Adapting the Covariance Matrix in Evolution Strategies

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Abstract: Evolution strategies belong to the best performing modern natural computing methods for continuous optimization. This paper addresses the covariance matrix adaptation which is central to the algorithm. Nearly all approaches so far consider the sample covariance as one of the main factors for the adaptation. However, as known from modern statistics, this estimate may be of poor quality in many cases. Unfortunately, these cases are encountered often in practical applications. This paper explores the use of different previously unexplored estimates.

1 INTRODUCTION

Black-Box optimization is an important subcategory of optimization. Over the years, several methods have been developed - ranging from simple pattern search over mesh adaptive methods to natural computing, see e.g. (Audet, 2013; Conn et al., 2009; Eiben and Smith, 2003). This paper focuses on evolution strategies (ESs) which represent well-performing metaheuristics for continuous, non-linear optimization. In recent workshops on black-box optimization, see e.g. (Hansen et al., 2010), variants of this particular subtype of evolutionary algorithms have emerged as one the best performing methods among a broad range of competitors stemming from natural computing. Evolution strategies rely primarily on random changes to move through the search space. These random changes, usually normally distributed random variables, must be controlled by adapting both, the extend and the direction of the movements.

Modern evolution strategies apply therefore covariance matrix and step-size adaptation – with great success. However, most methods use the common estimate of the population covariance matrix as one component to guide the search. Here, there may be room for further improvement, especially with regard to common application cases of evolution strategies which usually concern optimization in highdimensional search spaces. For efficiency reasons, the population size λ , that is, the number of candidate solutions, is kept below the search space dimensionality N and scales usually with $O(\log(N))$ or with O(N). In other words, either $\lambda \ll N$ or $\lambda \approx N$ which may represent a problem when using the sample covariance matrix. This even more so, since the sample size used in the estimation is just a fraction of the population size. Furthermore, the result is not robust against outliers which may appear in practical optimization which has often to cope with noise. This paper introduces and explores new approaches addressing the first problem by developing a new estimate for the covariance matrix. To our knowledge, these estimators have not been applied to evolution strategies before.

The paper is structured as follows: First, evolution strategies are introduced and common ways to adapt the covariance matrix are described and explained. Afterwards, we point out a potential dangerous weakness of the traditionally used estimate of the population covariance. Candidates for better estimates are presented and described in the following section. We propose and investigate several approaches ranging from a transfer of shrinkage estimators over a maximum entropy covariance selection principle to a new combination of both approaches. The quality of the resulting algorithms is assessed in the experimental test section. Conclusions and possible further research directions constitute the last part of the paper.

1.1 Evolution Strategies

Evolutionary algorithms (EAs) (Eiben and Smith, 2003) are population-based stochastic search and optimization algorithms including today genetic algorithms, genetic programming, (natural) evolution strategies, evolutionary programming, and differential evolution. As a rule, they require only weak pre-

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conditions on the function to be optimized. Therefore, they are applicable in cases when only pointwise function evaluations are possible.

An evolutionary algorithm starts with an initial population of candidate solutions. The individuals are either drawn randomly from the search space or are initialized according to previous information on good solutions. A subset of the parent population is chosen for the creation of the offspring. This process is termed parent selection. Creation normally consists of recombination and mutation. While recombination combines traits from two or more parents, mutation is an unary operator and is realized by random perturbations. After the offspring have been created, survivor selection is performed to determine the next parent population. Evolutionary algorithms differ in the representation of the solutions and in the realization of the selection, recombination, and mutation operators.

Evolution strategies (ESs) (Rechenberg, 1973; Schwefel, 1981) are a variant of evolutionary algorithms that is predominantly applied in continuous search spaces. Evolution strategies are commonly notated as $(\mu/\rho, \lambda)$ -ESs. The parameter μ stands for the size of the parent population. In the case of recombination, p parents are chosen randomly and are combined for the recombination result. While other forms exist, recombination usually consists of determining the weighted mean of the parents (Beyer and Schwefel, 2002). The result is then mutated by adding a normally distributed random variable with zero mean and covariance matrix $\sigma^2 C$. While there are ESs that operate without recombination, the mutation process is essential and can be seen as the main search operator. Afterwards, the individuals are evaluated using the function to be optimized or a derived function which allows an easy ranking of the population. Only the rank of an individual is important for the selection.

There are two main types of evolution strategies: Evolution strategies with "plus"-selection and ESs with "comma"-selection. The first select the μ -best offspring and parents as the next parent population, where ESs with "comma"-selection discard the old parent population completely and take only the best offspring. Figure 1 shows the general algorithm. The symbol S_m denotes the control parameters of the mutation. Evolution strategies need to adapt the covariance matrix for the mutation during the run. Evolution strategies with ill-adapted parameters converge only slowly or may fail in the optimization. Methods for adapting the scale factor σ or the full covariance matrix have received a lot of attention (see (Meyer-Nieberg and Beyer, 2007)). The main approaches are described in the following section.



Figure 1: A generic $(\mu/\rho + \lambda)$ -ES (cf. (Beyer, 2001, p. 8)). The notation is common in evolution strategies and denotes a strategy with μ parents and λ offspring using either plus or comma-selection. Recombination uses ρ parents for each offspring.

1.2 Updating the Covariance Matrix

First, the update of the covariance matrix is addressed. In evolution strategies two types exist: one applied in the *covariance matrix adaptation evolution strategy* (CMA-ES) (Hansen and Ostermeier, 2001) which considers past information from the search and an alternative used by the *covariance matrix selfadaptation evolution strategy* (CMSA-ES) (Beyer and Sendhoff, 2008) which focusses more on the present population.

