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Niching for finding robust optima

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Preface

In this paper a robustness scheme with niching is presented for extending an evolution strategy to an evolution strategy with a niching technique and robustness scheme. This gives the algorithm more explorative power and better chances of finding robust optima. The proposed schemes are implemented and experiments are run on nine different test functions. The conclusion is that, for the majority of the test functions the extended algorithm perform wells and outperform the benchmark algorithms. However, interestingly enough, the extended algorithm did not outperform the benchmark algorithms on the multipeak functions, although that was the hypothesis.

Chapter 1

Introduction

Evolution strategies are optimization techniques to find a high quality solutions for complex non-linear optimization problems. Given an objective function $f(\mathbf{x}) \rightarrow \min, \mathbf{x} \in \mathbb{R}^N$ the evolution strategy (ES), will try to minimize this function and find the best solution. However, the input variables are not always fully controllable. Practical realizations of solutions can deviate, requiring a robust solution that performs well under these deviations.

The normal fitness function does not take the possible deviations into account. Therefore, a robust individual will not be rewarded with a higher fitness. A new fitness function is created that estimates the fitness under deviations. The new fitness function is called the *effective fitness function* [5] and is an expected fitness function. $f_{\text{eff}} = \mathbf{E}[f(\mathbf{x}+\mathbf{z})]$, where $\mathbf{z} \sim \mathbf{pdf}(\boldsymbol{\delta})$ is some continuous probability variable.

Robustness schemes proposed in literature [4,9] perform well on locally zooming into the robust optimum, but they are not able to consistently determine the more robust parts of the search area. In this paper it is investigated whether niching can help with identifying the more robust parts of the search area.

Niching is a technique that enforces spatial diversity within a population. In the approach of Shir [7], at every generation niche leaders are chosen that are at least a distance ρ from each other. These spatiality separated niche leaders are thereafter used for generating several separated sub-populations. This prevents the whole population from converging to one point or area, therewith giving the algorithm more exploratory power. In this paper, niching will be combined with sampling schemes for finding robust solutions. The intuition is that this will improve the algorithm's ability to find the more robust parts of the search space, which will result in better robust optima. The studies performed in this paper serve to underpin this hypothesis.

The remainder of the paper is structured as follows: Chapter 2 explains the chosen evolution strategy. Chapter 3 shows how the niching is implemented. Chapter 4 explains the robustness scheme that was used. In Chapter 5 niching and robustness are combined. Chapter 6 presents the experiments and their results, ending with a conclusion and outlook in Chapter 7.

Chapter 2

Evolution Strategy

The Evolution Strategy (ES) that is used for the implementation is the Covariance Matrix Adaptation Evolution Strategy (CMA-ES) [3]. It is a state-of-the-art algorithm for unconstrained continuous optimization that is suitable for extending it with niching techniques and robustness schemes.

Algorithm 1 CMA-ES

Input parameters(λ, μ)

- 1: **Initialize** internal parameters: $\sigma, \mathbf{C}$ and $\mathbf{x}_{mean}$
- 2: **while** not terminate **do**
- 3: **for** $i = 1 : \lambda$ **do**
- 4: $\mathbf{z}_i \sim N(\mathbf{0}, \mathbf{I})$
- 5: $\mathbf{x}_i \leftarrow \mathbf{x}_{mean} + \sigma \cdot \sqrt{\mathbf{C}} \cdot \mathbf{z}_i$
- 6: $\mathbf{f}_i \leftarrow \text{evaluate}(\mathbf{x}_i)$
- 7: **end for**
- 8: $\mathbf{x}_{mean} \leftarrow$ weighted average of the μ best individuals
- 9: **update** σ
- 10: **update** $\mathbf{C}$
- 11: **end while**

Output (best $\mathbf{x}$)

Algorithm 1 subsumes the working mechanism of the CMA-ES. After initializing the global stepsize σ , the covariance matrix $\mathbf{C}$ and the recombinant $\mathbf{x}_{mean}$ the main evolution loop begins. The λ offspring are created by adding a random vector $\mathbf{z}, \mathbf{z} \sim N(\mathbf{0}, \sigma \mathbf{C})$ to $\mathbf{x}_{mean}$. The new offspring are evaluated by the fitness function and the μ best are recombined into a new recombinant, $\mathbf{x}_{mean}$, for the next generation. The step size σ and the covariance matrix $\mathbf{C}$ are updated and a new iteration of the loop is started until the stopping conditions are met, then the best found solution is returned. For a detailed descriptions of the working mechanism of the algorithm see [3].

Chapter 3

Niching

A property of evolution strategies is that populations converge with a high probability to a (local) optimum. When that happens diversity of the population is lost. As explained earlier, when looking for robust optima it could be very useful to maintain diversity in the population. A technique to keep diversity in the population is niching.

Niching as defined by [7], works by evolving q different subpopulations parallel to each other, and forcing these subpopulations to stay separated. This creates a $(\{\mu_1, \dots, \mu_q\}, q \cdot \lambda)$ -strategy, where $\mu_1, \dots, \mu_q$ denotes the number of parents of the subpopulations. Algorithm 2 describes the identification of the best individuals per niche (see appendix A for a matlab implementation of the algorithm).

Algorithm 2 works as follows: It assumes that the population Pop is sorted by fitness (the fittest individual is Pop₁). The population is an array that consists of $\lambda \cdot q$ vectors. Each vector is an candidate solution $\{\mathbf{x}_1, \dots, \mathbf{x}_{\lambda \cdot q}\}$. The algorithm calculates the DPS. The DPS is a set of vectors, which are candidate solutions. Initially the DPS is set to $\emptyset$. Then, for every individual i in the population, it is checked, if its distance to all the elements in the DPS is bigger then the niching radius ρ . If this is the case and the number of elements in DPS is smaller than q , then i th individual is also a niche leader and is added to the DPS.

In Figure 3.1, the working mechanism of the algorithm is illustrated. Figure 3.1a shows the population. Then in, Figure 3.1b, the best individual is checked. At this point the DPS is still empty, so its distance to all elements in DPS is larger than ρ . This makes the best individual a new niche leader. It is colored blue. The blue circle around it shows the niching radius and is added to the DPS. In Figure 3.1c, the second best individual is checked and it is within the niching radius of one of the members of the DPS. Hence, it is not a new niche leader and it is not added to the DPS. After that, the next best individual is checked in Figure 3.1d. It lies outside the niching radius of the member in the DPS, so the individual becomes a niche leader. It is colored red and the niching radius is shown around it with a circle, then it is added to the DPS.

Algorithm 2 Dynamic Peak Identification**Input** (Pop, λ, q, ρ) {assume that Pop is sorted on fitness}

```

1:  $i \leftarrow 1$ 
2:  $numpeaks \leftarrow 0$ 
3:  $DPS \leftarrow \emptyset$ 
4: while ( $numpeaks < q$  and  $i \leq \lambda \cdot q$ ) do
5:    $is\_niche\_leader \leftarrow \mathbf{true}$ 
6:   for  $k = 1 : numpeaks$  do
7:     if  $distance(Pop_i, DPS_k) \leq \rho$  then
8:        $is\_niche\_leader \leftarrow \mathbf{false}$ 
9:     end if
10:  end for
11:  if  $is\_niche\_leader == \mathbf{true}$  then
12:     $DPS \leftarrow DPS \cup Pop_i$ 
13:     $numpeaks \leftarrow numpeaks + 1$ 
14:  end if
15:   $i \leftarrow i + 1$ 
16: end while
Output DPS

```

This process continues in the other Figures 3.1e and 3.1f.

3.1 Niching radius

An important parameter for niching is the niching radius ρ . In [7], a suggestion is made how to set this parameter. Given the number of peaks q in the search space, every peak is considered to have a n -dimensional hypersphere surrounding the peaks with radius ρ , which encloses $\frac{1}{q}$ of the volume of the search space. Two assumptions are made: 1) the number of peaks q can be estimated or is given, and 2) the peaks lie at least a distance of 2ρ from each other.

