m}^{(t)}) = m^{(t+1)} .
\]

For the fourth statement, we obtain that \(\nabla^2 \tilde{f}^{(t)}(x) = A^{(t)} H (A^{(t)})^T\). Since by Lemma 5
\[
C^{(t)} = (A^{(t)})^T A^{(t)} \xrightarrow{t \to \infty} \alpha H^{-1}
\]
we obtain \(\nabla^2 \tilde{f}^{(t)}(x) \xrightarrow{t \to \infty} \alpha I\). \qed

In other words, instead of considering an update of the covariance matrix, we can apply the \((1+1)\)-ES to a sequence of functions that converge to the sphere function. This requires that the chosen sequence of functions does not change the behaviour of the optimizer. For this, statements 1 and 3 are crucial, because they can be used to show that single-step improvements on the set of functions can be related to improvements on the target function. This result does not extend to the two-step progress and \(f(m^{(t+2)}) - f(m^{(t)}) = \tilde{f}^{(t)}(\tilde{m}^{(t+2)}) - \tilde{f}^{(t)}(\tilde{m}^{(t)})\) as the two steps are taken in different coordinate systems. Figure 3 gives a visual depiction of this sequence of functions.

The analysis of Morinaga and Akimoto (2019) does not use the function-values directly, but instead uses a different function to show convergence. This is to allow their analysis to be invariant to strictly monotonically increasing transformations of the function values. This is an important property in their analysis, because otherwise transforming a function would have an impact on the measured convergence speed. To achieve this, we define the function
\[
f_\mu(m) = \frac{d}{\mu(\{x \in \mathbb{R}^d \mid f(x) < f(m)\})} ,
\]
which denotes the \(d\)-th root of the Lebesgue measure of the set of points that improve upon \(m\). For this function it holds that \(f(x) < f(y) \iff f_\mu(x) < f_\mu(y)\). For the sphere function, \(f_\mu\) can be computed analytically and we obtain \(f_\mu(m) = \gamma_d \cdot \|m - x^*\|\), where \(\gamma_d\) is a dimension-dependent
constant. This justifies the use of \( f_\mu(m) \) as a measure of distance of \( m \) to the optimum. For a general convex quadratic function it holds that

\[
f_\mu(m) = \frac{\gamma d}{\sqrt{\det(H)}} \cdot \sqrt{f(m) - f^*}.
\]

The question arises, whether this transformation is compatible with the set of functions defined in Corollary 7. The answer is given by the following lemma:

**Lemma 8.** Let \( \tilde{f}^{(t)} = f \circ [g^{(t)}]^{-1} \), \( \tilde{m}^{(t)} \), \( t \in \mathbb{N} \) the set of functions and vectors as defined in Corollary 7 and

\[
\tilde{f}_\mu^{(t)}(m) = \frac{1}{\sqrt{\det(A^{(t)}_0)}} f_\mu(m^{(t)})
\]

It holds that

1. \( \tilde{f}_\mu^{(t)}(\tilde{m}^{(t)}) = \tilde{f}_\mu^{(t-1)}(\tilde{m}^{(t)}) \)
2. \( \tilde{f}_\mu^{(t)}(\tilde{m}^{(t)}) = \frac{1}{\sqrt{\det(A^{(t)}_0)}} f_\mu(m^{(t)}) \)

**Proof.** Let \( \varphi^{(t)} = g^{(t-1)} \circ [g^{(t)}]^{-1} \). With this, it holds that \( \tilde{f}^{(t)} = \tilde{f}^{(t-1)} \circ \varphi^{(t)} \). It is easy to verify that \( \varphi^{(t)}(\tilde{m}^{(t)}) = \tilde{m}^{(t)} \) and

\[
\nabla \varphi^{(t)}(x) = [A^{(t-1)}_0]^{-1} A^{(t)}_0 = G^{(t)} ,
\]

where \( G^{(t)} \) is the matrix computed by \texttt{computeG} via equation (3) in iteration \( t \). We obtain

\[
\tilde{f}^{(t)}_\mu(\tilde{m}^{(t)}) = \frac{d}{\mu} \left( \left\{ x \, | \, \tilde{f}^{(t)}(x) < \tilde{f}^{(t)}(\tilde{m}^{(t)}) \right\} \right)
\]

\[
= \frac{d}{\mu} \left( \left\{ x \, | \, \tilde{f}^{(t-1)}(\varphi^{(t)}(x)) < \tilde{f}^{(t-1)}(\varphi^{(t)}(\tilde{m}^{(t)})) \right\} \right)
\]

