

Evolution Strategies and Covariance Matrix Adaptation

Investigating New Shrinkage Techniques

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Abstract: This paper discusses the covariance matrix adaptation in evolution strategies, a central and essential mechanism for the search process. Basing the estimation of the covariance matrix on small samples w.r.t. the search space dimension is known to be problematic. However, this situation is common in optimization raising the question, whether the performance of the evolutionary algorithms could be improved. In statistics, several approaches have been developed recently to improve the quality of the maximum-likelihood estimate. However, they are seldom applied in evolutionary computation. Here, we focus on linear shrinkage which requires relatively little additional effort. Several approaches and shrinkage targets are integrated into evolution strategies and analyzed in a series of experiments.

1 INTRODUCTION

Evolution strategies (ESs) belong to the class of evolutionary algorithms. Their performance compared to other black-box optimization techniques is good as it has been observed in practice and in several competitions as e.g. (Hansen et al., 2010). Since they operate mainly in continuous search spaces, their central search operator is mutation which is typically realized as a multivariate normal distribution with mean \mathbf{m} and covariance matrix $\sigma^2\mathbf{C}$. In order to progress fast and reliably towards the optimal point, the extent as well as the directions of the mutations must be adapted so that the distribution of the random variables is suitable to fitness landscape of the particular function. Techniques for controlling the mutation process have therefore received a lot of attention in research on evolution strategies. The focus lies on the control of covariance matrix. The covariance matrix adaptation techniques developed typically make use of a variant of the sample covariance. However, the estimation problem is ill-posed: Due to efficiency, the sample size is relatively small w.r.t. the search space dimension. This leads to a well-known problem in statistics: The covariance matrix estimate may differ considerably from the underlying true covariance (Stein, 1956; Stein, 1975). Taking a closer look at the adaptation equations, reveals that nearly all adaptation techniques introduce correction or regularization techniques by falling back to the previous covari-

ance matrix and/or by strengthening certain promising directions. These procedures exhibit similarities to shrinkage estimation in statistical estimation theory leading to the research question of the present paper: If evolution strategies perform a kind of implicit shrinkage, can they profit from the introduction of explicit shrinkage operators?

The current analysis extends the work carried out in (Meyer-Nieberg and Kropat, 2014; Meyer-Nieberg and Kropat, 2015a) and augments the investigation conducted in (Meyer-Nieberg and Kropat, 2015b; Meyer-Nieberg and Kropat, 2015c) for the case of thresholding estimators. (Meyer-Nieberg and Kropat, 2014; Meyer-Nieberg and Kropat, 2015a) presented the first approaches to apply Ledoit-Wolf shrinkage estimators in evolution strategies. There, the shrinkage estimators were combined with an approach stemming from a maximum entropy covariance selection principle. A literature review resulted in only two papers aside from our previous approaches: An application in the case of Gaussian estimation of distribution algorithms albeit with quite a different goal (Dong and Yao, 2007). There, the learning of the covariance matrix during the run lead to non positive definite matrices. For this reason, a shrinkage procedure was applied to “repair” the covariance matrix towards the required structure. The authors used a similar approach as in (Ledoit and Wolf, 2004b) but made the shrinkage intensity adaptable. More recently Kramer considered Ledoit-Wolf-estimator based on (Ledoit and

Wolf, 2004a) for an evolution strategy which does not follow a population-based approach but uses a variant of the (1+1)-ES with covariance matrix adaptation for which past search points are taken into account (Kramer, 2015).

Here, we focus on an approach in the eigenspace of the covariance matrix. Several shrinkage targets are analyzed and compared with each other and with the original ES version. The paper is structured as follows: First, a brief introduction into evolution strategies with covariance matrix adaptation is provided. Afterwards, we focus on the problem of estimating high-dimensional covariance matrices. Several shrinkage targets are introduced and their integration into evolution strategies is described. The strategies are assessed and compared to the original ES version in the experimental section. The paper ends with the conclusions and an outlook regarding open research points.

2 EVOLUTION STRATEGIES

Let $f: \mathbb{R}^N \rightarrow \mathbb{R}$ be a continuous function that allows only the evaluation of the function itself but not the derivation of higher order information. In this context, metaheuristics as evolution strategies and similar approaches can be applied. Evolution strategies (ESs) are stochastic optimization methods that usually use a sample or population of search points also called candidate solutions. They distinguish between a population of μ parents and λ offspring. In many applications in continuous search spaces, the parent population is discarded after the offspring have been created. Therefore, $\lambda > \mu$ is required. Evolution strategies use a multivariate normal distribution with mean $\mathbf{m}^{(g)}$ and covariance matrix $(\sigma^{(g)})^2 \mathbf{C}^{(g)}$ to obtain new search points. The mean is taken as the (weighted) centroid of the parent population whereas the covariance matrix is updated by following one of the established techniques. Sampling λ times from the normal distribution, results in the offspring population

$$\mathbf{x}_l = \mathbf{m}^{(g)} + \sigma^{(g)} \mathcal{N}(0, \mathbf{C}^{(g)}), l = 1, \dots, \lambda. \quad (1)$$

Afterwards, the new search points are evaluated using the function f to be optimized. The μ best of the λ offspring are selected for the following parent population.