The volume of a hypersphere is

$$V = c(n)r^n. \quad (3.1)$$

where $c(n)$ is a positive constant depending on the dimensions and r is given by:

$$r = \frac{1}{2} \sqrt{\sum_{i=1}^n (\mathbf{x}l_i - \mathbf{x}u_i)^2}, \quad (3.2)$$

where $\mathbf{x}u$ denotes the upper bound and $\mathbf{x}l$ denotes the lower bound. V is divided into q spheres

$$c(n)\rho^n = \frac{1}{q}c(n)r^n. \quad (3.3)$$

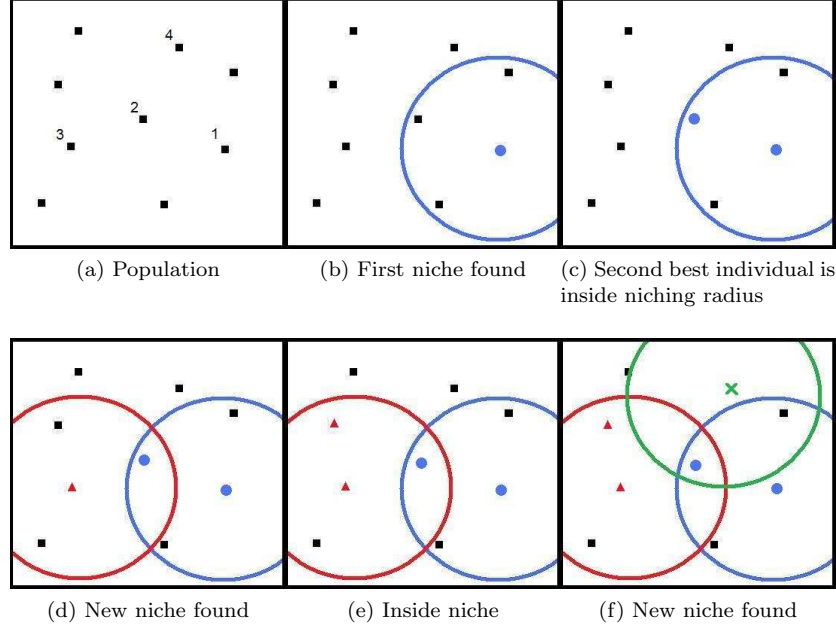


Figure 3.1: Illustration of the dynamic peak identification procedure with three niches found

To calculate ρ :

$$\rho = \frac{r}{\sqrt[q]{q}}. \quad (3.4)$$

When dealing with a search space that is a cube the volume of the circumscribed sphere is taken as the volume of the search space, however, the volume of the circumscribed sphere is much larger than the volume of the cube. This can result in a ρ that is too large.

For example the 10-dimensional problem with the lower bound for every dimension being -5 and the upper bound for every dimension 5 and dividing that into 4 volumes, $q = 4$.

$$\rho = \frac{\frac{1}{2} \sqrt{\sum_{i=1}^n (\mathbf{x}\mathbf{l}_i - \mathbf{x}\mathbf{u}_i)^2}}{\sqrt[q]{q}} = \frac{15.8114}{\sqrt[10]{4}} = 13.7646. \quad (3.5)$$

Since the maximum distance for two points the search space is 31.6228 and the suggested niching radius for $q = 4$ is 13.7646, the chances that the peaks lie a distance of at least 2ρ from each other are not so high. The sphere function only has one peak, but the ρ is not depended on the function only on the bounds of the search space and the number of niches.

As an alternative we propose another procedure to calculate ρ , by taking the incircle of the search space instead of the circumscribed circle. The r is now be given by:

$$r = \frac{1}{2} \cdot \frac{1}{n} \sum_{i=1}^n |\mathbf{x}\mathbf{u}_i - \mathbf{x}\mathbf{l}_i|. \quad (3.6)$$

For the 10-dimensional problem with the same bounds this results into a ρ of:

$$\rho = \frac{\frac{1}{2} \cdot \frac{1}{n} \sum_{i=1}^n |\mathbf{x}\mathbf{u}_i - \mathbf{x}\mathbf{l}_i|}{\sqrt[q]{q}} = \frac{5}{\sqrt[10]{4}} = 4.3528, \quad (3.7)$$

which appears to be a better value for ρ .

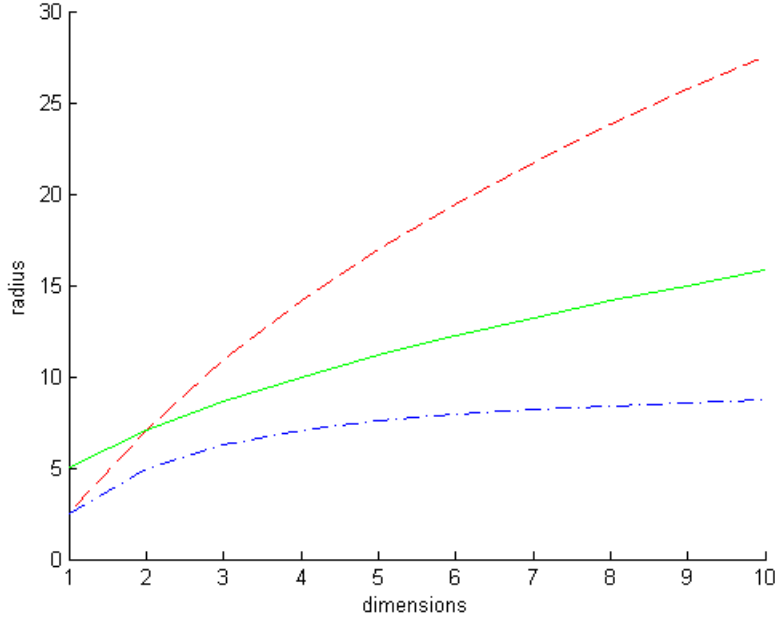


Figure 3.2: A plot of two different niching radii versus the diagonal of the search space. The blue dashed line shows the niching radius derived from the inner circle. The red dashed line indicates the niching radius derived from the circumscribed circle. The green line indicates $\frac{1}{q}$ times the length of the diagonal of the search space, $q = 4$ the lowerbounds are -10 and the upperbounds are 10 .

Figure 3.2, shows that ρ taken from the circumscribed circle grows faster for higher dimensions than ρ derived from the incircle. The green constant line shows the growth of the diagonal of the search space. The blue line stays closer to the green line than the red line.

3.2 CMA-ES with niching

Algorithm 3 shows the niching technique implemented into the CMA-ES. To add the niching technique to the CMA-ES, some changes have to be made to the CMA-ES as presented in Algorithm 1. Instead of having one σ , $\mathbf{x}_{mean}$ and $\mathbf{C}$, every niche has its own σ , $\mathbf{x}_{mean}$ and $\mathbf{C}$. When creating new offspring the σ , $\mathbf{x}_{mean}$ and $\mathbf{C}$ of the niche leader are used.

Algorithm 3 CMA-ES with niching

Input parameters(λ, μ, q)

- 1: **Initialize** internal parameters: $\sigma_1, \dots, \sigma_q, \mathbf{C}_1, \dots, \mathbf{C}_q, \mathbf{x}_{mean_1}, \dots, \mathbf{x}_{mean_q}, \rho$
- 2: **while** not terminate **do**
- 3: **for** $j = 1 : q$ **do**
- 4: **for** $i = 1 : \lambda$ **do**
- 5: $\mathbf{z}_{j,i} \sim N(\mathbf{0}, \mathbf{I})$
- 6: $\mathbf{x}_{j,i} \leftarrow \mathbf{x}_{mean_j} + \sigma_j \cdot \sqrt{\mathbf{C}_j} \cdot \mathbf{z}_{j,i}$
- 7: $\mathbf{f}_{j,i} \leftarrow \text{evaluate}(\mathbf{x}_{j,i})$
- 8: **end for**
- 9: **end for**
- 10: $(\mathbf{x}_{1:1}, \dots, \mathbf{x}_{q:\lambda}) \leftarrow \text{sort}(\mathbf{x}_{1,1}, \mathbf{f}_{1,1}), \dots, (\mathbf{x}_{q,\lambda}, \mathbf{f}_{q,\lambda})$ {In ascending order}
- 11: $\text{DPS} = \text{dpi}(\mathbf{x})$
- 12: **for** $j = 1 : q$ **do**
- 13: $\mathbf{x}_{mean,j} \leftarrow \text{DPS}_j$
- 14: **update** σ_j
- 15: **update** $\mathbf{C}_j$
- 16: **end for**
- 17: **end while**

Output (best individual)

Two problems occur when updating $\mathbf{x}_{mean}$ and creating offspring. How to deal with the case when there are less than μ individuals in a niche? This problem can be overcome by taking the mean of the individuals that exist in the niche, instead of taking the mean of μ individuals.

The other problem is more difficult. When the new offspring are created and regrouped in q niches, it is possible that two individuals that are now in the same niche have different parents. Updating σ and $\mathbf{C}$ becomes a problem, because it is not reasonable to combine two (or multiple) covariance matrices and two step sizes. The solution is to allow for only one parent per niche, $\mu = 1$. Changing the CMA-ES from a (μ, λ) -strategy into the CMA-ES with niching, which is a $(\{\mu_1, \dots, \mu_q\}, q \cdot \lambda)$ -strategy, where every $\mu = 1$.

Chapter 4

Robustness

A robust solution is a solution that performs well when the variables are effected by a disturbance δ . In Figure 4.1, two peaks are shown, the left peak has a better optimum. The right peak is more robust, and might be a better robust solution depending on the disturbance δ . Note that is assumed that δ is known, but that assumption holds for many of real life problems, without a known δ it would not be possible to have an effective fitness function.

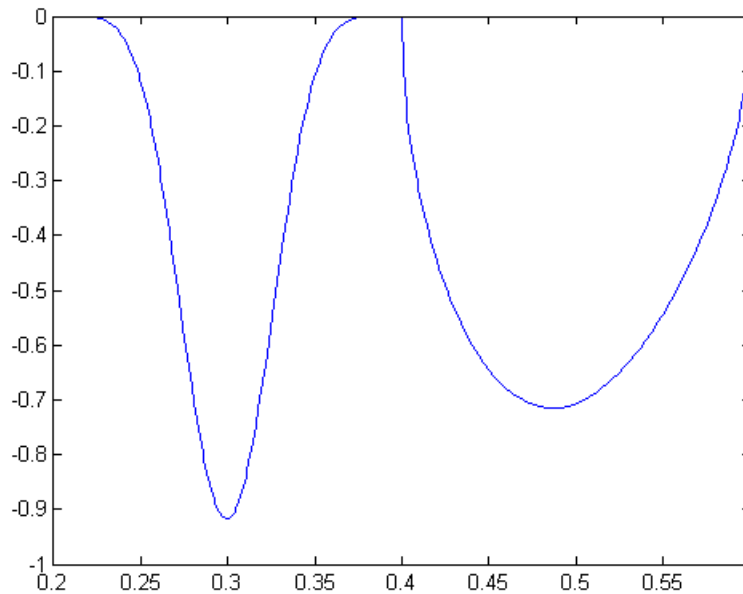


Figure 4.1: Two peaks: The left peak has the better optimum for minimization. The right peak is the more robust peak.

