Multi-armed Bandit Based Covariance Matrix Adaptation Evolution Strategy

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Outline

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Real-valued Function Optimization

- Real-valued function
  - $f\colon \mathcal{S} \subset \mathbb{R}^n \to \mathbb{R}, x \mapsto f(x)$
  - $\mathcal{S}$: search space
  - Elements of $\mathcal{S}$: candidates or solutions
- Optimization
  - $\arg\min_x f(x)$, where x are within given bounds.
  - Maximizing f is equivalent to minimizing $-f$.
- Example
  - $\arg\min_x 2x^3 - 3x^2 - 36x - 14$.
  - Design of aircraft wings.

Black-box Optimization

- Without interior information.
- Unavailable to optimize using mathematical methods.
- The only information is the interaction between input and output.

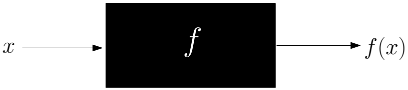

Figure: Black-box function

Difficulties

- Non-convex
- Ruggedness
- Dimensionality and non-separable
- Ill-conditioned

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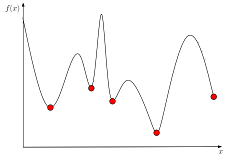

Figure: Non-convex function

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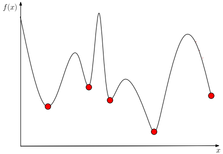

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Difficulties

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  - Non-smooth.
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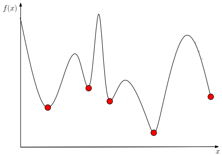


Figure: Non-convex function

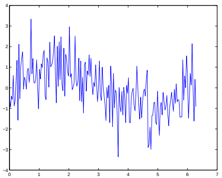
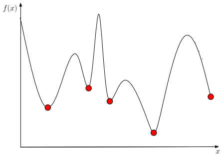


Figure: $sin(x)$ with noise

Difficulties

- Non-convex
  - Multi-modal problems
- Ruggedness
  - Perturbated by noise.
  - Non-smooth.
- Dimensionality and non-separable
- Ill-conditioned
  - Unable to extract gradient information



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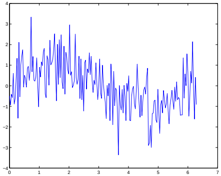

Figure: $sin(x)$ with noise

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Related Approaches

- Optimizing black-box problems
  - No deterministic way to evolve global optimum.
  - Applying random search for approximation.
- Stochastic algorithms
  - Ant Colony Optimization, Bat Algorithm, etc.
  - Iteratively generating better solutions.
- Two major approaches
  - Estimation of distribution algorithm (EDA).
  - Evolution strategy (ES).

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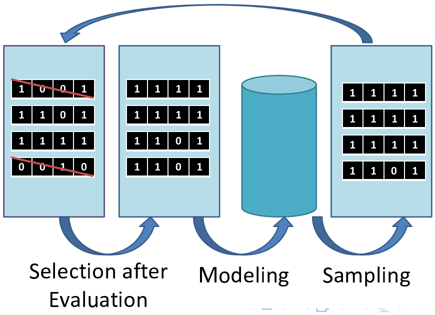

Extended Compact Genetic Algorithm (ECGA)

- Each EDA is different from the others in model building.
- ECGA was proposed by Harik (1999).
- Good probabilistic model inspires good linkage learing
  - Model is built according to population distribution.
  - Applying greedy search to refine model iteratively.
- ECGA focuses on bitstring, discrete problems.
  - χ-ECGA.
  - An interface for real-valued function is demanded.

Discretization

- Continuous domain → Discrete domain
- Finding good solutions → Finding promising regions
- 2 traditional discretization methods
  - Fixed Height Histogram (FHH)
  - Fixed Width Histogram (FWH)

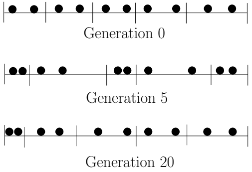

Figure: illustration of FHH

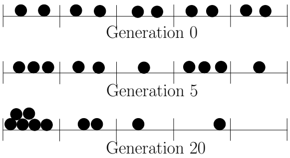

Figure: illustration of FWH

Split on Demand

- Solutions in each bin should not exceed γN.
  - N is the population size.
  - γ defines the rate of one region.
- γ decays with a factor ϵ.