The covariance matrix update of the CMA-ES is explained first. The CMA-ES uses weighted intermediate recombination, in other words, it computes the weighted centroid of the μ best individuals of the population. This mean $\mathbf{m}^{(g)}$ is used for creating all offspring by adding a random vector drawn from a normal distribution with covariance matrix $(\sigma^{(g)})^2 \mathbf{C}^{(g)}$, i.e., the actual covariance matrix consists of a general scaling factor (or step-size or mutation strength) and the matrix denoting the directions. Following usual notation in evolution strategies this matrix $\mathbf{C}^{(g)}$ will be referred to as *covariance matrix* in the following.

The basis for the CMA update is the common estimate of the covariance matrix using the newly created population. Instead of considering the whole population for deriving the estimates, though, it introduces a bias towards good search regions by taking only the μ best individuals into account. Furthermore, it does not estimate the mean anew but uses the weighted mean $\mathbf{m}^{(g)}$. Following (Hansen and Ostermeier, 2001),

$$\mathbf{y}_{m:\lambda}^{(g+1)} := \frac{1}{\mathbf{\sigma}^{(g)}} \left(\mathbf{x}_{m:\lambda}^{(g+1)} - \mathbf{m}^{(g)} \right) \tag{1}$$

are determined with $\mathbf{x}_{m:\lambda}$ denoting the *m*th best of the λ particle according to the fitness ranking. The rank- μ update the obtains the covariance matrix as

$$\mathbf{C}_{\mu}^{(g+1)} := \sum_{m=1}^{\mu} w_m \mathbf{y}_{m:\lambda}^{(g+1)} (\mathbf{y}_{m:\lambda}^{(g+1)})^{\mathrm{T}}$$
(2)

To derive reliable estimates larger population sizes are usually necessary which is detrimental with regard to the algorithm's speed. Therefore, past information, that is, past covariance matrizes are usually also considered

$$\mathbf{C}^{(g+1)} := (1 - c_{\mu})C^{(g)} + c_{\mu}\mathbf{C}^{(g+1)}_{\mu} \qquad (3)$$

with parameter $0 \le c_{\mu} \le 1$ determining the effective time-horizon. In CMA-ESs, it has been found that an enhance of the general search direction in the covariance matrix is usual beneficial. For this, the concepts of the *evolutionary path* and the *rank-one-update* are introduced. As its name already suggests, an evolutionary path considers the path in the search space the population has taken so far. The weighted means serve as representatives. Defining

$$\mathbf{v}^{(g+1)} := \frac{\mathbf{m}^{(g+1)} - \mathbf{m}^{(g)}}{\mathbf{\sigma}^{(g)}}$$

the evolutionary path reads

$$\mathbf{p}_{c}^{(g+1)} := (1 - c_{c})\mathbf{p}_{c}^{(g)} + \sqrt{c_{c}(2 - c_{c})\mu_{\text{eff}}} \left(\frac{\mathbf{m}^{(g+1)} - \mathbf{m}^{(g)}}{\mathbf{\sigma}^{(g)}}\right).$$
(4)

For details on the parameters, see e.g. (Hansen, 2006). The evolutionary path gives a general search direction that the ES has taken in the recent past. In order to bias the covariance matrix accordingly, the rank-one-update

$$\mathbf{C}_{1}^{(g+1)} := \mathbf{p}_{c}^{(g+1)} (\mathbf{p}_{c}^{(g+1)})^{\mathrm{T}}$$
(5)

is performed and used as a further component of the covariance matrix. A normal distribution with covariance $\mathbf{C}_{1}^{(g+1)}$ leads towards a one-dimensional distribution on the line defined by $\mathbf{p}_{c}^{(g+1)}$. With (5) and (3), the final covariance update of the CMA-ES reads

$$\mathbf{C}^{(g+1)} := (1 - c_1 - c_\mu) \mathbf{C}^{(g)} + c_1 \mathbf{C}_1^{(g+1)} + c_\mu \mathbf{C}_\mu^{(g+1)}.$$
(6)

The CMA-ES is one of the most powerful evolution strategies. However, as pointed out in (Beyer and Sendhoff, 2008), its scaling behavior with the population size is not good. The alternative approach of the CMSA-ES (Beyer and Sendhoff, 2008) updates the covariance matrix differently. Considering again the definition (1), the covariance update is a convex combination of the old covariance and the population covariance, i.e., the rank- μ update

$$\mathbf{C}^{(g+1)} := (1 - \frac{1}{c_{\tau}})\mathbf{C}^{(g)} + \frac{1}{c_{\tau}} \sum_{m=1}^{\mu} w_m \mathbf{y}_{m:\lambda}^{(g+1)} (\mathbf{y}_{m:\lambda}^{(g+1)})^{\mathrm{T}}$$
(7)

with the weights usually set to $w_m = 1/\mu$. See (Beyer and Sendhoff, 2008) for information on the free parameter c_{τ} .

1.3 Step-size Adaptation

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The CMA-ES uses the so-called *cumulative step-size adaptation* (CSA) to control the scaling parameter (also called *step-size*, *mutation strength* or *step-length*) (Hansen, 2006). To this end, the CSA determines again an evolutionary path by summating the movement of the population centers

$$\mathbf{p}_{\sigma}^{(g+1)} = (1 - c_{\sigma})\mathbf{p}_{\sigma}^{(g)} + \sqrt{c_{\sigma}(2 - c_{\sigma})\mu_{\text{eff}}}(\mathbf{C}^{(g)})^{-\frac{1}{2}} \times \frac{\mathbf{m}^{(g+1)} - \mathbf{m}^{(g)}}{\sigma^{(g)}}$$
(8)

eliminating the influence of the covariance matrix and the step length. For a detailed description of the parameters, see (Hansen, 2006). The length of the path in (8) is important. In the case of short path lengths, several movement of the centers counteract each other which is an indication that the step-size is too large and should be reduced. If on the other hand, the ES takes several consecutive steps in approximately the same direction, progress and algorithm speed would be improved, if larger changes were possible. Long path lengths, therefore, are an indicator for a required increase of the step length. Ideally, the CSA should result in uncorrelated steps.