\[
= \frac{d}{\mu} \left( \left\{ x \, | \, \tilde{f}^{(t-1)}(y) < \tilde{f}^{(t-1)}(\tilde{m}^{(t)}) \text{ for } y = \varphi^{(t)}(x) \right\} \right)
\]

\[
\overset{(*)}{=} \frac{d}{\mu} \left( \left\{ y \, | \, \tilde{f}^{(t-1)}(y) < \tilde{f}^{(t-1)}(\tilde{m}^{(t)}) \right\} \right)
\]

\[
= \tilde{f}^{(t-1)}_\mu(\tilde{m}^{(t)})
\]

for all \( t \). The set changes from the left-hand-side to the right-hand-side of equation (\(*\)). The equality of the Lebesgue measures of the two sets holds because the matrix \( G^{(t)} \) has unit determinant, and hence the transformation \( \varphi^{(t-1)} \) preserves the Lebesgue measure.

We can apply the decomposition argument via \( \varphi^{(t)} \) iteratively and arrive at \( \tilde{f}^{(t)} = \tilde{f}^{(0)} \circ \varphi^{(1)} \circ \ldots \circ \varphi^{(t)} \), where

\[
\tilde{f}^{(0)}(m) = \left( f \circ [g^{(0)}]^{-1} \right)(m) = f(A^{(0)}(m - m^{(0)}) + m^{(0)}) ,
\]

follows from the definition of \( g^{(t)} \) and starting-conditions of \((1+1)\)-ES and \((1+4)\)-HE-ES. As \( \nabla \varphi^{(t)} \) has unit determinant for all \( t > 0 \), it holds that \( \tilde{f}^{(t)}_\mu(\tilde{m}^{(t)}) = \tilde{f}^{(0)}_\mu(g^{(0)}(m^{(t)})) \). Finally, the
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Lebesque-measure of \( \tilde{f}^{(0)} \) is given by:

\[
\tilde{f}^{(0)}(m) = d \sqrt{\mu}\left( \left\{ x \mid \tilde{f}^{(0)}(x) < \tilde{f}^{(0)}(m) \right\} \right)
= d \sqrt{\mu}\left( \left\{ x \mid f(A^{(0)}(x - m^{(0)}) + m^{(0)}) < f([g^{(0)}]^{-1}(m)) \right\} \right)
= d \sqrt{\det A^{(0)} \mu}\left( \left\{ y \mid f(y) < f([g^{(0)}]^{-1}(m)) \right\} \right)
= \frac{1}{d \sqrt{\det A^{(0)}}} f_{\mu}([g^{(0)}]^{-1}(m)).
\]

4.1 Adaptation of the Analysis of Morinaga and Akimoto (2019)

Before we state our main theorem, we need to recap the results of Morinaga and Akimoto (2019) and how their proof is structured. A key definition for this is the normalized step size

\[
\bar{\sigma} = \frac{\sigma}{f_{\mu}(m)}
\]

which uses \( f_{\mu}(m) \) as a measure of distance from the optimum. Using this definition, the convergence proof for the (1+1)-ES with 1/5-success rule is structured into the following steps:

1. It is proven that for any \( 0 < p_u < 1/5 < p_l < 1/2 \) we can find normalized step-sizes \( 0 < \bar{\sigma}_l < \bar{\sigma}_u < \infty \) such, that for \( \bar{\sigma} \in [\bar{\sigma}_l, \bar{\sigma}_u] \) the success-probability of the (1+1)-ES is

\[
P( f(X) < f(m) ) \in [p_u, p_l],
\]

where \( X \sim N(m, f_{\mu}(m)\bar{\sigma}I) \) for all \( m \in \mathbb{R}^d \) such, that \( f(m) \leq f(m^{(0)}) \). In other words, for any point that might get accepted during an optimization run, the success probability must be within \([p_u, p_l]\) when \( \bar{\sigma} \in [\bar{\sigma}_l, \bar{\sigma}_u] \).

2. Morinaga and Akimoto (2019) now pick \( l \leq \bar{\sigma}_l \) and \( u \geq \bar{\sigma}_u \) with \( u/l \geq c_{5/4} \) and some constant \( v > 0 \) to be quantified later to define the potential function

\[
V(m, \bar{\sigma}) = \log f_{\mu}(m) + v \max \left\{ 0, \log \frac{c_{5/4} l}{\bar{\sigma}}, \log \frac{c_{5/4} \bar{\sigma}}{u} \right\}
\]

It is clear that \( V(m, \bar{\sigma}) \geq \log f_{\mu}(m) \) and thus, if \( \Psi \)-linear convergence is shown with the potential \( \Psi = V \), then it also holds for \( \Psi(m) = \log f_{\mu}(m) \). The second term penalizes \( \bar{\sigma} \notin [l, u] \) and thus allows to measure progress when \( \sigma \) has too large or too small value so that progress in \( f_{\mu}(m) \) is unlikely or very small.