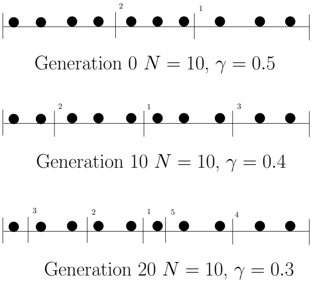

Figure: illustration of SoD

Real-coded ECGA with SoD

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1. Preparing discretization

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2. Integrating discretized results into ECGA.

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4. Sampling accordingly.
5. For every L generations, a local optimizer is adopted to obtain high resolution solutions
6. If model does not converge, goto 1.

Evolution Strategy (ES)

- A search template for black-box optimization.
  - Encoded in continuous domain.
- New search points are generated based on current population.
- (μ, λ)-ES and $(\mu, \mu + \lambda)$-ES.
- $x_i^{t+1} = m^t + \sigma N_i(0, C)$.
  - x_i: i-th generated solution at generation $t + 1$.
  - m: weighted mean of population at generation t.
  - σ: step size.
  - C: Estimated distribution.

Covariance Matrix Adaptation Evolution Strategy (CMA-ES)

- A famous derivation of ES.
- Importance of σ and C.
  - Larger step size reinforces exploration while smaller reinforces exploitation.
    - Choosing an fixed, appropriate number?
  - Covariance matrix determines the shape of estimated distribution.
    - Determining the length of each axis.
    - Representing the dependency among decision variables.
- CMA-ES features in the adoption of historical information.
  - σ and C are adjusted accordingly.

Illustration of σ and C

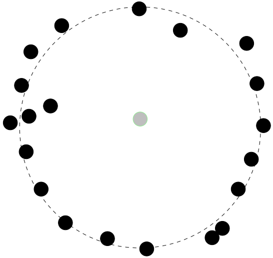


Figure: $t = 0$

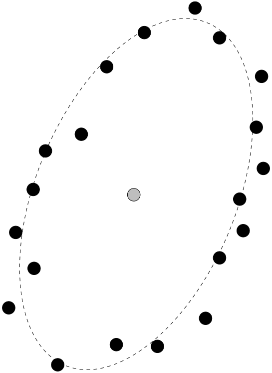


Figure: $t = 10$

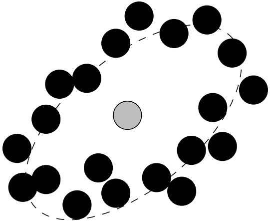


Figure: $t = 20$

Outline

Motivation

- Exploration and Exploitation
  - Exploration: the ability to have an overview to the search space.
  - Exploitation: the ability to generate high resolution solutions.
  - CMA-ES preforms outstandingly on exploitation.
- Easily trapped into local optima due to the ability of exploitation.
  - Lack of diversity
  - Typical evolutionary algorithms adopt a larger initial population size.
  - CMA-ES benefits nothing from a larger initial population size.

Hypothesis

- Increasing diversity by maintaining multiple groups.
    - kind of discretization.
    - How to define the number of groups?
    - What is the criteria for individuals to form a group?
- There is implicit information hidden between groups.
    - How to extract the information?
    - How to benefit from the information and obtain better solutions?
        - Inspired by discretization, we aim to find a more promising region.
- 2-layer CMA-ES is introduced
    - Inner layer for exploitation
    - Outer layer for exploration

Outline

Flow of Proposed Template

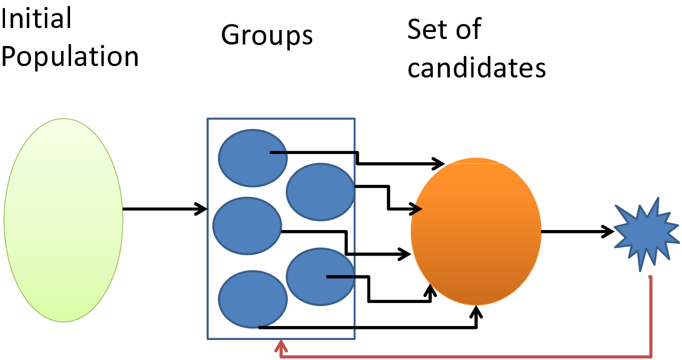


Figure: Flow

Pseudo-code of Template

```
begin
    Initializing population;
    Clustering;
    while not terminate do
        while any group has not been evolved for certain generation do
            Evolving each group;
        end
        Selecting candidates for each group;
        Evolving the selected solutions;
    end
end
Algorithm: Overview for the system
```