After some calculations, see (Hansen, 2006), the ideal situation is revealed as standard normally distributed steps, which leads to

$$\ln(\boldsymbol{\sigma}^{(g+1)}) = \ln(\boldsymbol{\sigma}^{(g)}) + \frac{c_{\boldsymbol{\sigma}}}{d_{\boldsymbol{\sigma}}} \Big(\frac{\|\mathbf{p}_{\boldsymbol{\sigma}}^{(g+1)}\| - \mu_{\boldsymbol{\chi}_n}}{\mu_{\boldsymbol{\chi}_n}} \Big) \qquad (9)$$

as the CSA-rule. The change is multiplicative in order to avoid numerical problems and results in nonnegative scaling parameters. The parameter μ_{χ_n} in (9) stands for the mean of the χ -distribution with *n* degrees of freedom. If a random variable follows a χ_n^2 distribution, its square root is χ -distributed. The degrees of freedom coincide with the search space dimension. The CSA-rule works well in many application cases. It can be shown, however, that the original CSA encounter problems in large noise regimes resulting in a loss of step-size control and premature convergence. Therefore, uncertainty handling procedures and other safeguards are advisable.

An alternative approach for adapting the step-size is self-adaptation first introduced in (Rechenberg, 1973) and developed further in (Schwefel, 1981). It subjects the strategy parameters of the mutation to evolution. In other words, the scaling parameter or in its full form, the whole covariance matrix, undergoes recombination, mutation, and indirect selection processes. The working principle is based on an indirect stochastic linkage between good individuals and appropriate parameters: On average good parameters should lead to better offspring than too large or too small values or misleading directions. Although selfadaptation has been developed to adapt the whole covariance matrix, it is used nowadays mainly to adapt the step-size or a diagonal covariance matrix. In the case of the mutation strength, usually a log-normal distribution

$$\sigma_l^{(g)} = \sigma_{\text{base}} \exp(\tau \mathcal{N}(0, 1))$$
(10)

is used for mutation. The parameter τ is called the *learning rate* and is usually chosen to scale with $1/\sqrt{2N}$. The variable σ_{base} is either the parental scale factor or the result of recombination. For the stepsize, it is possible to apply the same type of recombination as for the positions although different forms – for instance a multiplicative combination – could be used instead. The self-adaptation of the step-size is referred to as σ -self-adaptation (σ SA) in the remainder of this paper.

The newly created mutation strength is then directly used in the mutation of the offspring. If the resulting offspring is sufficiently good, the scale factor is passed to the next generation. The baseline σ_{base} is either the mutation strength of the parent or if recombination is used the recombination result. Self-adaptation with recombination has been shown to be "robust" against noise (Beyer and Meyer-Nieberg, 2006) and is used in the CMSA-ES as update rule for the scaling factor. In (Beyer and Sendhoff, 2008) it was found that the CMSA-ES performs comparably to the CMA-ES for smaller populations but is less computational expensive for larger population sizes.

2 WHY THE COVARIANCE ESTIMATOR SHOULD BE CHANGED

The covariance matrix C_{μ} which appears in (2) and (7) can be interpreted as the sample covariance matrix with sample size μ . Two differences are present. The first using μ instead of $\mu - 1$ can be explained by using the known mean instead of an estimate. The second lies in the non-identically distributed random variables of the population since order statistics appear. We will disregard that problem for the time being.

In the case of identically independently distributed random variables, the estimate converges almost surely towards the "true" covariance Σ for $\mu \to \infty$. In addition, the sample covariance matrix is related (in our case equal) to the maximum likelihood (ML) estimator of Σ . Both facts serve a justification to take C_{μ} as the substitute for the unknown true covariance for large μ . However, the quality of the estimate can be quite poor if $\mu < N$ or even $\mu \approx N$.

This was first discovered by Stein (Stein, 1956; Stein, 1975). Stein's phenomenon states that while the ML estimate is often seen as the best possible guess, its quality may be poor and can be improved in many cases. This holds especially for high-dimensional spaces. The same problem transfers to covariance matrix estimation, see (Schäffer and Strimmer, 2005). Also recognized by Stein, in case of small ratios μ/N the eigenstructure of C_{μ} may not agree well with the true eigenstructure of Σ . As stated in (Ledoit and Wolf, 2004), the largest eigenvalue has a tendency towards too large values, whereas the smallest shows the opposite behavior. This results in a larger spectrum of the sample covariance matrix with respect to the true covariance for $N/\mu \not\rightarrow 0$ for $\mu, N \rightarrow \infty$ (Bai and Silverstein, 1998). As found by Huber (Huber, 1981), a heavy tail distribution leads also to a distortion of the sample covariance.

In statistics, considerable efforts have been made to find more reliable and robust estimates. Owing to the great inportance of the covariance matrix in data mining and other statistical analyses, work is still ongoing. The following section provides a short introduction before focussing on the approach used for evolution strategies.

3 ESTIMATING THE COVARIANCE

As stated above, the estimation of high-dimensional covariance matrices has received a lot of attention, see e.g. (Chen et al., 2012). Several types have been introduced, for example: shrinkage estimators, banding and tapering estimators, sparse matrix transform estimators, and the graphical Lasso estimator. This paper concentrates on shrinkage estimators and on an idea inspired by a maximum entropy approach. Both classes can be computed comparatively efficiently. Future research will consider other classes of estimators.