3. Using this potential, the expected truncated single-step progress is derived. To be more exact, we pick \( A > 0 \) and define the sequence

\[
Y^{(t+1)} = Y^{(t)} + \max \left\{ V(m^{(t+1)}, \bar{\sigma}^{(t+1)}) - V(m^{(t)}, \bar{\sigma}^{(t)}), -A \right\}, \quad Y^{(0)} = V(m^{(0)}, \bar{\sigma}^{(0)})
\]

(21)
This bounds the single-step progress by $-A$ and prevents technical difficulties in the proof due to very good steps which occur with low probability. With this sequence, the expected single-step progress is bounded by

$$
E \left[ Y^{(t+1)} - Y^{(t)} \mid Y^{(t)} \right] \leq -B .
$$

The result is obtained by maximizing the progress over $v$ and it is shown that for each $f$ there exists an interval $v \in (0, v_u)$ such, that $B > 0$.

4. Finally, with this bound in place, Theorem 1 in Akimoto et al. (2018) is applied to bound convergence.

Most important for us, the final step only depends on $A$ and $B$ and is thus independent of $V$. The third step in turn computes the expected progress of a single iteration, thus changing $V$ between two iterations does not affect this, as long as we ensure that the progress measured by a chosen $V^{(t)}$ relates to progress on $V(m, \bar{\sigma})$. Our proof strategy is therefore the following. We consider the $(1+1)$-ES in the setting of Corollary 7. We define the normalized step-size

$$
\bar{\sigma}^{(t)} = \frac{\sigma^{(t)}}{\sqrt{\det A^{(0)} f^{(t)}_{\mu}(\bar{m}^{(t)})}}
$$

as well as a sequence of potential-functions

$$
V^{(t)}(\bar{m}, \bar{\sigma}) = \log \bar{f}_{\mu}(\bar{m}) - \log \sqrt{\det A^{(0)} f^{(t)}_{\mu}(\bar{m}^{(t)})} + \max \left\{ 0, \log \frac{c_{f, l}}{\bar{\sigma}}, \log \frac{c_{f, u}}{\bar{\sigma}} \right\} . \tag{22}
$$

As due to Lemma 8 statement 2, $f_{\mu}(m^{(t)}) = \sqrt{\det A^{(0)} f^{(t)}_{\mu}(\bar{m}^{(t)})}$, our definition of $\bar{\sigma}$ coincides with equation (20). Applying Lemma 8 to $V^{(t)}$, we obtain the properties

$$
V^{(t)}(\bar{m}^{(t)}, \bar{\sigma}^{(t)}) = V(m^{(t)}, \bar{\sigma}^{(t)}) \quad \text{and} \quad V^{(t+1)}(\bar{m}^{(t+1)}, \bar{\sigma}^{(t+1)}) = V^{(t)}(\bar{m}^{(t+1)}, \bar{\sigma}^{(t+1)}) .
$$

Thus, the sequence of truncated single step progress in (21) coincides with

$$
Y^{(t+1)} = Y^{(t)} + \max \left\{ V^{(t)}(\bar{m}^{(t+1)}, \bar{\sigma}^{(t+1)}) - V^{(t)}(\bar{m}^{(t)}, \bar{\sigma}^{(t)}), -A \right\} , \quad Y^{(0)} = 0 . \tag{23}
$$

With this in place, we will find a feasible $v > 0$ and bound

$$
E \left[ Y^{(t+1)} - Y^{(t)} \mid Y^{(t)} \right] \leq -B^{(t)} \leq -B < 0 ,
$$

which produces the final result. We formalize this argument further in the proof of the final theorem:

**Theorem 9.** Consider minimization of the convex quadratic function

$$
f(x) = \frac{1}{2} (x - x^*)^T H(x - x^*) + f^*
$$

with the $(1+4)$-HE-ES. Let $\Psi(m) = \log \| f_{\mu}(m) \|$. The sequence $(m^{(t)})_{t \in \mathbb{N}}$ converges $\Psi$-linearly to $x^*$ with a convergence rate independent of $H$. 