Undetermined Components

- The method for making division
- The criterion of selecting representative solutions for each group
- The method for evolving the selected candidates

Making Division

- The initial population is expected to categorized according to position.
    - Roughly expresses the diversity
    - A population in a specific region is expected driven toward the identical local optimum.
    - In other words, a group can be roughly viewed as points near by one specific valley.
- Space locality plays an important role.
    - Applying clustering

k-means

- *k-means* clustering is a basic method for vector quantization.
  - Partitioning n solutions into k mutual independent clusters.
  - Serving as a prototype
- Number of clusters
  - As known as number of groups.
  - Without k, finding optimal is said to be NP-hard.
  - To define a proper k is difficult.
- Heuristic algorithms for approximation.
  - Forgy method for initialization
  - iteratively refinements until convergence

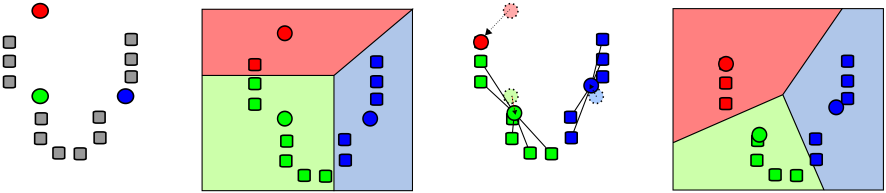
Algorithm of Approximation to k-means

Input: k, d, $\{o_1, o_2, \ldots, o_n\}$ as observations
Output: $\mathcal{S}$

```
Initial: m_1, m_2, ..., m_k are random selected from observations as initial
centers ;                                                   // Forgy method
while At least one of the observations moves to other group do
    for j = 1 to k do
        S_j = ∅ ;
    end
    for i = 1 to n do
        assign o_i to S_j if o_i is closest to m_j among the k centers;
    end
    for j = 1 to k do
        m_j is updated by the arithmetic mean of all vectors ∈ S_j;
    end
end
```

Algorithm: Clustering heuristic function

Illustration for The Algorithm



Remaining Criteria

- How to select representativeness from each group?
  - Using the optimal solution found so far as the representativeness in each group
- How to evolve selected candidates?
  - Evolving them with CMA-ES
  - The so-called 'outer CMA-ES'
  - Aims to observe if better regions can be reached
- The number of solutions in a group is fixed after clustering.
  - Once a better solution is generated, the worst one should be replaced.

An Implementation of the Template

Input: n,t

Output: best solution ever evolved

Uniformly sampled population of size n;

$k = \sqrt{\frac{n}{2}}$;

Integrating *k-means* with *Frogy-method* to cluster the n individuals into k groups;

$C \leftarrow$ array with size k;

for *i = 1 to k* **do**

  Optimizing group$_i$ by adopting CMA-ES for t generations;

  $C_i \leftarrow$ best solution;

  Applying CMA-ES to evolve the population consisting of local optima of groups, as known as C, until terminated.;

end

Algorithm: 2-layer CMA-ES

- 2-layer CMA-ES addresses the diversity for the search.
- Next we lay emphasis on finding more promising regions.

Exploring

- Based on current groups, we aim to figure out better solutions.
  - According to our hypothesis, the implicit information is hidden between groups.
  - What is a good way to evolve groups?
- We consider the priority
  - Put less concentration on groups which performs badly
  - Lay emphasis on possible regions
  - Without any prior knowledge, a selection strategy is demanded.
- The ability to generate new groups adaptively
  - We assume a fixed number of groups.
  - A replacement strategy is demanded accordingly.

The Selection Strategy

- The selection strategy is with the feature that
  - Given a set of groups, the performance of each group is evaluated through trials
  - Lays emphasis on better performance groups
  - groups with worse performance would not be ignored permanently
- This is just identical to the Multi-armed Bandit (MAB) problem.

Multi-armed Bandit Problem

- Investigate the trade-off between exploration and exploitation
- Assume there are k independent slot machines
- Each machine generates reward according to its own unknown probability distribution.
- We can only observe the playing sequence and the correlated reward.
- The goal is to maximize reward in limited play times.