3.1 Shrinkage Estimators

Most (linear) shrinkage estimators use the convex combination

$$\mathbf{S}_{est}(\mathbf{\rho}) = \mathbf{\rho}\mathbf{F} + (1-\mathbf{\rho})\mathbf{C}_{\mu} \qquad (11)$$

with **F** the *target* to correct the estimate provided by the sample covariance. The parameter $\rho \in]0,1[$ is called the *shrinkage intensity*. Equation (11) is used to shrink the eigenvalues of **C**_µ towards the eigenvalues of **F**. The shrinkage intensity ρ should be chosen to minimize

$$\mathbf{E}\Big(\|\mathbf{S}_{est}(\boldsymbol{\rho}) - \boldsymbol{\Sigma}\|_F^2\Big) \tag{12}$$

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

$$\|\mathbf{A}\|_{F}^{2} = \frac{1}{N} \operatorname{Tr} \left[\mathbf{A} \mathbf{A}^{\mathrm{T}} \right], \qquad (13)$$

see (Ledoit and Wolf, 2004). To solve this problem, knowledge of the true covariance Σ would be required which is unobtainable in most cases.

Starting from (12), Ledoit and Wolf obtained an analytical expression for the optimal shrinkage intensity for the target $\mathbf{F} = \text{Tr}(\mathbf{C}_{\mu})/N\mathbf{I}$. The result does not make assumptions on the underlying distribution. In the case of $\mu \approx N$ or vastly different eigenvalues, the shrinkage estimator does not differ much from the sample covariance matrix, however.

Other authors introduced different estimators, see e.g. (Chen et al., 2010) or (Chen et al., 2012)). Ledoit and Wolfe themselves considered non-linear shrinkage estimators (Ledoit and Wolf, 2012). Most of the approaches require larger computational efforts. In the case of the non-linear shrinkage, for example, the authors are faced with a non-linear, non-convex optimization problem, which they solve by using sequential linear programming (Ledoit and Wolf, 2012). A general analytical expression is unobtainable, however. Shrinkage estimators and other estimators aside from the standard case have not been used in in evolution strategies before. A literature review resulted in one application in the case of Gaussian based 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. 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, 2004) but made the shrinkage intensity adaptable.

Interestingly, (3), (6), and (7) of the ES algorithm can be interpreted as a special case of shrinkage. In the case of the CMSA-ES, for example, the estimate is shrunk towards the old covariance matrix. The shrinkage intensity is determined by

$$= 1 + \frac{N(N+1)}{2\mu}$$
(14)

as $\rho = 1 - 1/c_{\tau}$. As long as the increase of μ with the dimensionality *N* is below $O(N^2)$, the coefficient (14) approaches infinity for $N \to \infty$. Since the contribution of the sample covariance to the new covariance in (7) is weighted with $1/c_{\tau}$, its influence fades out for increasing dimensions. It is the aim of the paper to investigate whether a further shrinkage can improve the result.

Our first experiments were concerned with transferring shrinkage estimators to ESs. The situation in which the estimation takes place in the case of evolution strategies differs from the assumptions in literature. The covariance matrix $\Sigma = \mathbf{C}^{g-1}$ that was used to create the offspring is known. This would enable the use of oracle estimators normally used to start the calculations deriving the estimates. However, since the sample is based on rank-based selection, the covariance matrix of the sample will differ to some extend. Neglecting the selection pressure in a first approach, the sample $\mathbf{x}_1, \ldots, \mathbf{x}_{\mu}$ would represent normally distributed random variables. For this scenario, the sample covariance matrix C_{μ} would be shrunk towards the shrinkage target **F** by choosing ρ as the minimizer of (12).

Since most shrinkage approaches consider diagonal matrices as shrinkage targets, we choose the matrix $\mathbf{F} = \text{diag}(\mathbf{C}_{\mu})$, that is, the diagonal elements of the sample covariance matrix are unchanged and only the off-diagonal entries are decreased. Following (Fisher and Sun, 2011), the optimal intensity of the oracle reads

$$\rho = 1 - \frac{\alpha_D^2 + \gamma_S^2}{\delta_D^2} \tag{15}$$

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with

$$\alpha_D^2 = \frac{1}{\mu N} \Big(\mathrm{Tr}(\Sigma \Sigma^{\mathrm{T}}) + \mathrm{Tr}(\Sigma)^2 \Big), \qquad (16)$$

$$\gamma_D^2 = -\frac{2}{\mu N} \operatorname{Tr}\left(\operatorname{diag}(\Sigma)^2\right), \qquad (17)$$

and

$$\delta_D^2 = \frac{1}{\mu N} \Big((\mu + 1) \operatorname{Tr}(\Sigma \Sigma^{\mathrm{T}}) + \operatorname{Tr}(\Sigma)^2 - (\mu + 2) \operatorname{Tr}(\operatorname{diag}(\Sigma)^2) \Big).$$
(18)

A first approach for evolution strategies would be to apply the shrinkage above, starting with the "ideal" shrinkage intensity and to use then the shrinkage result as the new population covariance in the rank- μ update. However, a shrinkage towards a diagonal does not appear to be a good idea for optimizing functions that are not oriented towards the coordinate system. Experiments with ESs validated this assumption.

3.2 A Maximum Entropy Covariance Estimation

Therefore, we make use of another concept following (Thomaz et al., 2004). Confronted with the problem of determining a reliable covariance matrix by combining a sample covariance matrix with a pooled variance matrix, the authors introduced a *maximum entropy covariance selection principle*. Since a combination of covariance matrices also appears in evolution strategies, a closer look at their approach is interesting. Defining a population matrix C_p and the sample covariance matrix S_i , the mixture

$$\mathbf{S}_{mix}(\mathbf{\eta}) = \mathbf{\eta} \mathbf{C}_p + (1 - \mathbf{\eta}) \mathbf{S}_i \tag{19}$$

was considered. In departure from usual approaches, focus lay on the combination of the two matrixes that maximizes the entropy. To this end, the coordinate system was changed to the eigenspace of $\mathbf{S}_{mix}(1)$. Let \mathbf{M}_S denote the (normalized) eigenvectors of the mixture matrix. The representations of \mathbf{C}_p and \mathbf{S}_i in this coordination system read

$$\Phi^{C} = \mathbf{M}_{S}^{\mathrm{T}} \mathbf{C}_{p} \mathbf{M}_{S}$$
$$\Phi^{S} = \mathbf{M}_{S}^{\mathrm{T}} \mathbf{S}_{i} \mathbf{M}_{S}.$$
(20)