As stated previously, the parameters of the normal distribution must be adapted in order to allow progress towards the optimal point. The mean is obtained as the centroid of the parent population. In contrast, the covariance matrix requires more effort. Methods for adapting the scale factor σ or the full

covariance matrix have received a lot of attention in work on evolution strategies (see (Meyer-Nieberg and Beyer, 2007)). The investigation in this paper centers on the *covariance matrix self-adaptation evolution strategy* (CMSA-ES) (Beyer and Sendhoff, 2008).

2.1 Covariance Matrix Update

The covariance matrix $(\sigma^{(g)})^2 \mathbf{C}^{(g)}$ can be interpreted as the product of a general scaling factor $\sigma^{(g)}$ (or step-size or mutation strength) and direction matrix $\mathbf{C}^{(g)}$. Previous research in evolution strategies has shown that both should be treated separately. The adaptation therefore takes two distinct processes into account: the first for the step-size, the second for the matrix itself. Following established practice in evolution strategies, the matrix $\mathbf{C}^{(g)}$ will be referred to as the *covariance matrix* in the remainder of the paper.

Once the new sample has been created, the parameters of the distribution must be updated. First, the μ best offspring provide the sample which is used to estimate the covariance matrix. Considering only the better candidate solutions shall introduce a bias towards good search regions. It is necessary to re-estimate the mean $\mathbf{m}^{(g)}$, thus, the number of degrees of freedom remains μ . Let $\mathbf{x}_{m:\lambda}$ denote the m th best of the λ offspring w.r.t. the fitness and let

$$\mathbf{z}_{m:\lambda}^{(g+1)} := \frac{1}{\sigma^{(g)}} (\mathbf{x}_{m:\lambda}^{(g+1)} - \mathbf{m}^{(g)}), \quad (2)$$

stand for the normalized offspring. The covariance update is then determined as

$$\mathbf{C}^{(g+1)} := \left(1 - \frac{1}{c_\tau}\right) \mathbf{C}^{(g)} + \frac{1}{c_\tau} \sum_{m=1}^{\mu} w_m \mathbf{z}_{m:\lambda}^{(g+1)} (\mathbf{z}_{m:\lambda}^{(g+1)})^T \quad (3)$$

combining the old covariance and the population covariance and with the weights usually reading $w_m = 1/\mu$ (Beyer and Sendhoff, 2008). The parameter c_τ is described in more detail later in the paper.

2.2 Step-size Adaptation

The CMSA-ES applies *self-adaptation* in order to tune the mutation strength $\sigma^{(g)}$. Self-Adaptation has been developed by Rechenberg (Rechenberg, 1973) and Schwefel (Schwefel, 1981). It takes place at the level of the individuals meaning that each population member operates with its distinct set. The strategy parameters are adapted by including them in the genome and subjecting them to evolution. That is, they undergo recombination and mutation processes. Afterwards, they are used in the mutation of the search

Require: $\lambda, \mu, \mathbf{C}^{(0)}, \mathbf{m}^{(0)}, \sigma^{(0)}, \tau, c_\tau$
 1: $g = 0$
 2: **while** termination criteria not met **do**
 3: **for** $l = 1$ **to** λ **do**
 4: $\sigma_l = \sigma^{(g)} \exp(\tau \mathcal{N}(0, 1))$
 5: $\mathbf{x}_l = \mathbf{m}^{(g)} + \sigma_l \tilde{\mathcal{N}}(0, \mathbf{C}^{(g)})$
 6: $f_l = f(\mathbf{x}_l)$
 7: **end for**
 8: Select $(\mathbf{x}_{1:\lambda}, \sigma_{1:\lambda}), \dots, (\mathbf{x}_{\mu:\lambda}, \sigma_{\mu:\lambda})$ according to their fitness f_l
 9: $\mathbf{m}^{(g+1)} = \sum_{m=1}^{\mu} w_m \mathbf{x}_{m:\lambda}$
 10: $\sigma^{(g+1)} = \sum_{m=1}^{\mu} w_m \sigma_{m:\lambda}$
 11: $\mathbf{z}_{m:\lambda} = \frac{\mathbf{x}_{m:\lambda} - \mathbf{m}^{(g)}}{\sigma^{(g)}}$ for $m = 1, \dots, \mu$
 12: $\mathbf{C}_\mu = \sum_{i=1}^{\mu} w_i \mathbf{z}_i \mathbf{z}_i^T$
 13: $\mathbf{C}^{(g+1)} = (1 - \frac{1}{c_\tau}) \mathbf{C}^{(g)} + \frac{1}{c_\tau} \mathbf{C}_\mu^{(g+1)}$
 14: $g = g + 1$
 15: **end while**