Robustness is important because it is not always possible to control the input variables. Especially in industrial applications where candidate solutions cannot be realized with arbitrary precision.

When there are a lot of peaks it is very hard to find the more robust peaks. Robustness schemes perform well on zooming in locally into the robust optimum. But they perform poorly in identifying the more robust parts of the search space.

What niching can add to this is, is that keeping the population spread out over the search space it finds more peaks. This should result in better chances of finding more robust peaks.

The robustness scheme that was chosen is the multi-evaluation-model (MEM). It does not just calculate the fitness from an individual $\mathbf{x}$, but it takes m different random samples of the disturbance $\boldsymbol{\delta}$ from an individual. MEM calculates the fitness of those m points and takes the mean of those values as the fitness for the individual $\mathbf{x}$, i.e.,

$$f_{\text{eff}}(\mathbf{x}) = \frac{1}{m} \sum_{i=1}^m f(\mathbf{x} + \boldsymbol{\delta}_i), \boldsymbol{\delta}_i \sim \boldsymbol{\delta}. \quad (4.1)$$

The evaluation can be done with the recycling of the disturbance samples or for every individual take a new disturbance sample. In the first case, denoted MEM^+ , the same disturbance is added to every individual and its fitness is then calculated. In the second case, denoted MEM^- , every individual has its own disturbance which is evaluated. For this algorithm the recycling method, MEM^+ , is chosen.

Chapter 5

Niching and finding robust optima

In Algorithm 4, the result of combining the MEM scheme with Algorithm 3 is shown (see appendix B for a matlab implementation of the algorithm).

In the MEM scheme, the parameter m , the number of samples, needs to be set. To find the best setting for m the algorithm, with $q = 4$, is tested on a 10 dimensional instance of Branke's multipeak problem. It's a modification of the Branke function [1] and it has many peaks. The peaks are positioned like a grid. All the peaks are positioned at the -1 and 1 coordinates. The more -1 coordinates the more robust the peak is. Hence, the global optimum is $\mathbf{x} = (-1, -1, -1, -1, -1, -1, -1, -1, -1, -1)$. So each found peak has a score for the number of dimensions the coordinate is smaller than zero. The most robust peak has a score of 10.

The algorithm is a run 100 times for each setting of m . The most robust niche was identified by counting in how many dimensions $\mathbf{x} < 0$. For how many dimensions that was true is plotted in Figure 5.1

As can be seen in Figure 5.1, $m = 1$ is the best. It finds the most robust peak the most often and has a lower average fitness. MEM with $m = 1$ is a special case of the MEM-scheme, called single evaluation method (SEM).

Algorithm 4 CMA-ES with niching and the MEM evaluation scheme for finding robust optima

Input parameters(λ, μ, q, m)

```

1: Initialize internal parameters:  $\sigma_1, \dots, \sigma_q, \mathbf{C}_1, \dots, \mathbf{C}_q, \mathbf{x}_{mean_1}, \dots, \mathbf{x}_{mean_q}, \rho$ 
2: while not terminate do
3:    $\delta_l \sim \delta, l = 1, \dots, m$ 
4:   for  $j = 1 : q$  do
5:     for  $i = 1 : \lambda$  do
6:        $sumf = 0$ 
7:        $\mathbf{z}_{j,i} \sim N(0, \mathbf{I})$ 
8:        $\mathbf{x}_{j,i} \leftarrow \mathbf{x}_{mean_j} + \sigma_j \cdot \sqrt{\mathbf{C}_j} \cdot \mathbf{z}_{j,i}$ 
9:       for  $l = 1 : m$  do
10:         $sumf = sumf + \text{evaluate}(\mathbf{x}_{j,i} + \delta_l)$ 
11:      end for
12:    end for
13:     $\mathbf{fo}_{j,i} \leftarrow \frac{sumf}{m}$ 
14:  end for
15:   $(\mathbf{x}_{1:1}, \dots, \mathbf{x}_{q:\lambda}) \leftarrow \text{sort}(\mathbf{x}, \mathbf{fo}) \{\text{In ascending order}\}$ 
16:   $DPS = \text{dpi}(\mathbf{x})$ 
17:  for  $j = 1 : q$  do
18:    update  $\mathbf{x}_{mean,j}$ 
19:    update  $\sigma_j$ 
20:    update  $\mathbf{C}_j$ 
21:  end for
22: end while

```

Output (best individual)

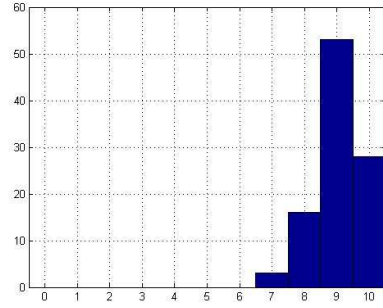
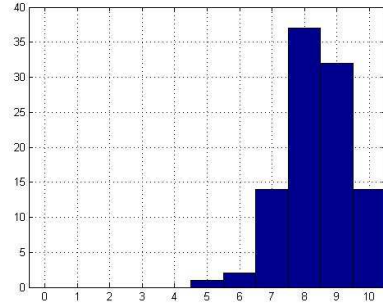
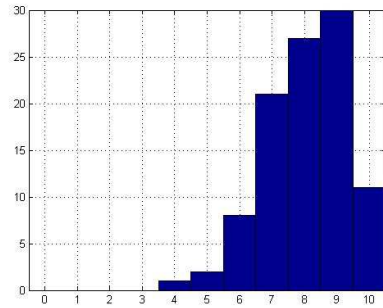
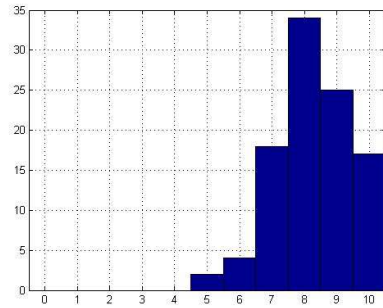
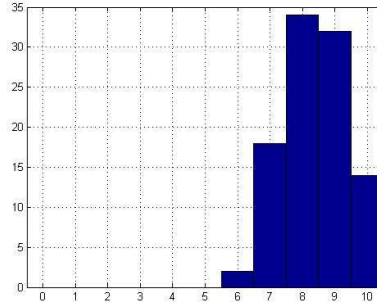
(a) $m = 1$, average fitness = 0.4601(b) $m = 2$, average fitness = 0.4791(c) $m = 3$, average fitness = 0.4845(d) $m = 4$, average fitness = 0.4730(e) $m = 5$, average fitness = 0.4649

Figure 5.1: Number of times peak found versus robustness score of the peaks for different instances of the CMA-ES with niching and the MEM⁺ for finding robust optima.

Chapter 6

Experimental results

6.1 Proof of concept

An experiment on a two-dimensional problem is done to see if the CMA-ES with niching and MEM has potential to find the more robust parts of the search space. Three algorithms are compared namely, the CMA-ES, the CMA-ES with niching and the CMA-ES with niching and the MEM⁺. The three algorithms are run on a two-dimensional instances of Branke's multipeak function, and again by counting in how many dimensions the solution is smaller than zero it is calculated which peak is found. The more dimensions smaller than zero, the more robust the optimum is. The two dimensional instance of Branke's multipeak function has four peaks: $(1, 1)$, $(-1, 1)$, $(1, -1)$, $(-1, -1)$. Each peak is given a score equal to the number of -1 they have. The three algorithms need to find as often as possible the peak with score two. The settings for the algorithms are: $q = 2$ and $m = 1$. For the niching algorithms the peak with the higher score is chosen. The results are plotted in Figure 6.1.

The results shown in Figure 6.1, indicate that niching alone is not enough to identify the more robust parts of the search area. The algorithm with niching and MEM however, performs better than the normal CMA-ES in finding the more robust parts of the search area. The differences are marginal, and a more systematic testing approach is needed and will be conducted in Chapter 6.2.

6.2 Experiments

The CMA-es with niching and the MEM evaluation scheme is compared with a normal CMA-ES, a CMA-ES with niching and a CMA-ES with the MEM scheme (without niching). The four algorithms are compared on nine artificial test functions.