Both matrices are usually not diagonal. To construct the new estimate for the covariance matrix,

$$\Lambda^{C} = \operatorname{diag}(\Phi^{C})$$

$$\Lambda^{S} = \operatorname{diag}(\Phi^{S})$$
(21)

were determined. By taking $\lambda_i = \max(\lambda_i^C, \lambda_i^S)$, a covariance matrix estimate could finally be constructed via $\mathbf{M}_S \Lambda \mathbf{M}_S^T$. The approach maximizes the possible contributions to the principal direction of the mixture matrix and is based on a maximum entropy derivation for the estimation.

3.3 New Covariance Estimators

This paper proposes a combination of a shrinkage estimator and the basis transformation introduced (Thomaz et al., 2004) for a use in evolution strategies. The aim is to switch towards a suitable coordinate system and then either to discard the contributions of the sample covariance that are not properly aligned or to shrink the off-diagonal components. Two choices for the mixture matrix represent themselves. The first

$$\mathbf{S}_{mix} = \mathbf{C}^g + \mathbf{C}_\mu \tag{22}$$

is be chosen in accordance to (Thomaz et al., 2004). The second takes the covariance result that would have been used in the original CMSA-ES

$$\mathbf{S}_{mix} = (1 - c_{\tau})\mathbf{C}^g + c_{\tau}\mathbf{C}_{\mu} \tag{23}$$

and is considered even more appropriate for very small samples. Both choices will be investigated in this paper. They in turn can be coupled with several further ways to proceed. Switching towards the eigenspace of S_{mix} , results in the covariance matrix representations $\Phi_{\mu} := \mathbf{M}_{S}^{T} \mathbf{C}_{\mu} \mathbf{M}_{S}$ and $\Phi_{\Sigma} := \mathbf{M}_{S}^{T} \mathbf{C}^{g} \mathbf{M}_{S}$. The first approach for constructing a new estimate of the sample covariance is to apply the principle of maximal contribution to the axes from (Thomaz et al., 2004) and to determine

$$\Lambda_{\mu} = \max\left(\operatorname{diag}(\Phi_{\mu}), \operatorname{diag}(\Phi_{\Sigma})\right).$$
(24)

The sample covariance matrix can then be computed as $\mathbf{C}'_{\mu} = \mathbf{M}_{S} \Lambda_{\mu} \mathbf{M}_{S}^{T}$. Another approach would be to discard all entries of Φ_{μ} except the diagonal

$$\Lambda_{\mu} = \operatorname{diag}(\Phi_{\mu}). \tag{25}$$

A third approach consists of applying a shrinkage estimator like

$$\Phi_{\mu}^{S} = (1 - \rho)\Phi_{\mu} + \rho \operatorname{diag}(\Phi_{\mu})$$
(26)

with ρ for example determined by (15) with $\Sigma = \mathbf{M}_{S}^{T} \mathbf{C}^{g} \mathbf{M}_{S}$. This approach does not discard the offdiagonal entries completely. The shrinkage intensity ρ remains to be determined. First experiments will start with (15).

4 EXPERIMENTS

This section describes the experiments that were performed to explore the new approaches. For our investigation, the CMSA-ES version is considered since it operates just with the population covariance matrix and effects from changing the estimate should be easier to discerned. The competitors consist of algorithms which use shrinkage estimators as defined in (22) to (26). This code is not optimized for performance with respect to absolute computing time, since this paper aims at a proof of concept. The experiments are performed for the search space dimensions N = 2, 5, 10, and 20. The maximal number of fitness evaluations is $FE_{max} = 2 \times 10^4 N$. The CMSA-ES versions use $\lambda = \lfloor \log(3N) + 8 \rfloor$ offspring and $\mu = \lceil \lambda/4 \rceil$ parents. The start position of the algorithms is randomly chosen from a normal distribution with mean zero and standard deviation of 0.5. A run terminates prematurely if the difference between the best value obtained so far and the optimal fitness value $|f_{best} - f_{opt}|$ is below a predefined precision set to 10^{-8} . For each fitness function and dimension, 15 runs are used.

4.1 Test Suite

The experiments are performed with the black box optimization benchmarking (BBOB) software framework and the test suite introduced for the black box optimization workshops, see (Hansen et al., 2012). The aim of the workshop is to benchmark and compare metaheuristics and other direct search methods for continuous optimization. The framework allows the plug-in of algorithms adhering to a common interface and provides a comfortable way of generating the results in form of tables and figures.

The test suite contains noisy and noise-less functions with the position of the optimum changing randomly from run to run. This paper focuses on the 24 noise-less functions (Finck et al., 2010). They can be divided into four classes: 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). Among the unimodal functions with only one optimal point, there are separable functions which are given as

$$f(\mathbf{x}) = \sum_{i=1}^{N} f_i(x_i) \tag{27}$$

and can therefore be solved by optimizing each component separately. The simplest member of this class is the (quadratic) sphere with $f(\mathbf{x}) = ||\mathbf{x}||^2$. Other functions include ill-conditioned functions, like for instance the elliposoidal function, and multimodal functions (Rastrigin) which represent particular challenges for the optimization (Table 1).

4.2 Performance Measure

The following performance measure is used in accordance to (Hansen et al., 2012). The expected runTable 1: Some of the test functions used for the comparison of the algorithms. The variable z denotes a transformation of x in order to keep the algorithm from exploiting certain particularities of the function, see (Finck et al., 2010).