Figure 1: The main steps of a CMSA-ES. Normally, the weights w_m are set to $w_m = 1/\mu$ for $m = 1, \dots, \mu$.

space position. The influence on the selection is indirect: Self-adaptation is based on the assumption of a stochastic linkage between good objective values and appropriately tuned strategy parameters: Self-adaptation is mainly used to adapt the step-size or a diagonal covariance matrix. Here, the mutation strength is considered. Its mutation process is realized with the help of the log-normal distribution following

$$\sigma_l^{(g)} = \sigma^{(g)} \exp(\tau \mathcal{N}(0, 1)). \quad (4)$$

The parameter τ , the *learning rate*, should scale with $1/\sqrt{2N}$ (Meyer-Nieberg and Beyer, 2005). Self-adaptation with recombination has been shown as “robust” against noise (Beyer and Meyer-Nieberg, 2006). In the case of ES with recombination, the variable $\sigma^{(g)}$ in (4) is the result of the recombination of the mutation strengths. Here, the same recombination type may be used as for the objective values, that is, $\sigma^{(g+1)} = \sum w_m \sigma_{m:\lambda}$ with $\sigma_{m:\lambda}$ standing for the mutation strength associated with the m th best individual. Figure 1 summarizes the main steps of the covariance matrix self-adaptation ES (CMSA-ES).

3 COVARIANCE ESTIMATION: SHRINKAGE

Estimating the covariance matrix in high-dimensional search spaces, requires an appropriate sample size. Using the population covariance matrix necessitates $\mu \gg N$ for obtaining a high quality estimator. If this is

not the case, estimate and “true” covariance may not agree well. Among others, the eigen structure may be significantly distorted, see e.g. (Ledoit and Wolf, 2004b). However, this is the case in evolution strategies. Typical recommendations for the population sizing are to use an offspring population size λ of either $\lambda = \mathcal{O}(\log(N))$ or $\lambda = \mathcal{O}(N)$ and setting $\mu = \lceil c\lambda \rceil$ with $c \in (0, 0.5)$. Thus, either $\mu/N \rightarrow c$ or even $\mu/N \rightarrow 0$ for $N \rightarrow \infty$ holds, showing that the textbook estimation equation is not applicable in high-dimensional settings.

As stated above, the estimation of high-dimensional covariance matrices has received a lot of attention, see e.g. (Chen et al., 2012). Several approaches can be found in the literature, see e.g. (Pourahmadi, 2013; Tong et al., 2014). This paper focuses on linear shrinkage estimators that can be computed comparatively efficiently and thus do not burden the algorithm strongly. Other classes, as e.g. thresholding operators for sparse covariance matrix estimation, are currently considered in separate analyses.

Based on (Stein, 1956; Ledoit and Wolf, 2004b), linear shrinkage approaches consider an estimate of the form

$$\mathbf{S}_{\text{est}}(\rho) = \rho \mathbf{F} + (1 - \rho) \mathbf{C}_\mu \quad (5)$$

with \mathbf{F} the *target* to correct the estimate provided by the sample covariance \mathbf{C}_μ . The parameter $\rho \in (0, 1)$ is called the *shrinkage intensity*. Equation (5) is used to shrink the eigenvalues of \mathbf{C}_μ towards the eigenvalues of \mathbf{F} . The intensity ρ should be chosen to minimize

$$\mathbb{E}(\|\mathbf{S}_{\text{est}}(\rho) - \Sigma\|_F^2) \quad (6)$$

with $\|\cdot\|_F^2$ denoting the squared Frobenius norm with

$$\|\mathbf{A}\|_F^2 = \frac{1}{N} \text{Tr}[\mathbf{A}\mathbf{A}^T], \quad (7)$$

see (Ledoit and Wolf, 2004b). Note the factor $1/N$ is additionally introduced in (Ledoit and Wolf, 2004b) to normalize the norm w.r.t. the dimension.

Based on (6) and taking into account that the true covariance is unknown in practice, Ledoit and Wolf were able to obtain an optimal shrinkage intensity for the target $\mathbf{F} = \text{Tr}(\mathbf{C}_\mu)/N \mathbf{I}$ for general probability distributions.

Several other approaches can be identified in literature. One the one hand, different targets can be considered, see e.g. (Schäffer and Strimmer, 2005; Fisher and Sun, 2011; Ledoit and Wolf, 2003; Touloumis, 2015). Schäffer and Strimmer analyze among others diagonal matrices with equal and unequal variance or special correlation models (Schäffer and Strimmer, 2005). Fisher and Sun also allow for several targets

(Fisher and Sun, 2011) assuming a multivariate normal distribution. Touloumis relaxed the normality assumption, considered several targets, and provided a new non-parametric family of shrinkage estimators (Touloumis, 2015). Other authors introduced different estimators, see e.g. (Chen et al., 2010) or (Chen et al., 2012)). Recently, Ledoit and Wolf extended their work to include non-linear shrinkage estimators (Ledoit and Wolf, 2012; Ledoit and Wolf, 2014). A problem arises concerning the complexity of the approaches. Especially the non-linear estimates require solving an associated optimization problem. Since the estimation has to be performed in every generation of the ES, only computationally simple approaches can be taken into account. Therefore, the paper focuses on linear shrinkage with shrinkage targets and intensities taken from (Ledoit and Wolf, 2004a; Ledoit and Wolf, 2004b; Fisher and Sun, 2011; Touloumis, 2015).