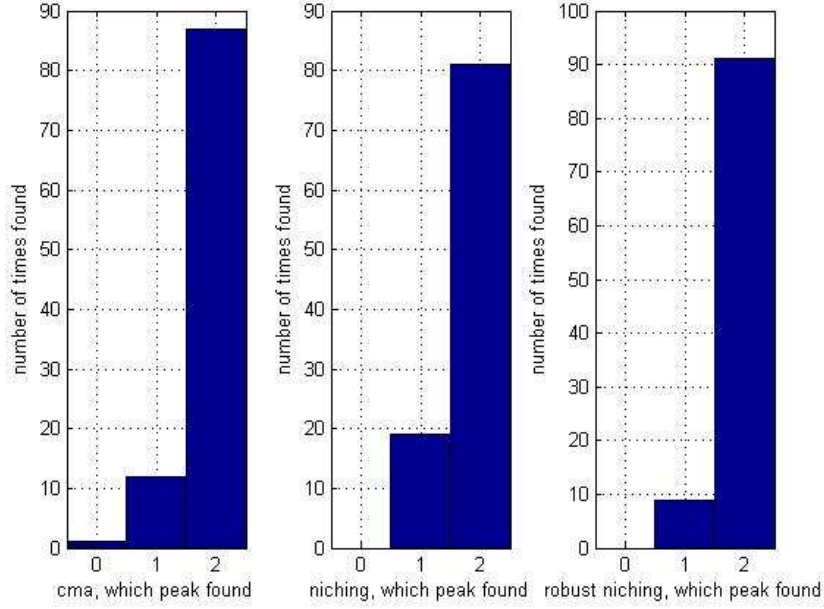


Figure 6.1: Number of times peak found vs robustness score of the peaks.

6.3 Test functions

f1: Sphere problem (from [6])

$$f_1(\mathbf{x}) = \sum_{i=1}^n x_i^2,$$

$$\mathbf{x} \in [-5, 5]^N, \boldsymbol{\delta} \sim U(-1, 1), \text{ and } \mathbf{x}_{\mathbf{ro}} = \mathbf{0}.$$

f2: Heavyside sphere problem (from [4])

$$f_2(\mathbf{x}) = \frac{1}{n} \sum_{i=1}^n \frac{1}{1 + e^{\left(\frac{2}{5}(x_i + 3)\right)}} + \frac{1}{1 + e^{10(x_i - 4)}},$$

$$\mathbf{x} \in [-10, 10]^N, \boldsymbol{\delta} \sim U(-1, 1), \text{ and } \mathbf{x}_{\mathbf{ro}} = [1, 1, 0, \dots, 0].$$

f3: Sawtooth problem (from [2])

$$f_3(\mathbf{x}) = 1 - \frac{1}{n} \sum_{i=1}^n \begin{cases} (x_i + 0.8) & \text{if } x_i < 0.2 \wedge x_i \geq -0.8 \\ 0 & \text{else} \end{cases},$$

$$\mathbf{x} \in [-1, 1]^N, \boldsymbol{\delta} \sim U(-0.2, 0.2), \text{ and } \mathbf{x}_{\mathbf{ro}} = \mathbf{0}.$$

f4: Volcano problem (from [5])

$$f_4(\mathbf{x}) = \begin{cases} \sqrt{\|\mathbf{x}\|} - 1 & \text{if } \|\mathbf{x}\| > 1 \\ 0 & \text{else} \end{cases},$$

$$\mathbf{x} \in [-10, 10]^N, \boldsymbol{\delta} \sim U(-\mathbf{1.5}, \mathbf{1.5}), \text{ and } \mathbf{x}_{\mathbf{ro}} = \mathbf{0}.$$

f5: Modded branke multipeak problem (from [1])

$$f_5(\mathbf{x}) = \frac{1}{n} \sum_{i=1}^n c - \begin{cases} 1 - (x+1)^2 & \text{if } x_i < 0 \wedge x_i \geq -2 \\ c \cdot 2^{(-8 \cdot |x_i - 1|)} & \text{if } x_i \geq 0 \wedge 2 \geq x_i \end{cases},$$

$$c_1 = 1.3, \mathbf{x} \in [-2, 2]^N, \boldsymbol{\delta} \sim U(-\mathbf{0.5}, \mathbf{0.5}), \text{ and } \mathbf{x}_{\mathbf{ro}} = -\mathbf{1}.$$

f6: Pickelhaube problem (from [5])

$$f_6(\mathbf{x}) = c_{1a} - \max(f_{base}, f_{1a}, f_{1b}, f_2),$$

$$f_{1a} = c_{1a} \cdot \left(1 - \frac{\|\mathbf{x} + \mathbf{5}\|}{5 \cdot \sqrt[3]{N}}\right),$$

$$f_{1b} = c_{1b} \cdot \left(1 - \frac{\|\mathbf{x} + \mathbf{5}\|}{5 \cdot N^2}\right),$$

$$f_2 = c_2 \cdot \left(1 - \frac{\|\mathbf{x} - \mathbf{5}\|}{5 \cdot (\sqrt{N})^{d_2}}\right),$$

$$f_{base} = 0.1 \cdot \exp(-\frac{1}{2} \cdot \|\mathbf{x}\|),$$

$$c_{1a} = \frac{5}{5 - \sqrt{5}}, c_{1b} = \frac{625}{624},$$

$$c_2 = 1.5975528761621545, d_2 = 1.1513175769876054,$$

$$\mathbf{x} \in [-10, 10]^N, \boldsymbol{\delta} \sim U(-\mathbf{1}, \mathbf{1}), \text{ and } \mathbf{x}_{\mathbf{ro}} = \mathbf{5}.$$

f7: FNIM f2 problem

$$f_7(\mathbf{x}) = -\frac{(a - x_2) + \frac{1}{n} \sum_{i=3}^n x_i^2}{(x_i^2 + b) - x_1^2},$$

$$a = 5, b = 1, \mathbf{x} \in [-5, 5]^N, \boldsymbol{\delta} \sim U(-\mathbf{1}, \mathbf{1}), \text{ and } \mathbf{x}_{\mathbf{ro}} = \mathbf{5}.$$

f8: Multipeak f1 problem (from [8])

$$f_8(\mathbf{x}) = \frac{1}{n} \sum_{i=1}^n \begin{cases} e^{(-2 \ln 2 (\frac{x-0.1}{0.8})^2)} \sqrt{|\sin(5\pi x_i)|} & \text{if } 0.4 < x_i \leq 0.6 \\ e^{(-2 \ln 2 (\frac{x-0.1}{0.8})^2)} \sin^6(5\pi x_i) & \text{else} \end{cases},$$

$$\mathbf{x} \in [0, 1]^N, \boldsymbol{\delta} \sim U(-\mathbf{0.0625}, \mathbf{0.0625}), \text{ and } \mathbf{x}_{\mathbf{ro}} \approx \mathbf{0.4911}.$$

f9: Multipeak f2 problem

$$f_9(\mathbf{x}) = \frac{1}{n} \sum_{i=1}^n 2 \sin(10 \exp(-0.2x_i) \cdot x_i) \cdot \exp(-0.25x_i).$$

$$\mathbf{x} \in [-10, 10]^N, \boldsymbol{\delta} \sim U(-\mathbf{1}, \mathbf{1}), \text{ and } \mathbf{x}_{\mathbf{ro}} = \mathbf{5}.$$

In Figure 6.2 the nine test problems are shown in two dimensions.

6.4 Results

Each of the four algorithms is run 25 times on each of the nine test problems. Each run has 10,000 function evaluations. The parameters q and m are respectively set to 4 and 3. In Figures 6.3 to 6.11, the average fitness versus the function evaluations are shown.

6.5 Discussion of the results

In Figures 6.3 to 6.11, it can be seen that the CMA-ES with niching and the MEM evaluation scheme performs the best on four out of the nine test functions, namely the heavy side sphere problem, the volcano problem, the FNIM problem and Multipeak f2. The CMA-ES with the MEM evaluation scheme, without niching, only is the best for two test problems, namely the sawtooth problem and the multipeak f1 problem. The CMA-ES with niching and MEM scheme, outperforms the CMA-ES with the MEM scheme in a total of 6 out of 9. Adding niching give the algorithm an improvement for the majority of the test problems.

What is very interesting to see is that the CMA-ES with niching and the MEM evaluation scheme does not perform well on Branke's multipeak function and the Multipeak f1 function. While the intuition was that niching would help in a multipeak problems it seems like that is not always the case. The reason for this is not clear. It is possible that a niche leader gets stuck at a local minimum that has a distance to the global minimum that is smaller then ρ . In that case the niching radius prevents other niches from finding the global minimum. The niche which has the global minimum in its niching radius might have zoomed in too far at a local minimum to be able to jump to the global minimum. This presumption gets reinforced by the fact that the CMA-ES with niching and MEM does perform well on the Multipeak f2 function, where the global minimum is located further away from other peaks.