Sphere $f(\mathbf{x}) = \|\mathbf{z}\|^2$ Rosenbrock $f(\mathbf{x}) = \sum_{i=1}^{N-1} 200(z_i^2 - z_{i+1})^2 + (z_i - 1)^2$ Ellipsoidal $f(\mathbf{x}) = \sum_{i=1}^{N} 10^{6\frac{i-1}{N-1}} z_i^2$ Discus $f(\mathbf{x}) = 10^6 z_1^2 + \sum_{i=2}^{N} z_i^2$ Rastrigin $f(\mathbf{x}) = 10(N - \sum_{i=1}^{N} \cos(2\pi z_i)) + \|\mathbf{z}\|^2$



Figure 2: The CMSA-shr-ES. ERT loss ratio (in number of *f*-evaluations divided by dimension) divided by the best ERT seen in GECCO-BBOB-2009 for the target f_t , or, if the best algorithm reached a better target within the budget, the budget divided by the best ERT. Line: geometric mean. Box-Whisker error bar: 25-75%-ile with median (box), 10-90%-ile (caps), and minimum and maximum ERT loss ratio (points). The vertical line gives the maximal number of function evaluations in a single trial in this function subset.

ning time (ERT) gives 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, we use

$$ERT = \frac{\#(FEs(f_{best} \ge f_{target}))}{\#succ}$$
(28)

as an estimate by summing up the fitness evaluations $FEs(f_{\text{best}} \ge f_{\text{target}})$ of each run until the fitness of the best individual is smaller than the target value, divided by all successfull runs.



Figure 3: The CMSA-ES. ERT loss ratio (in number of f-evaluations divided by dimension) divided by the best ERT seen in GECCO-BBOB-2009 for the target f_t , or, if the best algorithm reached a better target within the budget, the budget divided by the best ERT. Line: geometric mean. Box-Whisker error bar: 25-75%-ile with median (box), 10-90%-ile (caps), and minimum and maximum ERT loss ratio (points). The vertical line gives the maximal number of function evaluations in a single trial in this function subset.

4.3 **Results and Discussion**

Due to space restrictions, Figure 4 and Tables 2-3 show only the results from the best experiments which were achieved for the variant which used (26) together with (23) as the transformation matrix (called CMSAshr-ES in the following). First of all, it should be noted that there is no significant advantage to either algorithm for the test suite functions. Tables 2 and 3 show the ERT loss ratio with respect to the best result from the BBOB 2009 workshop for predefined budgets given in the first column. The median performance of both algorithms improves with the dimension until the budget of 10^3 – which is interesting. An increase of the budget goes along with a decreased performance which is less pronounced for the CMSA-shr-ES in the case of the larger dimensional space. This indicates that the CMSA-shr-ES may perform more favorable in larger search spaces as envisioned. Further experiments which a larger maximal number of fitness evaluations and larger dimensional spaces will be conducted which should shed more light on the behavior. Furthermore, the decrease in performance with the budget hints at a search stagnation probably due to convergence into local optima. Restart strategies may be beneficial, but since they

have to be fitted to the algorithms, we do not apply them in the present paper.

Figure 4 shows the expected running time for reaching the precision of 10^{-8} for all 24 functions and search space dimensionalities. In the case of the separable functions (1-5), both algorithms show a very similar behavior, succeeding in optimizing the first two functions and exhibiting difficulties in the case of the difficult rastrigin variants. On the linear slope, the original CMSA-ES shows fewer expected function evaluations for smaller dimensions which starts to change when the dimensionality is increased. For the functions with ids 6-9, with moderate condition numbers, there are advantages to the CMSA-shr-ES, with the exception of the rotated rosenbrock (9). Most of the functions with high conditioning, ids 10-12, and 14, can be solved by both variants with slightly better results for the CMSA-ES. The sharp ridge (id 13) appears as problematic, with the CMSA-shr-ES showing fewer fitness evaluations for hitting the various precisions goals in Table 2.

Interestingly, the CMSA-shr variant seems to perform better for the difficult multimodal functions, e.g., Gallaghers 101 peak function, a finding which should be explored in more detail. The results for the last two multimodal functions can be explained in part in that the computing resources were insufficient for the optimization. Even the best performing algorithms from the BBOB workshop needed more resources than we used in our experiments.

Further experiments will be conducted in order to shed more light on the behavior. Special attention will be given to the choice of the shrinkage factor, since (15) is unlikely to be optimal and may have influenced the outcome strongly. Furthermore, the question remains whether the population size should be increased for the self-adaptation process. Also, larger search space dimensionalities than N = 20 are of interest.

5 CONCLUSIONS

Evolution strategies are well performing variants of evolutionary algorithms used in continuous optimization. They ultilize normally distributed mutations as their main search procedure. Their performance depends on the control of the mutation process which is governed by adapting step-sizes and covariance matrices. One possible improvement concerns the covariance matrix adaptation which makes use of the sample covariance matrix. In statistical research, this estimate has been identified as not agreeing well with the true covariance for the case of large dimensional



Figure 4: Expected running time (ERT in number of *f*-evaluations) divided by dimension for target function value 10^{-8} as \log_{10} values versus dimension. Different symbols correspond to different algorithms given in the legend of f_1 and f_{24} . Light symbols give the maximum number of function evaluations from the longest trial divided by dimension. Horizontal lines give linear scaling, slanted dotted lines give quadratic scaling. Black stars indicate statistically better result compared to all other algorithms with p < 0.01 and Bonferroni correction number of dimensions (six). Legend: .

spaces and small sample sizes, or more correctly for sample sizes that do not increase sufficiently fast with the dimensionality. While modern approaches for covariance matrix adaptation correct the estimate, the question arises whether the performance of these evolutionary algoTable 2: ERT in number of function evaluations divided by the best ERT measured during BBOB-2009 given in the respective first row with the central 80% range divided by two in brackets for different Δf values. #succ is the number of trials that reached the final target $f_{\text{opt}} + 10^{-8}$. 1:CMSA-S is CMSA-shr-ES and 2:CMSA is CMSA-ES. Bold entries are statistically significantly better compared to the other algorithm, with p = 0.05 or $p = 10^{-k}$ where $k \in \{2, 3, 4, ...\}$ is the number following the \star symbol, with Bonferroni correction of 48. A \downarrow indicates the same tested against the best BBOB-2009.