Interestingly, Equation (3) of the ES algorithm represents a special case of shrinkage with the old covariance matrix as the target. The shrinkage intensity is determined by

$$c_\tau = 1 + \frac{N(N+1)}{2\mu} \quad (8)$$

as $\rho = 1 - 1/c_\tau$. The paper investigates whether an additional shrinkage could improve the performance. Transferring shrinkage estimators to ESs must take the situation in which the estimation occurs into account since it differs from the assumptions in statistical literature. First, the covariance matrix $\Sigma = \mathbf{C}^{g-1}$ that was used to create the offspring is known. Second, the sample is based on truncation selection. Therefore, the variables cannot be assumed to be identically and independently distributed (iid). Only if there were no selection pressure, the sample $\mathbf{x}_1, \dots, \mathbf{x}_\mu$ would represent normally distributed random variables. In this context, it is interesting to note that during the discussion in (Hansen, 2006) with respect to the setting of the CMA-ES parameters it is argued to choose the parameters so that the distribution of the random variables remains unchanged if no selection pressure were present. This paper uses a similar argument to justify the usage of the shrinkage intensities obtained for assuming iid random or even normally distributed random variables. Since we are aware of the fact that the situation may differ vastly from the analysis assumptions of the statistical literature, other settings will be considered in future work.

Before continuing, it is worthwhile to take a closer look at the covariance matrix update (3). As stated, it can be interpreted as a shrinkage equation. Its effects become more clear, if we move into the eigenspace of $\mathbf{C}^{(g)}$. Since the covariance matrix is a positive

definite matrix, we can carry out a spectral composition of $\mathbf{C}^{(g)}$ with $\mathbf{C}^{(g)} = \mathbf{M}^T \Lambda \mathbf{M}$. The modal matrix $\mathbf{M} = (\mathbf{v}_1, \dots, \mathbf{v}_N)$ contains the eigenvectors of $\mathbf{C}^{(g)}$, whereas $\Lambda = \text{diag}(\lambda_1, \dots, \lambda_N)$ represents the diagonal matrix with the corresponding eigenvalues $\lambda_1, \dots, \lambda_N$. The representation $\mathbf{C}_C^{(g+1)}$ of $\mathbf{C}^{(g+1)}$ in the eigenspace of $\mathbf{C}^{(g)}$ then reads

$$\begin{aligned} \mathbf{C}_C^{(g+1)} &= \rho \Lambda + (1 - \rho) \mathbf{C}_\mu^C \\ &= \text{diag}(\mathbf{C}_\mu^C) + \rho \left(\Lambda - \text{diag}(\mathbf{C}_\mu^C) \right) + \\ &\quad (1 - \rho) \left(\mathbf{L}_\mu^C + \mathbf{U}_\mu^C \right) \end{aligned} \quad (9)$$

with $\mathbf{C}_\mu^C = \mathbf{M}^T \mathbf{C}_\mu \mathbf{M}$. The matrix \mathbf{L}_μ^C denotes the matrix with the entries of \mathbf{C}_μ^C below the diagonal, whereas \mathbf{U}_μ^C comprises the elements above. In other words, the covariance matrix update decreases the off-diagonal elements of the transformed population covariance. In the case of the diagonal entries, two cases may appear: if $c_{\mu_{ii}}^C < \lambda_i$, the new entry is in the interval $[c_{\mu_{ii}}^C, \lambda_i]$ and thus the estimate increases towards λ_i , otherwise it is shrunk towards λ_i . Thus, in the eigenspace of $\mathbf{C}^{(g)}$, Equation (9) behaves similar to shrinkage with a diagonal matrix as target matrix and therefore in original space it shrinks the eigenvalues of the population matrix towards those of the target. In contrast to shrinkage, the target matrix is not computed via the sample but with the old covariance (which is not obtainable in the general case).

Applying shrinkage requires among others the choice of an appropriate target. Most shrinkage approaches consider regular structures as e.g. the scaled unity matrix, diagonal matrices, or matrices with constant correlations as shrinkage targets. However, a shrinkage towards a regular structure concerning the coordinate system does not appear as an optimal choice concerning the optimization of arbitrary functions.