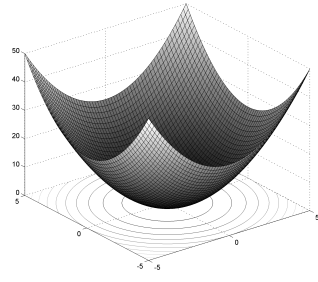
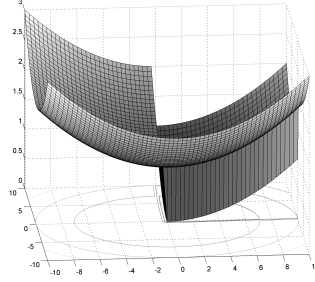
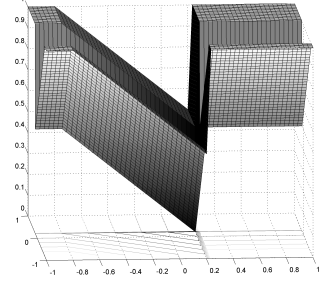
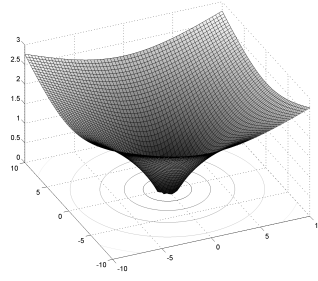
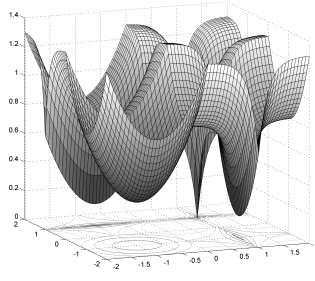
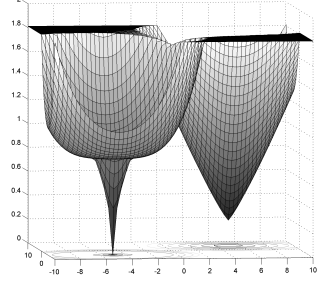
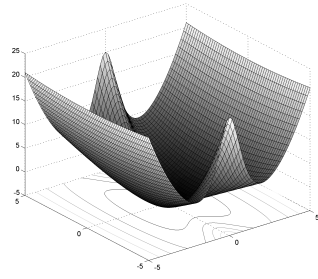
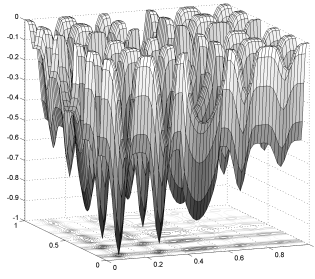
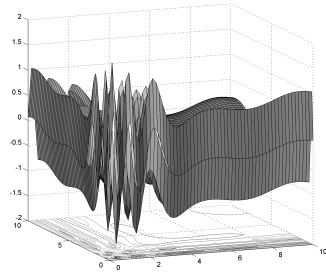
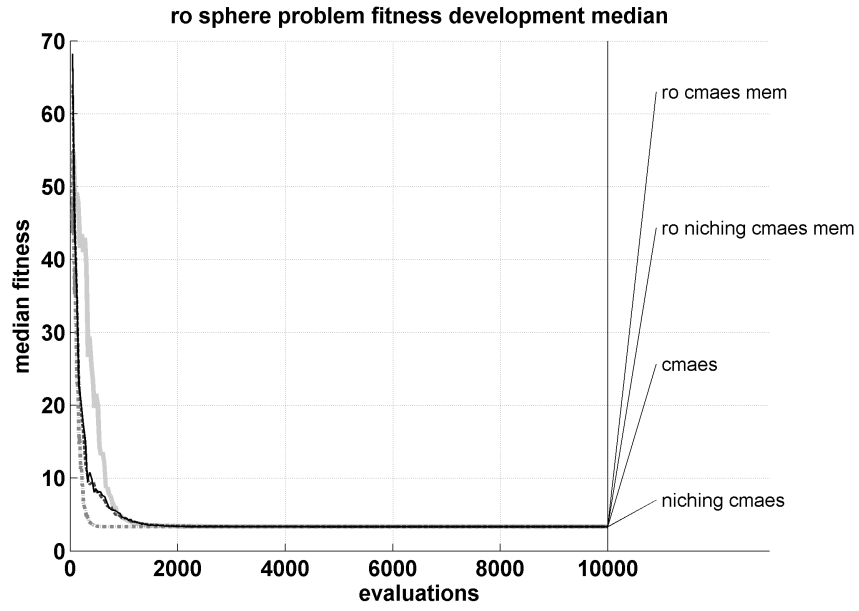
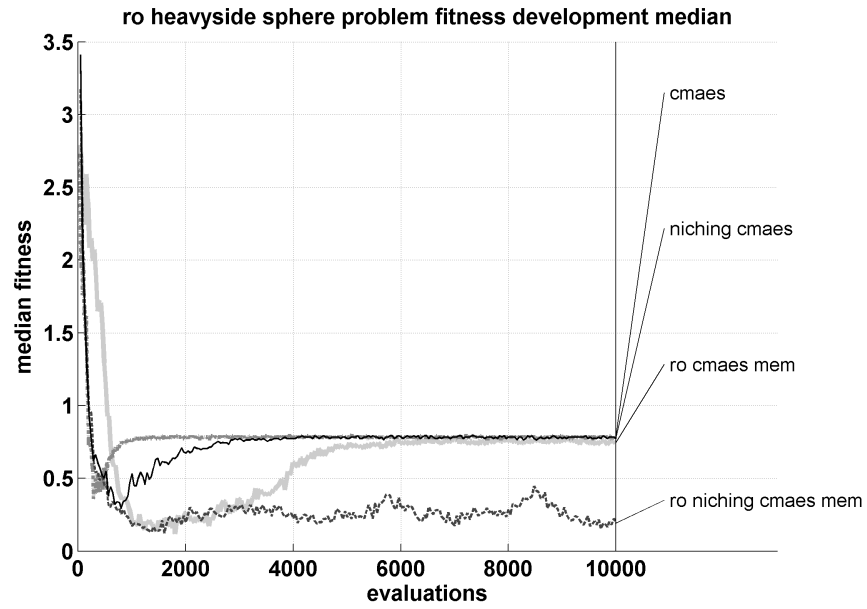
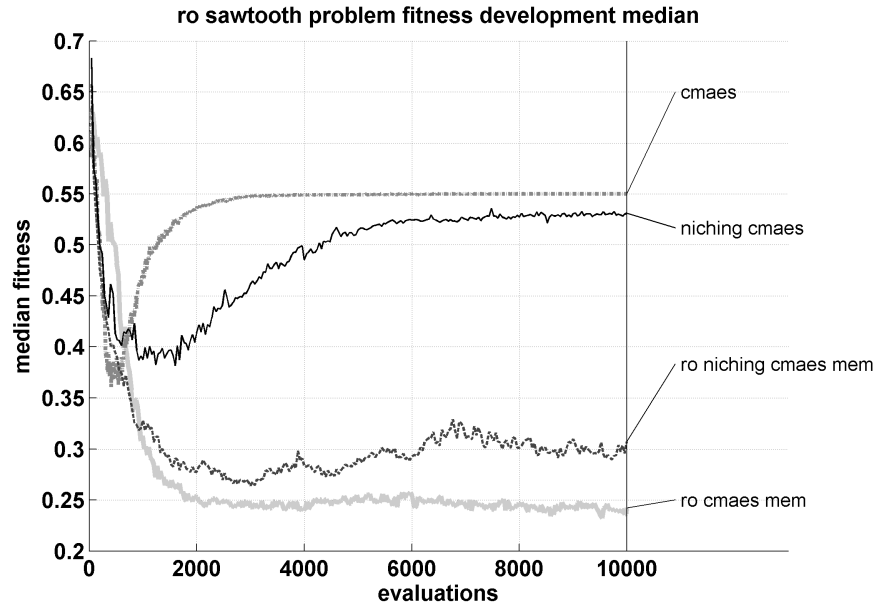
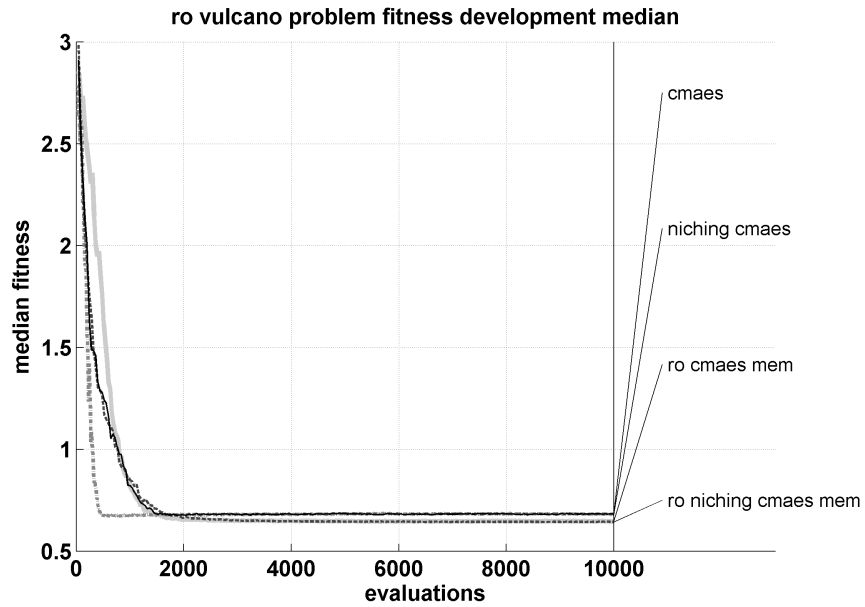
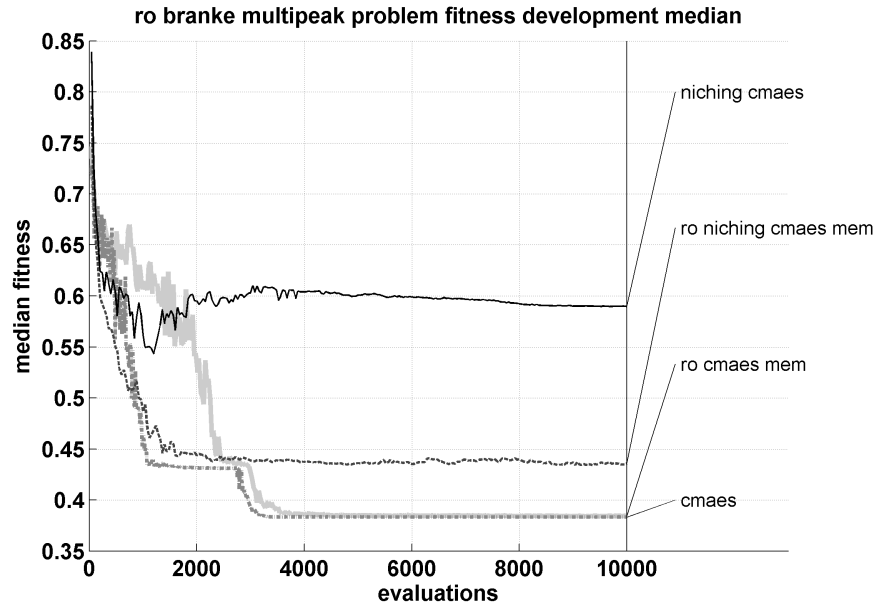
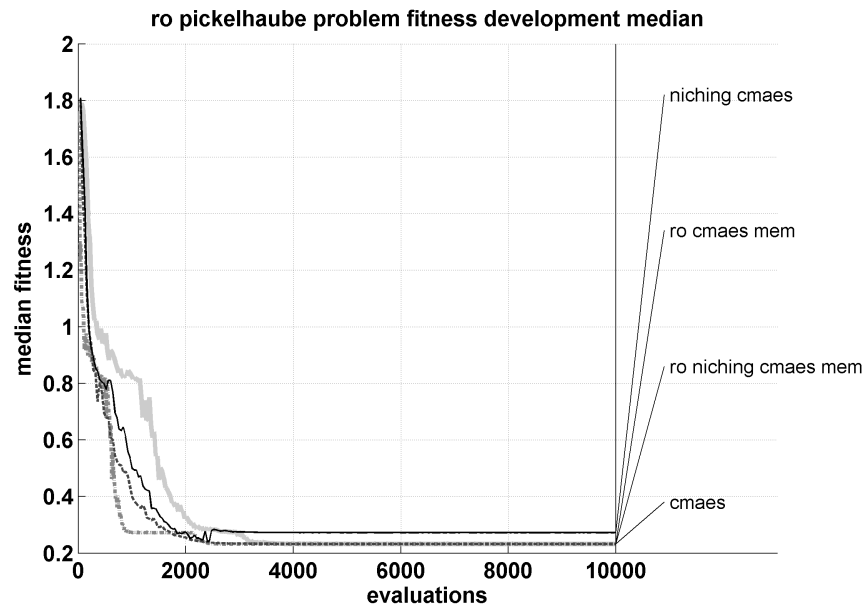
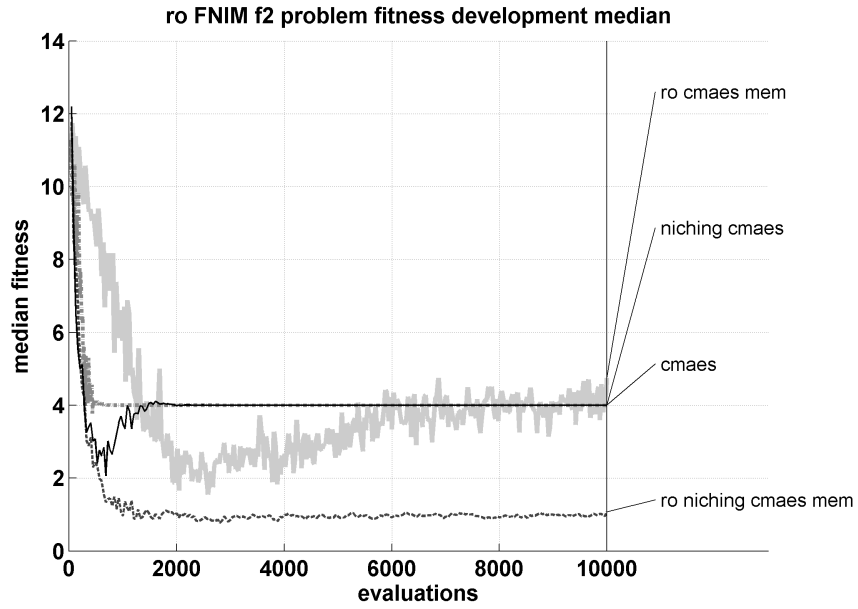
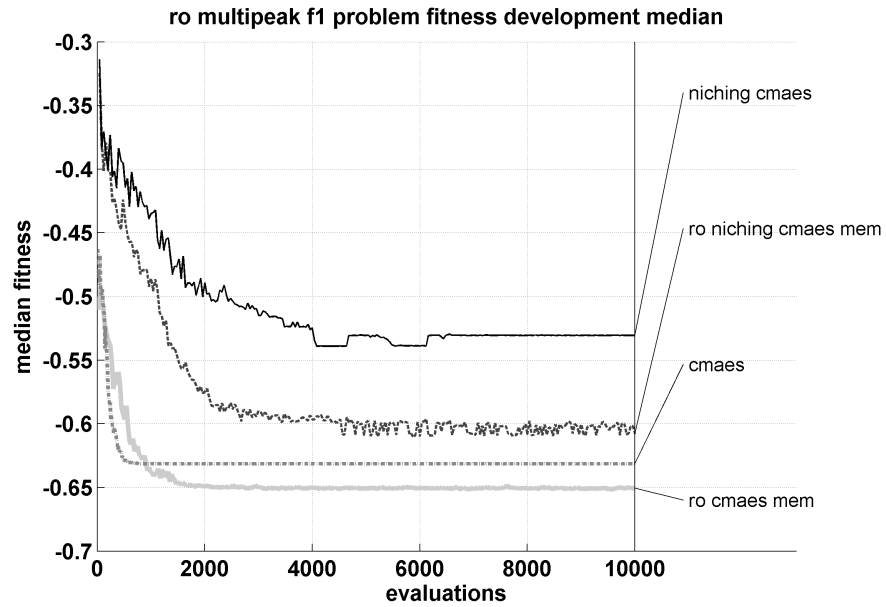
(a) Sphere problem, f_1 .(b) Heavy side sphere problem f_2 .(c) Sawtooth problem, f_3 .(d) Volcano problem, f_4 .(e) Branke multipeak problem, f_5 .(f) Pickelhaube problem, f_6 .(g) FNIM f2 problem, f_7 .(h) Multipeak f1 problem, f_8 .(i) Multipeak f2 problem, f_9 .