		5-D						20-D								
	Δf	1e+1	1e-1	1e-3	1e-5	1e-7	#succ	Δf	1e+1	1e-1	1e-3	1e-5	1e-7	#succ		
	1: CMSA-S	2.4(2)	12 12(4)	12 25(6)	12 38(8)	53(8)	15/15	1: CMSA-S	4.3 4.7(1)	43 15(3)	43 27(3)	43 38(2)	43 48(3)	15/15		
	2: CMSA	2.4(2)	12(4) 88	26(7) 90	40(8) 92	54(15) 94	15/15	2: CMSA	4.7(0.9)	14(2)	24(2)	35(3)	46(3)	15/15		
	1: CMSA-S	26(21)	44(24)	53(30)	56(30)	57(29)	15/15	1: CMSA-S	331(232)	567(121)	647(81)	704(91)	755(82)	15/15		
	2: CMSA	19(15)	47(19)	54(23)	60(23)	63(30)	15/15	2: CMSA	332(106)	561(127) 7635	637(154)	687(182)786(186)	14/15		
	1: CMSA-S	22(70)	0007	∞	∞	∞1.0e5	0/15	1: CMSA-S	∞	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	∞4.0e5	0/15		
	2: CMSA	94(140)	∞ 1699	∞ 1917	00	∞1.0e5	0/15	2: CMSA	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	∞4.0e5	0/15		
	1: CMSA-S	46(62)	000	∞	∞	∞1.0e5	0/15	1: CMSA-S	4722	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	∞	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	∞4.0e5	0/15		
	2: CMSA	186(247)	∞	∞	∞	∞1.0e5	0/15	2: CMSA		00	×	∞ 41	∞4.0e5	0/15		
	1: CMSA-S	8.6(3)	10 16(6)	17(6)	10 17(6)	17(6)	15/15	1: CMSA-S	41 10(3)	41 13(4)	41 13(4)	41 13(4)	41 13(4)	15/15		
	2: CMSA	8.2(3)	13(6)	14(6)	14(6)	14(6)	15/15	2: CMSA	11(3)	16(4)	16(4)	16(4)	16(4)	15/15		
	1: CMSA-S	2.0(1.0)	281 2.6(1.0)	3.2(3)	2.5(1)) 3.2(3)	15/15	1: CMSA-S	1.6(1)	6.4(10)	5220 63(78)	0728 388(475)682(690)	0/15		
	2: CMSA	1.6(0.9)	2.2(0.9)	3.2(3)	3.7(3)	5.8(4)	15/15	2: CMSA	1.7(0.4)	7.0(6)	231(278)	00	∞4.0e5	0/15		
	1; CMSA-S	24 57(5)	1171 1217(1281)	1572	1572	1597 ∞1.0e5	0/15	1: CMSA-S	1351 649(862)	9503 ∞	16524 ∞	16524 ∞	16969 ∞4.0e5	0/15		
	2: CMSA	123(3)	00	~~	00	∞1.0e5	0/15	2: CMSA	299(444)	00	00	00	∞4.0e5	0/15		
	f ₈ 1: CMSA-S	73	336 88(152)	391 79(133)	410 76(125	422	15/15	1: CMSA-S	2039	4040 = 49(50)	4219 50(47)	4371 50(49)	4484 50(51)	15/15		
	2: CMSA	3.0(1)	85(151)	77(131)	74(124) 72(122)	12/15	2: CMSA	23(14)	67(62)	67(60)	66(58)	66(57)	11/15		
عداد	1: CMSA-S	35 2 7(2)	214	300	335	369 15(7)	15/15	f9 1: CMSA-S	1716	- 3277 63(64)	3455 64(60)	3594 64(57)	3727 64(54)	15/15	1T	NS
	2: CMSA	2.9(1)	17(9)	16(7)	16(7)	15(7)	15/15	2: CMSA	27(7)	52(8)	54(8)	54(9)	54(8)	14/15		
	f ₁₀	349 67(6)	574 6 7(5)	626 7.6(5)	829 6 3(4)	880 6 3(3)	15/15	f ₁₀	7413	10735 19(5)	14920 15(4)	17073 15(3)	17476 15(3)	15/15		
	2: CMSA	7.2(4)	7.4(5)	8.3(5)	7.3(5)) 7.4(4)	15/15	2: CMSA	17(10)	21(5)	17(5)	16(5)	18(5)	14/15		
	f ₁₁	143	763 4 7(2)	1177 3 5(2)	1467	1673	15/15	f ₁₁ 1: CMSA-S	1002	6278 4 1(1)	9762 4 2(1)	12285	14831	15/15		
	2: CMSA	7.3(6)	4.0(3)	3.3(2)	3.0(2)	2.9(1) 2.8(1)	15/15	2: CMSA-5	13(5)	3.6(1)	3.8(1.0)	4.6(2	(3.3(3)) $(4.8(1))$	15/15		
	f ₁₂	108	371	461	1303	1494	15/15	f ₁₂	1042	2740	4140	12407	13827	15/15		
	2: CMSA	9.1(2)	17(21)	19(18)	9.4(9)) 10(8)	15/15	2: CMSA-S	5.8(15)	23(22)	26(15) 26(16)	12(5)	12(4) 13(6)	15/15		
	f ₁₃	132	250	1310	1752	2255	15/15	f ₁₃	652	2751	18749	24455	30201	15/15		
	2: CMSA	5.0(7)	27(25)	7.2(5)	7.2(4)) 7.0(3)	14/15	2: CMSA-S	704(921)	946(1163)	299(323) ∞	~	∞4.0e5 ∞4.0e5	0/15		
	f ₁₄	10	58	139	251	476	15/15	f ₁₄	75	304	932 5 0(2)	1648	15661	15/15		
	2: CMSA	1.3(2)	3.4(1)	5.4(2)	8.7(4)) 8.3(4)	15/15	2: CMSA-S	2.0(0.6)	2.6(0.3)	6.2(0.8)	16(5)	6.0(2)	14/15		
	f ₁₅	511	19369	20073	20769	21359	14/15	f ₁₅	30378	3.1e5	3.2e5	4.5e5	4.6e5	15/15		