4 SHRINKAGE ESTIMATION EVOLUTION STRATEGIES

Since we cannot assume that the covariance matrix adaptation would profit from a shrinkage towards regular structures in every application case, we do not perform the shrinkage in the original search space. Instead, we consider the eigenspace of a positive definite matrix. A similar approach was introduced in (Thomaz et al., 2004) and used as the foundation of (Meyer-Nieberg and Kropat, 2014; Meyer-Nieberg and Kropat, 2015a). In (Thomaz et al., 2004) the authors were faced with the task to obtain a reliable

covariance matrix. To this end, a sample covariance matrix \mathbf{S}_i was combined with a pooled variance matrix \mathbf{C}_p – similar to (3)

$$\mathbf{S}_{mix}(\xi) = \xi \mathbf{C}_p + (1 - \xi) \mathbf{S}_i \quad (10)$$

with the parameter ξ to be determined. To proceed, the authors switched to the eigenspace of the non-weighted mixture matrix where they followed a maximal entropy approach to determine an improved estimate of the covariance matrix. Furthermore, (Hansen, 2008) suggested that changing the coordinate system may result in an improved performance. Therefore, Hansen introduced an adaptive encoding for the CMA-ES. It is based on the spectral decomposition of the covariance matrix. New search points are created in the eigenspace of the covariance matrix.

Similar to (Hansen, 2008), we suggest the ES will profit from a change of the coordinate system. However, the covariance matrix adaptation and estimation which in (Hansen, 2008) occurs in the original space will be performed in the transformed space.

This paper considers a combination of a shrinkage estimator and the basis transformation for a use in the CMSA-ES. First results were obtained in (Meyer-Nieberg and Kropat, 2014; Meyer-Nieberg and Kropat, 2015a). Here, the work is extended by considering several mixture matrices, targets, and choices for the shrinkage intensity. The resulting shrinkage CMSA-ES (Shr-CMSA-ES) approaches follow the same general principle:

- First, the coordinate system is transformed,
- followed by a shrinkage towards a particular shrinkage target.

In order to conduct the search space transformation, a positive-definite matrix is required. This paper considers the following choices for the transformation matrix which arise as combinations of the population covariance matrix \mathbf{C}_μ and $\mathbf{C}^{(g)}$

$$\mathbf{S}_{mix} = \mathbf{C}^{(g)} + \mathbf{C}_\mu, \quad (11)$$

$$\mathbf{S}_{g+1} = (1 - c_\tau) \mathbf{C}^{(g)} + c_\tau \mathbf{C}_\mu, \quad (12)$$

$$\mathbf{S}_g = \mathbf{C}^{(g)}. \quad (13)$$

The variants (11) - (13) are based on different assumptions: The first (11) follows (Thomaz et al., 2004). The influence of the old covariance and the population covariance are balanced. Structural changes caused by \mathbf{C}_μ will be dampened but will influence the result more strongly than in the case of (12) and (13). The second (13) considers the covariance mixture that would have been used in the original CMSA-ES. Depending on the size of c_τ , which in turn is a function of μ and N , see (8), the influence of the population covariance matrix may be stronger or lesser. The third

considers the eigenspace of the old covariance matrix and reduces therefore the influence of the new estimate. Equations (11) - (13) are used to change the coordinate system. Assuming that for example (13) is used, the following steps are performed

- spectral decomposition: $\mathbf{M}, \mathbf{D} \leftarrow \text{spectral}(\mathbf{S}^{(g)})$,
- determination of $\mathbf{C}_\mu^S := \mathbf{M}_S^T \mathbf{C}_\mu \mathbf{M}_S$ and $\mathbf{C}_S := \mathbf{M}_S^T \mathbf{C}^{(g)} \mathbf{M}_S$,
- shrinkage resulting in \mathbf{C}_{shr} ,
- retransformation $\mathbf{C}_\mu = \mathbf{M}^T \hat{\mathbf{C}}_{shr} \mathbf{M}$,
- covariance adaptation

$$\mathbf{C}^{(g+1)} = \left(1 - \frac{1}{c_\tau}\right) \mathbf{C}^{(g)} + \frac{1}{c_\tau} \mathbf{C}_\mu.$$

The representations of the covariance matrices in the eigenspace are given as $\mathbf{C}_\mu^S := \mathbf{M}_S^T \mathbf{C}_\mu \mathbf{M}_S$ and $\mathbf{C}_S := \mathbf{M}_S^T \mathbf{C}^{(g)} \mathbf{M}_S$ with \mathbf{S} standing for one of the variants (11) - (13). Once the change is performed, different targets can be taken into account. In this paper, we consider the matrices

$$\mathbf{F}_u = v \mathbf{I}, \quad (14)$$

with $v = \text{Tr}(\mathbf{C}_\mu^S)/N$ (Ledoit and Wolf, 2004b),

$$\mathbf{F}_d = \text{diag}(\mathbf{C}_\mu^S) \quad (15)$$

the diagonal entries of \mathbf{C}_μ^S (Fisher and Sun, 2011; Touloumis, 2015), the constant correlation model with matrix \mathbf{F}_c the entries of which read

$$f_{ij} = \begin{cases} s_{ii} & \text{if } i = j \\ \bar{r} \sqrt{s_{ii} s_{jj}} & \text{if } i \neq j \end{cases} \quad (16)$$