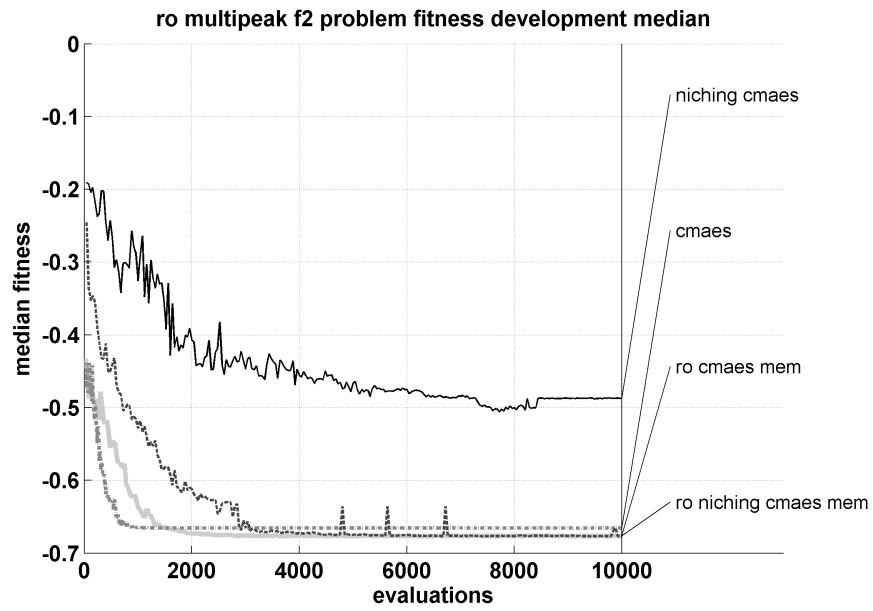
Figure 6.2: Two dimensional representations of the nine test problems.

Figure 6.3: Sphere problem, f_1 .Figure 6.4: Heavy side sphere problem f_2 .

Figure 6.5: Sawtooth problem, f_3 .Figure 6.6: Volcano problem, f_4 .

Figure 6.7: Branke multipeak problem, f_5 .Figure 6.8: Pickelhaube problem, f_6 .

Figure 6.9: FNIM f2 problem, f_7 .Figure 6.10: Multipeak f1 problem, f_8 .

Figure 6.11: Multipeak f2 problem, f_9 .