	2: CMSA-S	132(196)	72(80)	[∞] 70(77)	68(77)	∞1.0e5 66(77)	1/15	2: CMSA-S	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	00	80	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	∞4.0e5 ∞4.0e5	0/15		
	f ₁₆	120	2662	10449	11644	12095	15/15	f ₁₆	1384	77015	1.9e5	2.0e5	2.2e5	15/15		
	2: CMSA-S	3.3(3)	526(620) 245(282)	00	00 00	∞1.0e5 ∞1.0e5	0/15	2: CMSA-S	107(146)	00 00	00	00 00	∞4.0e5 ∞4.0e5	0/15		
	f ₁₇	5.2	899	3669	6351	7934	15/15	f ₁₇	63	4005	30677	56288	80472	15/15		
	2: CMSA-S	2.6(3)	223(278)	000 177(218)	00 00	∞1.0e5 ∞1.0e5	0/15	2: CMSA-S	1.1(1)	650(749)	00	00 00	∞4.0e5 ∞4.0e5	0/15		
	f ₁₈	103	3968	9280	10905	12469	15/15	f ₁₈	621	19561	67569	1.3e5	1.5e5	15/15		
	1: CMSA-S 2: CMSA	0.90(0.7)) 22(38)	∞ 151(172)	00 00	∞1.0e5 ∞1.0e5	0/15	1: CMSA-S 2: CMSA	0.96(0.5) ∞	00 00	00 00	∞4.0e5 ∞4.0e5	0/15		
	f ₁₉	1	242	1.2e5	1.2e5	1.2e5	15/15	f ₁₉	1	3.4e5	6.2e6	6.7e6	6.7e6	15/15		
	1: CMSA-S 2: CMSA	3.1(2) 3.0(3)	2730(3097) 1186(1448)	00 00	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	∞1.0e5 ∞1.0e5	0/15	1: CMSA-S 2: CMSA	4.8(4) 6.4(9)	00 00	00 00	00 00	∞4.0e5 ∞4.0e5	0/15		
	f ₂₀	16	38111	54470	54861	55313	14/15	f ₂₀	82	3.1e6	5.5e6	5.6e6	5.6e6	14/15		
	1: CMSA-S 2: CMSA	1.6(1) 1.9(1)	00 00	00 00	~~ ~~	∞1.0e5 ∞1.0e5	0/15	1: CMSA-S 2: CMSA	2.0(0.6) 2.0(0.9)	00 00	∞ ∞	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	∞4.0e5 ∞4.0e5	0/15		
	f ₂₁	41	1674	1705	1729	1757	14/15	f ₂₁	561	14103	14643	15567	17589	15/15		
	1: CMSA-S 2: CMSA	377(1220) 612(1220)	388(448) 836(970)	382(469) 821(909)	376(434) 810(882))370(455)	2/15	1: CMSA-S 2: CMSA	51(1.0) 179(356)	43(57) 184(227)	41(55) 178(191)	39(51) 167(193	34(45))148(171)	6/15		
	f22	71	938	1008	1040	1068	14/15	f22	467	23491	24948	26847	1.3e5	12/15		
	1: CMSA-S 2: CMSA	514(705) 513(705)	693(853) 694(852)	645(793) 646(794)	626(673) 626(721))610(773)	2/15	1: CMSA-S 2: CMSA	430(857) 429(857)	00 00	00 00	00 00	∞4.0e5 ∞4.0e5	0/15		
	f23	3.0	14249	31654	33030	34256	15/15	f23	3.2	67457	4.9e5	8.1e5	8.4e5	15/15		
	1: CMSA-S 2: CMSA	2.0(2) 3.2(3)	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	00 00	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	∞1.0e5 ∞1.0e5	0/15	1: CMSA-S 2: CMSA	2.1(2) 2.3(3)	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	00 00	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	∞4.0e5 ∞4.0e5	0/15		
	£. CIVISA	1622	6.4e6	9.6e6	1.3e7	1.3e7	3/15	<u>f₂₄</u>	1.3e6	5.2e7	5.2e7	5.2e7	5.2e7	3/15		
	1: CMSA-S	33(62)	00	00	00	∞1.0e5	0/15	1: CMSA-S	00	00	00	00	∞4.0e5	0/15		
	2. UNISA	17(31)	30	00	00	~1.0es	10/13	2. CM3A	1 ³⁰	00	00	00	~~+.0es	0/15		

rithms may be further improved by applying other estimators for the covariance. This paper considered a combination of two estimation approaches to provide a first step on this way. Shrinkage estimators shrink the sample covariance matrix towards the identity matrix or diagonal matrix in the case of the paper. In cases, where the fitness function requires highly different eigenvalues and a rotation other than the cartesian coordinate system this may be problematic. Therefore, a switch towards the eigenspace of the covariance matrix was proposed in this paper and investigated in experiments on the BBOB test suite.

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