and $\bar{r} = 2/((N-1)N) \sum_{i=1}^{N-1} \sum_{j=i+1}^N s_{ij} / \sqrt{s_{ii} s_{jj}}$ (Ledoit and Wolf, 2004a). The shrinkage intensities are taken from the corresponding publications. For (14) the parameter is based on (Ledoit and Wolf, 2004b), for (15) it follows (Fisher and Sun, 2011) and (Touloumis, 2015) while it is taken from (Ledoit and Wolf, 2004a) in the case of (16). The question remains whether the additional term consisting of the old covariance matrix in (3) remains necessary or whether the ES may operate solely with shrinkage. Our preliminary investigations indicate that the latter strategies perform worse than the original CMSA-ES but more detailed investigations will be carried out.

5 EXPERIMENTAL ANALYSIS

Experiments were performed to investigate the shrinkage estimators introduced. First, the question of finding a suitable transformation was addressed. To

this end, a comparison of the effects of (11) - (13) was conducted for a combination of (15) and the shrinkage intensity from (Touloumis, 2015). The experiments showed that using (12) provided the best results for this combination. Therefore, the remaining discussion in this paper is restricted to ESs using the new covariance matrix. However, as we will see below, the increased variability provided by (11) should be considered together with (16) or (14) in further experiments. The analysis considers ES-algorithms which use shrinkage estimators as defined in (14) to (16). Aside from the CMSA-ES, we denote the strategies as follows

1. CI-ES: a CMSA-ES using (14) as shrinkage target,
2. CC-ES: the CMSA-ES with the constant correlation model (16),
3. FS-ES: the CMSA-ES which uses (15) and follows (Fisher and Sun, 2011) to determine the shrinkage intensity,
4. Tou-ES: a CMSA-ES based on (15) which uses the shrinkage intensity of (Touloumis, 2015).

The approaches were coded in MATLAB. In the case of the CI-ES and the CC-ES we used the estimation source code provided by the authors on their webpage¹. The implementation of the Tou-ES follows closely the R package².

5.1 Experimental Set-up

The parameters for the experiments read as follows. Each experiment uses 15 repeats. The initial population is drawn uniformly from $[-4, 4]^N$, whereas the mutation strength is chosen from $[0.25, 1]$. The search space dimensions were set to $N = 5, 10, 20$, and 40. The maximal number of fitness evaluations is set to $FE_{\max} = 2 \times 10^5 N$. All evolution strategies use $\lambda = \lceil \log(3N) + 8 \rceil$ offspring and $\mu = \lceil \lambda/4 \rceil$ parents. A run terminates prematurely if the difference between the best value so far and the optimal fitness value $|f_{\text{best}} - f_{\text{opt}}|$ is below a predefined precision set to 10^{-8} . Furthermore, we introduce a restart mechanism into the ESs so that the search is re-initialised when the search has stagnated for $10 + \lceil 30N/\lambda \rceil$ generations. Stagnation is determined by measuring the best function values in a generation. If the difference between minimal and maximal values of the sample lies below 10^{-8} for the given time-interval, the ES does not make significant movements anymore and the search is started anew.

¹<http://www.econ.uzh.ch/faculty/wolf/publications.html>

²<http://cran.r-project.org/web/packages/ShrinkCovMat>

The experiments are conducted with the help of the black box optimization benchmarking (BBOB) software framework and the test suite, see (Hansen et al., 2012). The framework allows the analysis of algorithms and provides means to generate tables and figures of the results.

This paper considers 24 noise-less functions (Finck et al., 2010). They consist of four subgroups: separable functions (function ids 1-5), functions with low/moderate conditioning (ids 6-9), functions with high conditioning (ids 10-14), and two groups of multimodal functions (ids 15-24).

The experiments use the expected running time (ERT) as performance measure. The ERT is defined as the expected value of the function evaluations (f -evaluations) the algorithm needs to reach the target value with the required precision for the first time, see (Hansen et al., 2012). In this paper, the estimate

$$ERT = \frac{\#(FES(f_{\text{best}} \geq f_{\text{target}}))}{\#succ} \quad (17)$$

is used, that is, the fitness evaluations $FES(f_{\text{best}} \geq f_{\text{target}})$ of each run until the fitness of the best individual is smaller than the target value are summed up and divided by the number of successful runs.

5.2 Results and Discussion

First of all, let us take a look at the behavior of the strategies for two exemplary functions, the sphere, $f(\mathbf{x}) = \|\mathbf{x}\|^2$, and the discus, $f(\mathbf{x}) = 10^6 x_1^2 + \sum_{i=2}^N x_i^2$. Figure 2 shows the ratio of the largest to the smallest eigenvalue of the covariance matrix for the CMSA-ES and for one of the shrinkage approaches, the CC-ES. In the case of the sphere, the figures illustrate that the largest and smallest eigenvalue develop differently and diverge for $N = 10$. Shrinkage causes the problem to be less pronounced. In the case of the discus, different eigenvalues are expected. Both strategies achieve this, the CC-ES shows again a lower rate of increase. This may be a hint that the adaptation process of the covariance matrix may be decelerated by the additional shrinkage. Whether this lowers the performance is investigated in the experiments with the complete test suite.