Chapter 7

Conclusion and Outlook

In this paper we have proposed an CMA-ES with niching and the MEM evaluation scheme. The proposed strategy has been tested against three other versions of the CMA-ES algorithm on nine 10 dimensional test problems. It has shown that the CMA-ES with niching and the MEM evaluation scheme can outperform on the majority of the test problems, but the original hypothesis is not completely confirmed. Because the original idea was that niching would help with finding the more robust parts of the search area, and thus perform better on the multipeak problems, but it does not perform better on the multipeak problems. The reason for this could not be found.

For future work it would be interesting to find the exact reason why the CMA-ES with niching and MEM does perform well on functions with sharp edges, but not so well on multipeak functions, while the intuition is the opposite.

Other future work could consist of exploring the possibilities of increasing the size of μ per niche. The problem of having multiple σ' s, $\mathbf{C}'$ s can be overcome by different ways. For example, taking the $\mathbf{C}$ and σ of the best individual of each niche, or taking the average of them. It is possible that this could improve the algorithm.

Another thing that is be worth looking into, is the role of q . How to set this parameter to have the most chance of finding the robust peak, but not wasting too many function evaluations. Having a variable q sounds like viable option. Starting with many niches to have big explorative power and then towards the end of the budget decreasing the size to continue with the best niches.

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Appendix A

Dynamic peak identification

```
1 function [num_peaks, dps] = dynamic_peak_identification(n, q, rho, xo, sortindex)
2 % [] = dynamic_peak_identification()
3 % Input:
4 % - N                               - Number of dimensions
5 % - n                               - Size of the population lambda * q
6 % - q                               - Number of peaks to identify
7 % - rho                             - The niching radius
8 % - xo                             - The current population
9 % - sortf                           - Order of the indices
10 %
11 % Output:
12 % - num_peaks                      - Number of peaks found
13 % - niches                         - Niches found
14
15 i = 1;
16 num_peaks = 0;
17 dps = -1 * ones(q,1);
18 while (num_peaks < q && i <= n)
19     is_niche_leader = true;
20     k = 1;
21     while (k <= num_peaks && is_niche_leader == true)
22         if (norm(xo(:,dps(k)) - xo(:,sortindex(i)))) < rho)
23             is_niche_leader = false;
24         end
25         k = k+1;
26     end
27     if (is_niche_leader)
28         num_peaks = num_peaks + 1;
29         dps(num_peaks) = sortindex(i);
30     end
31     i = i + 1;
32 end
33 end
```

Appendix B

CMA-ES with niching and MEM

```
1 function [stat] = ro_niching_cmaes_mem(problem_specification,
2                                     algorithm_parameters, run_parameters)
3 % [stat] = cmaes(problem_specification,
4 %               run_parameters, algorithm_parameters)
5 %
6 % Implementation of the mem scheme and niching into CMA-ES algorithm
7 %
8 % Input:
9 % - problem_specification      - A struct containing the problem
10 %                               definition with:
11 %   - problem_type            - A string holding description of
12 %                               the problem type
13 %   - problem_name            - A string holding the name of
14 %                               the test function
15 %   - objective_function       - A function handle to the
16 %                               objective function
17 %   - N                        - The number of dimensions
18 %                               of the search space
19 %   - lb                       - A vector of the upper bounds of
20 %                               the search interval
21 %   - ub                       - A vector of the lower bounds of
22 %                               the search interval
23 %
24 % - run_parameters            - A struct containing the run
25 %                               parameters with:
26 %   - max_generations_termination - The maximum number of generations
27 %   - max_evaluations_termination - The maximum number of evaluations
28 %   - min_fitness_termination    - Stop when a solution is found below
29 %                               this value
30 %   - history_statistics         - Maintain history statistics
31 %   - internal_parameters_statistics - Maintain statistics of the internal
```

```

32 %                                     parameters
33 % - report_intermediate               - Report statistics while running
34 % - report_after_termination          - Report after termination
35 % - report_fct                       - A handle to the report function
36 % - restart_log_intermediate          - Maintain a logfile to allow for
37 %                                     restarts
38 % - restart_log_after_termination     - Store a logfile to allow for
39 %                                     restarts after completing an optimization run
40 % - restart_log_logfile               - Filename of the restart logfile
41 %
42 % - algorithm_parameters              - A struct containing algorithm
43 %                                     specific parameters
44 % - bch_fct                          - A handle to the box constraint
45 %                                     handling function
46 % - sampling_fct                     - The sampling function used for
47 %                                     obtaining the samples for the robustness approximations
48 % - m                                - The number of samples used for the
49 %                                     robustness approximations
50 % - reuse_disturbances                - Specify whether or not to use the
51 %                                     same disturbances for all individuals in the population
52 %
53 % Output:
54 % - stat                             -
55 %
56 % Last modified: December 9, 2011
57
58 % Problem specification
59 fitnessfct = problem_specification.objective_fct;
60 N = problem_specification.N;
61 lb = problem_specification.lb;
62 ub = problem_specification.ub;
63 ur_sigma = problem_specification.ur_sigma;
64
65 % Run parameters
66 stopeval = run_parameters.max_evaluations_termination;
67 stopgen = run_parameters.max_generations_termination;
68 minfitness = run_parameters.min_fitness_termination;
69 history_statistics = run_parameters.history_statistics;
70 internal_parameter_statistics =
71     run_parameters.internal_parameter_statistics;
72 report_intermediate = run_parameters.report_intermediate;
73 report_after_termination = run_parameters.report_after_termination;
74 report_fct = run_parameters.report_fct;
75 restart_log_intermediate = run_parameters.restart_log_intermediate;
76 restart_log_after_termination =
77     run_parameters.restart_log_after_termination;
78 if (restart_log_intermediate || restart_log_after_termination)
79     restart_log_logfile = run_parameters.restart_log_logfile;
80 end
81

```

```

82 % Algorithm parameters
83 bch_fct = algorithm_parameters.bch_fct;
84 sampling_fct = algorithm_parameters.sampling_fct;
85 m = algorithm_parameters.m;
86 q = algorithm_parameters.q;
87
88 %count times of niche restart
89 restart = 0;
90 % Set lambda, mu and the weights for recombination
91 r = 0.5 * norm(ub - lb);
92 rho = r / q^(1/N);
93 lambda = 4 + floor(3 * log(N));
94 mu = 1; %only works for mu = 1
95 weights = log(mu + 1) - log(1:mu)';
96 weights = weights / sum(weights);
97 mueff = sum(weights)^2 / sum(weights.^2);
98
99 % Set parameters
100 cc = 4 / (N + 4);
101 cs = (mueff + 2) / (N + mueff + 3);
102 mucov = mueff;
103 ccov = (1 / mucov) * 2 / (N + 1.4)^2 + (1 - 1 / mucov)
104         * ((2 * mueff - 1) / ((N + 2)^2 + 2 * mueff));
105 damps = 1 + 2 * max(0, sqrt((mueff - 1) / (N + 1)) - 1) + cs;
106 chiN = N^0.5 * (1 - 1 / (4 * N) + 1 / (21 * N^2));
107
108 % Initialize xmean and step size
109 if (isfield(algorithm_parameters, 'xmean_init'))
110     xmean = algorithm_parameters.xmean_init;
111 else
112     xmean = repmat(lb, 1, q) + repmat(ub - lb, 1, q) .* rand(N,q);
113 end
114
115 if (isfield(algorithm_parameters, 'sigma_init'))
116     sigma = algorithm_parameters.sigma_init;
117 else
118     sigma = repmat((norm(ub - lb)) / (3 * q * sqrt(N)), 1, q);
119 end
120
121 % Test reuse_disturbances parameter
122 if (isfield(algorithm_parameters, 'reuse_disturbances'))
123     reuse_disturbances = algorithm_parameters.reuse_disturbances;
124 else
125     reuse_disturbances = true;
126 end
127
128 % Initialize matrices and vectors of the CMA-ES
129 pc = zeros(N,q);
130 ps = zeros(N,q);
131 B = ones(N,N,q);

```

```

132     D = ones(N,N,q);
133     C = ones(N,N,q);
134     for i=1:q,
135         pc(:,i) = zeros(N,1);
136         ps(:,i) = zeros(N,1);
137         B(:, :, i) = eye(N,N);
138         D(:, :, i) = eye(N,N);
139         C(:, :, i) = eye(N,N);
140     end
141
142     % Initialize counters
143     evalcount = 0;
144     gencount = 0;
145
146     % Statistics administration parameters
147     stat.optimizer_name = 'ro_niching_CMA-ES';
148     stat.run_status = 'Incomplete';
149     estimated_stopeval = max(stopeval, stopgen * lambda);
150     estimated_stopgen = max(stopgen, ceil(stopeval / lambda));
151     stat.gencount = 0;
152     stat.evalcount = 0;
153     stat.x_opt = zeros(N,q);
154     stat.f_opt = zeros(1,q);
155     stat.rho = rho;
156     if (history_statistics)
157         stat.evalvsngen = zeros(1, estimated_stopgen);
158         stat.hist_x_opt = zeros(N, q, estimated_stopgen);
159         stat.hist_f_opt = zeros(q, estimated_stopgen);
160         stat.hist_x = zeros(N, estimated_stopeval);
161         stat.hist_f = zeros(1, estimated_stopeval);
162         stat.hist_xmean = zeros(N, estimated_stopgen);
163     end
164     if (internal_parameter_statistics)
165         stat.hist_sigma = zeros(1, q, estimated_stopgen);
166         stat.hist_ps = zeros(N, estimated_stopgen);
167         stat.hist_pc = zeros(N, estimated_stopgen);
168         stat.hist_C = zeros(N, N, estimated_stopgen);
169         stat.hist_B = zeros(N, N, estimated_stopgen);
170         stat.hist_D = zeros(N, N, estimated_stopgen);
171         stat.hist_dps = zeros(q, estimated_stopgen);
172         stat.hist_q = q;
173         stat.hist_N = N;
174     end
175
176     % If restart then load restart log logfile
177     if (run_parameters.do_restart && exist(restart_log_logfile, 'file'))
178         load(sprintf('%s', restart_log_logfile));
179         stat.run_status = 'Incomplete';
180     end
181