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Proof. We consider the (1+1)-ES in the setting of Corollary 7 and thus obtain a state-trajectory $(\tilde{m}(t), \sigma(t))_{t \in \mathbb{N}}$ with function-sequence $(\tilde{f}(t))_{t \in \mathbb{N}}$ so, that $\nabla^2 \tilde{f}(t) \rightarrow \alpha I$ and $\det(\nabla^2 \tilde{f}(t)) = \alpha^d$. Pick $\beta > 1$ arbitrarily and consider the function space

$$F(\alpha, \beta) = \left\{ \tilde{f}(x) = f^* + (x - x^*)^T Q(x - x^*) \mid x^* \in \mathbb{R}^d, \det(Q) = \alpha^d, \kappa(Q) \leq \beta \right\}.$$ 

We note that for given $\alpha$ and $\beta$, the choice of matrices $Q$ in $F(\alpha, \beta)$ is restricted to a compact set. Therefore, a continuous function of $Q$ attains its infimum and supremum. As $\nabla^2 \tilde{f}(t) \rightarrow \alpha I$, we have $\kappa_t = \kappa(\nabla^2 \tilde{f}(t)) \rightarrow 1$ due to continuity. Therefore, there exists a $T_0 \in \mathbb{N}$ such, that $\kappa_t < \beta$ and $\tilde{f}(t) \in F(\alpha, \beta)$ for all $t > T_0$.

From now on, we will only consider $t > T_0$. Proposition 4 and Proposition 12 in Morinaga and Akimoto (2019) establish that for each $\tilde{f} \in F(\alpha, \beta)$ and each choice $0 < p_u < 1/5 < p_l < 1/2$ there exists a $0 < \sigma_1 < \sigma_u < \infty$ such, that step 1 is fulfilled. We can thus pick $0 < l < u < \infty$ such, that $\tilde{f}(t) - \tilde{f}(t)$ is obtained for a specific $\tilde{f}(t) \in F(\alpha, \beta)$.

With this choice of $l$ and $u$ and $v > 0$, we can define $V(t)$ and $Y(t)$ as in equations (22) and (23), respectively. With chosen $A > 0$, and $v > 0$ sufficiently small, Proposition 6 in Morinaga and Akimoto (2019) gives a bound on the expected single-step progress of

$$\mathbb{E} \left[ Y(t+1) - Y(t) \mid Y(t) \right] < -B(t).$$

While the bound $B(t)$ is obtained for a specific $v(t) > 0$, Morinaga and Akimoto (2019) show that we still obtain positive progress for $0 < v \leq v(t)$. As $v(t) > 0$ is a continuous function of $\kappa(\nabla^2 \tilde{f}(t))$, it attains its minimum within the set $F(\alpha, \beta)$ and therefore we pick $v = \inf_{t \in \mathbb{N}} v(t) > 0$. Let $B_0(t) > 0$ denote the progress rates obtained for this choice of $v$. Again, due to continuity of $B_0(t)$ as a function of $\tilde{f} \in F(\alpha, \beta)$, we can define $B = \inf_{t \in \mathbb{N}} B_0(t) > 0$.

Finally, with $A$ and $B$ in place, we can apply Theorem 1 in Akimoto et al. (2018) to obtain linear convergence. Since $\beta$ was chosen independently of $H$, the rate of convergence is independent of the problem instance and its difficulty $\kappa(H)$.

Our result is the first proof of linear convergence of a CMA-based elitist ES, and the first proof of linear convergence of any ES at a rate that is independent of $H$. The result is of interest in a broader context, because it can naturally be extended to other CMA-algorithms as the proof itself only uses two properties: the determinant of $C(t)$ is constant and $C(t) \rightarrow \alpha H^{-1}$. The first condition poses no difficulties for algorithm design, as we can always use a matrix with normalized variance for sampling, i.e. sample offspring from $\mathcal{N}(m(t), (\sigma(t))^2 \cdot C(t) / \sqrt{\det(C(t)})$. Therefore, our proof can also be applied to the covariance-matrix adaptation algorithm proposed by Stich et al. (2016) when applied to the (1+1)-ES. We expect similar results for a hybrid-algorithm that could be constructed from an (1+1)-ES using the BOBYQA approximation of the Hessian matrix (Powell 2009).

5 Conclusion

We have established that the covariance matrix update of the recently proposed Hessian Estimation Evolution Strategy is stable. It makes the covariance matrix converge to a multiple of the inverse Hessian of a convex quadratic objective function, and even in face of randomly sampled
offspring the covariance matrix cannot degrade. This strong guarantee highlights that the update mechanism is very different from CMA-ES and similar algorithms. It also allows us to derive a strong convergence speed guarantee, namely linear convergence of a variable metric evolution strategy at the optimal convergence rate, in the sense that the convergence speed coincides with the speed of the same algorithm without covariance matrix adaptation applied to the sphere function. To the best of our knowledge, this is the first result of this type for a variable metric evolution strategy.

References