The results of the experiments are summarized by Tables 1 - 3. They provide the estimate of the expected running time (ERT) for several precision targets ranging from 10^1 to 10^{-7} . Also shown is the number of successful runs. Several functions represent challenges for the ESs considered. These comprise the Rastrigin functions (id 3, id 4, id 15, and id 24) of the test suite, the step ellipsoidal function with a condition number of 100 (id 7), and a multimodal function with a weak global structure based on

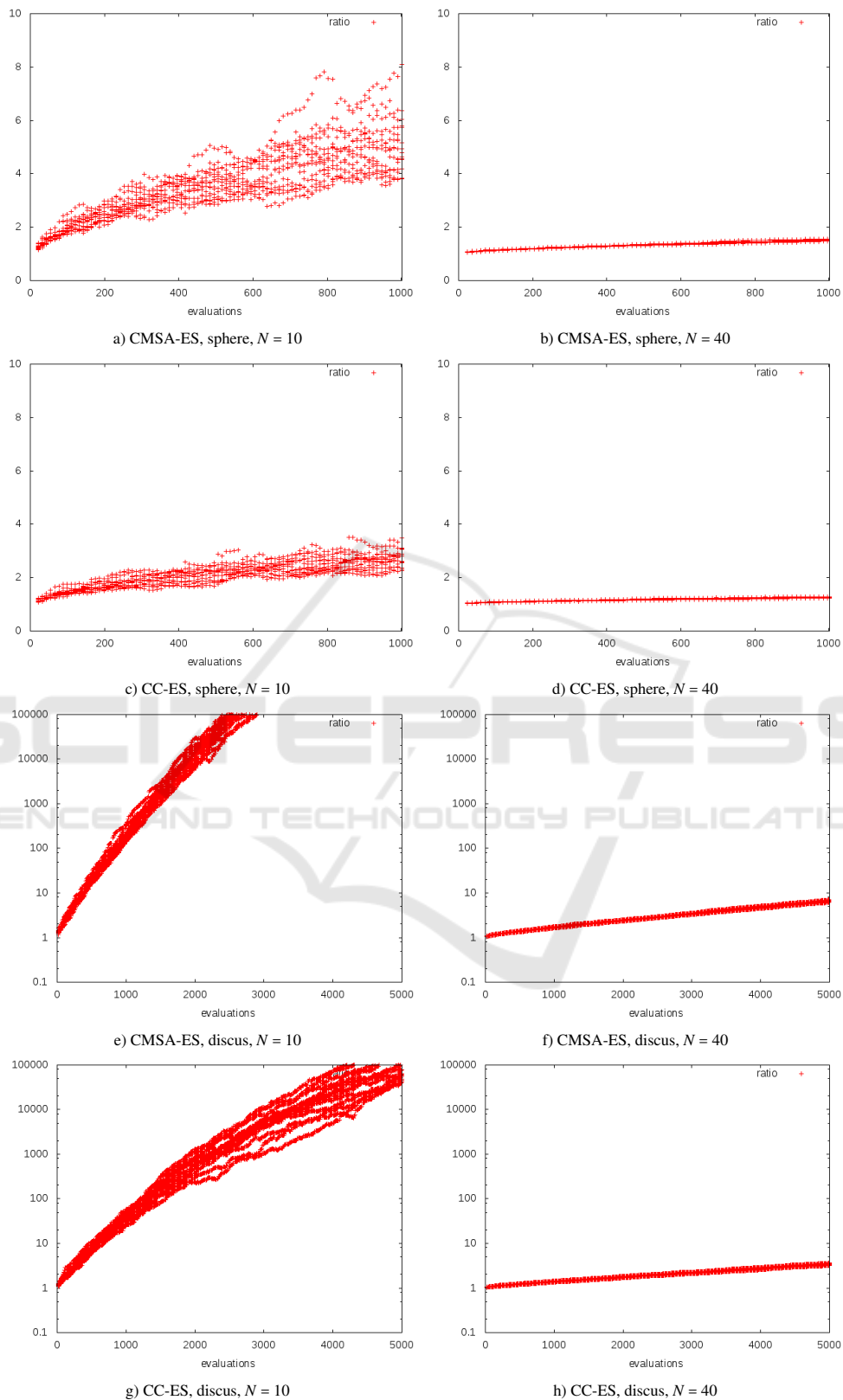


Figure 2: The development of the ratio of the largest to the smallest eigenvalue of the covariance on the sphere and the discus. Shown are the results from 15runs per dimensionality.