```

```

182 % Initialization for speedup
183 xo = zeros(N, q * lambda);
184 zo = zeros(N, q * lambda);
185 fo = zeros(1, q * lambda);
186 zmean = zeros(N,q);
187
188 % Evolution loop
189 while ((stopeval == -1 || evalcount < stopeval) ...
190     && (stopgen == -1 || gencount < stopgen) ...
191     && stat.f_opt(1) > minfitness)
192
193     % Statistics administration
194     gencount = gencount + 1;
195     stat.gencount = gencount;
196     if (internal_parameter_statistics)
197         for i=1:q,
198             stat.hist_sigma(:,i,gencount) = sigma(:,i);
199         end
200         stat.hist_ps(:,gencount) = ps(:,1);
201         stat.hist_pc(:,gencount) = pc(:,1);
202         stat.hist_C(:,gencount) = C(:,1);
203         stat.hist_B(:,gencount) = B(:,1);
204         stat.hist_D(:,gencount) = D(:,1);
205     end
206
207     % Generate a sample set of input parameter disturbances if they are reused
208     if (reuse_disturbances)
209         x_dists = sampling_fct(m, N, -ur_sigma', ur_sigma')';
210     end
211     fo_dists = zeros(1,m);
212     xo_dists = zeros(N,m);
213
214     % Generate and evaluate lambda offspring
215     for j=1:q
216         i = (j - 1) * lambda;
217         for k=1:lambda,
218             % Generate a sample set for every individual
219             if (~reuse_disturbances)
220                 x_dists = sampling_fct(m, N, -ur_sigma', ur_sigma')';
221             end
222             zo(:,k+i) = randn(N,1);
223             xo(:,k+i) = xmean(:,j) + sigma(:,j) * (B(:,j)
224                 * D(:,j) * zo(:,k+i));
225             xo(:,k+i) = feval(bch_fct, xo(:,k+i), lb, ub);
226
227             for l=1:m,
228                 xo_dists(:,l) = xo(:,k+i) + x_dists(:,l);
229                 fo_dists(l) = feval(fitnessfct, xo_dists(:,l));
230             end
231             fo(k+i) = mean(fo_dists);

```

```

232
233     % Statistics administration
234     evalcount = evalcount + 1;
235     stat.evalcount = evalcount;
236     if (history_statistics)
237         stat.hist_x(:,evalcount) = xo(:,k+i);
238         stat.hist_f(evalcount) = fo(k+i);
239     end
240 end
241 end
242
243 % Sort by fitness and compute weighted mean into xmean
244 [~, sortindex] = sort(fo); % M I N I M I Z A T I O N
245 [num_peaks, niches] = dynamic_peak_identification(lambda*q, q,
246                                                    rho, xo, sortindex);
247
248 parxmean = xmean;
249 parsigma = sigma;
250 parC = C;
251 parB = B;
252 parD = D;
253 parps = ps;
254 parpc = pc;
255
256 for i=1:num_peaks,
257     dps_parents = niches(i,:);
258     par = ceil(dps_parents / lambda);
259
260     zmean(:,i) = zo(:,dps_parents) * weights;
261
262     Bn = squeeze(parB(:,:,par));
263     Cn = squeeze(parC(:,:,par));
264     Dn = squeeze(parD(:,:,par));
265
266     xmean(:,i) = feval(bch_fct, parxmean(:,par)
267                       + parsigma(par) * (Bn * Dn * zmean(:,i)), lb, ub);
268
269     % Cumulation: Update evolution paths
270     ps(:,i) = (1 - cs) * parps(:,par) + sqrt(cs * (2 - cs)
271                                                * mueff) * (Bn * zmean(:,i));
272     hsig = norm(ps(:,i)) / sqrt(1 - (1 - cs)^(2 * evalcount / lambda))
273           / chiN < 1.4 + 2/(N + 1);
274     pc(:,i) = (1 - cc) * parpc(:,par) + hsig * sqrt(cc * (2 - cc)
275                                                    * mueff) * (Bn * Dn * zmean(:,i));
276
277     % Adapt covariance matrix C
278     Cn = (1 - ccov) * Cn + ccov * (1 / mucov) * ...
279         (pc(:,i) * pc(:,i)' + (1-hsig) * cc * (2 - cc) * Cn) +
280         ccov * (1-1/mucov) * ...
281         (Bn * Dn * zo(:,dps_parents)) * diag(weights)

```

```

282                                     * (Bn * Dn * zo(:,dps_parents))';
283
284     % Adapt step size sigma
285     sigma(i) = parsigma(par) * exp((cs / damp)
286                                     * (norm(ps(:,i)) / chiN - 1));
287
288     % Update B and D from C
289     Cn = triu(Cn) + triu(Cn,1)';
290     [Bn,Dn] = eig(Cn);
291     D(:, :, i) = diag(sqrt(diag(Dn)));
292     C(:, :, i) = Cn;
293     B(:, :, i) = Bn;
294 end
295
296 while (num_peaks < q)
297     num_peaks = num_peaks + 1;
298     restart = restart + 1;
299     xmean(:, num_peaks) = lb + (ub - lb) .* rand(N,1);
300     if (isfield(algorithm_parameters, 'sigma_init'))
301         sigma(num_peaks) = algorithm_parameters.sigma_init;
302     else
303         sigma(num_peaks) = (norm(ub - lb)) / (3 * q * sqrt(N));
304     end
305     pc(:, num_peaks) = zeros(N,1);
306     ps(:, num_peaks) = zeros(N,1);
307     B(:, :, num_peaks) = eye(N,N);
308     D(:, :, num_peaks) = eye(N,N);
309     C(:, :, num_peaks) = eye(N,N);
310 end
311
312 % Statistics administration
313 for i=1:q,
314     if(niches(i) < 0)
315         %stat.x_opt(:,i) = [inf, inf];
316     else
317         stat.x_opt(:,i) = xo(:, niches(i));
318     end
319 end
320
321 for i=1:q,
322     if (niches(i,1) < 0)
323         stat.f_opt(i) = Inf;
324     else
325         stat.f_opt(i) = fo(sortindex(niches(i,1)));
326     end
327 end
328
329 if (history_statistics)
330     stat.evalvsgen(stat.gencount) = evalcount;
331     stat.hist_x_opt(:, :, gencount) = stat.x_opt;
332     stat.hist_f_opt(:, :, gencount) = stat.f_opt;

```

```

332     stat.hist_xmean(:,gencount) = xmean(:,1);
333     stat.hist_dps(:,gencount) = niches(:,1);
334 end
335
336 % Store log for restart
337 if (restart_log_intermediate)
338     save(sprintf('%s',restart_log_logfile), 'xmean', 'sigma', 'pc',
339         'ps', 'B', 'D', 'C', 'evalcount', 'gencount', 'stat');
340 end
341
342 % Report statistics
343 if (report_intermediate)
344     report_fct(stat, problem_specification,
345         algorithm_parameters, run_parameters)
346 end
347 end
348
349 % Complete statistics struct
350 if (history_statistics)
351     stat.evalvsgen = stat.evalvsgen(1:gencount);
352     stat.hist_x = stat.hist_x(:,1:evalcount);
353     stat.hist_f = stat.hist_f(:,1:evalcount);
354     stat.hist_x_opt = stat.hist_x_opt(:,1:gencount);
355     stat.hist_f_opt = stat.hist_f_opt(:,1:gencount);
356     stat.hist_xmean = stat.hist_xmean(:,1:gencount);
357 end
358 if (internal_parameter_statistics)
359     stat.hist_sigma = stat.hist_sigma(:,1:gencount);
360     stat.hist_ps = stat.hist_ps(:,1:gencount,:);
361     stat.hist_pc = stat.hist_pc(:,1:gencount,:);
362     stat.hist_C = stat.hist_C(:,1:gencount,:);
363     stat.hist_B = stat.hist_B(:,1:gencount,:);
364     stat.hist_D = stat.hist_D(:,1:gencount,:);
365 end
366 stat.run_status = 'Complete';
367
368 % Store log
369 if (restart_log_intermediate || restart_log_after_termination)
370     save(sprintf('%s',restart_log_logfile), 'xmean', 'sigma', 'pc', 'ps',
371         'B', 'D', 'C', 'evalcount', 'gencount', 'stat');
372 end
373
374 % Plot statistics
375 if (report_after_termination)
376     report_fct(stat, problem_specification, algorithm_parameters,
377         run_parameters)
378 end
379 stat.hist_restart = restart;
380 end

```