Table 1: Expected running time (ERT in number of function evaluations) divided by the respective best ERT measured during BBOB-2009 in dimension 10. The ERT and in braces, as dispersion measure, the half difference between 90 and 10%-tile of bootstrapped run lengths appear for each algorithm and target, the corresponding best ERT in the first row. The different target Δf -values are shown in the top row. #succ is the number of trials that reached the (final) target $f_{opt} + 10^{-8}$. The median number of conducted function evaluations is additionally given in *italics*, if the target in the last column was never reached.

		10-D																
Δf_{opt}	1e1	1e0	1e-1	1e-2	1e-3	1e-5	1e-7	23	#succ	Δf_{opt}	1e1	1e0	1e-1	1e-2	1e-3	1e-5	1e-7	#succ
f1	22	23	23	23	23	23	23	23	15/15	f12	515	896	1240	1390	1569	3660	5154	15/15
CMSA	4.0(2)	8.6(3)	14(5)	19(3)	26(5)	38(6)	50(5)		15/15	CMSA	4.2(0.2)	10(6)	13(13)	15(13)	16(9)	8.8(5)	7.8(2)	15/15
CC-ES	3.7(2)	8.4(3)	13(3)	18(3)	23(3)	35(5)	45(3)		15/15	CC-ES	11(18)	37(15)	68(142)	161(241)	572(444)	∞	∞ 2e5	0/15
CI-ES	4.2(1)	9.3(4)	14(4)	19(5)	24(4)	34(6)	43(2)		15/15	CI-ES	29(97)	615(669)	2258(4031)	2020(1655)	∞	∞	∞ 2e5	0/15
Tou-ES	4.2(2)	9.1(3)	15(4)	21(3)	27(4)	40(7)	54(11)		15/15	Tou-ES	76(228)	177(170)	722(1674)	1016(1115)	910(970)	799(464)	569(378)	15/15
FS-ES	4.2(2)	10(2)	14(4)	19(2)	25(4)	37(5)	49(6)		15/15	FS-ES	2.3(2)	10(12)	13(8)	15(8)	16(10)	10(5)	10(6)	15/15

Schwefel (id 20). In these cases, all strategies are unable to progress further than the first intermediate precision of 10^1 . Additionally, for the multi-modal functions, 19 (Composite Griewank-Rosenbrock Function) and 23 (Katsuura), no strategy could reach 10^{-1} . The functions in question are removed from the tables.

To analyze the remaining functions, the four groups of the test suite are taken into account. The first class comprises the separable functions with id 1 to id 5. The three remaining functions, the sphere (f1), the separable ellipsoidal function (f2), and the linear slope (f5) differ in the degree of difficulty for the strategies. All strategies do not show any prob-

ities. However, more experiments should be carried out.

Functions with high conditioning constitute the next group. The ellipsoidal function (f10), the discus (f11), the bent cigar (f12), the sharp ridge (f13), and the different powers function (f14). Here, similar behaviors can be observed for the CMSA-ES and the FS-ES with no clear advantage for either variant. Both are able to reach the final target precision on the functions with the exception of the sharp ridge where only two successful runs are recorded for $N = 10$ in both cases. Again, these may be due to initialization effects and should be treated therefore with care.

In the case of the multi-modal functions (ids 15-24), all ESs encounter problems. Only for the two Gallagher's problems (id 21 and id 22) successes are recorded. Here, the CMSA-ES and the versions that use the diagonal elements of the sample covariance as shrinkage target show the best results. The FS-ES appears to be a good choice for $N = 10$. For $N = 20$ and $N = 40$, only a few runs of all ESs reach the final target precision. Therefore, a comparison for the higher-dimensional search spaces is difficult and is not carried out in this paper. We will conduct further experiments with a higher setting for the maximal number of fitness evaluations in future work.

6 CONCLUSIONS

Evolution strategies rely on mutation as their main search operator. This necessitates control and adaptation mechanisms. This paper considered the covariance matrix adaptation together with self-adaptation. Here, as for other approaches, the sample covariance plays an important role. This estimate should be treated with care, however, since it may not be reliable in all cases. This holds especially if the sample size is small with respect to the search space dimensionality and therefore for most application cases of evolution strategies. The paper provided an experimental analysis of shrinkage operators, an approach introduced in statistics for correcting the sample covariance. The covariance is shrunk towards a target and thus "corrected". The choice of the target and the combination weight, the shrinkage intensity, are crucial. Since the functions to be optimized may assume various structures, the approach must remain sufficiently adaptable. To achieve this, we considered a transformation of the original search space. The experimental analysis took several shrinkage targets into account using the intensity settings of the original publications. Pending further experiments that shall provide more information regarding the shrinkage intensity which

may have interfered with the findings, shrinkage targets in the transformed space that use a diagonal matrix consisting of the different entries of the transformed sample covariance appear as the best choices. Since the original covariance matrix adaptation performs a further type of shrinkage which lessens the influence of the sample covariance when the search space dimensionality increases, effects may be more pronounced for midsize dimensionalities. Future research will focus on the shrinkage intensity and its interaction with the covariance matrix adaptation.

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