Upper Confidence Bound

- A family of solutions to MAB problems
- UCB1 – the first Upper Confidence Bound (UCB) algorithm
- Play machine j which maximizes

$$\bar{x_j} + \sqrt{\frac{2 \ln n}{n_j}}$$

  - $\bar{x_j}$: the average reward of machine j.
  - n_j: the number of times machine j has been played.
  - n: the played times of overall system.

UCB1-tuned

- UCB1 takes no variance into consider.
  - UCB1-tuned is the version which adds variance as a factor.
  - UCB1-tuned is not proven working well but outperforms UCB1 in practice.
  - In UCB1-tuned, the machine j to be played is with the highest

$$\bar{x_j} + \sqrt{\frac{\ln n}{n_j} \min(\frac{1}{4}, V_j(n_j))}$$

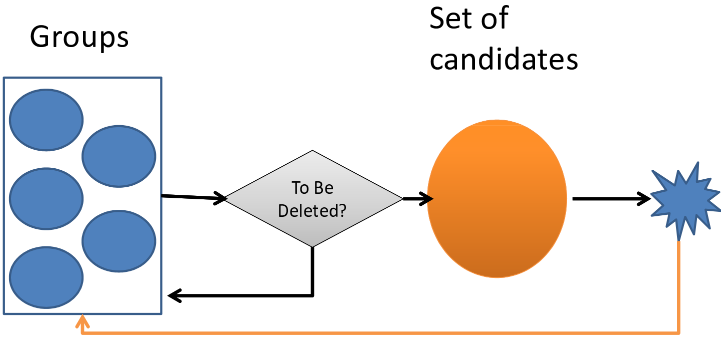
, where $V_j(t) = \sigma_j^2 + \sqrt{\frac{2 \ln n}{n_j}}$.

- UCB1-tuned is adopted in our work.

The Replacement Strategy

- By generating a new point and sampling around the new point, we claim to form a better group, and the worst one should be replaced.
- There are 2 judgement to distinguish if there is any group to delete.
  1. If a group does not sample a better solution anyway.
  2. If no group converges, check among groups if there is group has not been played for t rounds where t is a number larger than the number of the solutions the group contains.

Flow of MAB-based CMA-ES



Procedure of MAB-based CMA-ES

Algorithm: MAB-based CMA-ES

Input: n,t as a proper generation for each pulling action

Output: best solution ever evolved

Uniformly sampled population of size n;

$k = \sqrt{\frac{n}{2}}$;

Integrating *k-means* with *Frogy-method* to cluster the n individuals into k groups as known as bandits;

$C \leftarrow$ array with size k;

for *i = 1 to k* **do**

    pull(i);

    $C_i \leftarrow$ best solution;

end

while *not terminated* **do**

    for *i = 1 to k* **do**

        calculateUCB(i) ; `// calculate modified UCB1-tuned as illustrated above`

        record the index with max value in M;

    end

    pull(M);

    $C_M \leftarrow$ best solution in group$_M$;

    update();

end

```
Initial P ← a permutation array from 1 to k;
ToBeDeleted = 0;
for i = 1 to k do
    if deleting criterion 1 is met in group_{P_i} then
        ToBeDeleted = P_i;
    end
end
if ToBeDeleted = 0 then
    for i = 1 to k do
        if deleting criterion 2 is met in group_{P_i} then
            ToBeDeleted = P_i;
        end
    end
end
if ToBeDeleted = 0 then
    return;
end
else
    s ← ToBeDeleted;
    generate a new solution as a new group denoted as group* according
    to C_1, C_2, ..., C_{s_{i-1}}, C_{s_{i+1}}, ..., C_k ;
    for i = 1 to ||group_s|| − 1 do
        pull(group*) without replacing worst;
    end
    replace group_s with group*;
    return;
end
Algorithm: update
```

Outline

Testbed

- A set of benchmark proposed in CEC 2005 (Suganthan et al. 2005)
- 25 problems are categorized into 4 kinds of problem that
  - Unimodal functions (1–5)
  - Basic multi-modal functions (6–12)
  - Expanded functions (13–14)
  - Hybrid composition functions (15–25)
- Benchmark criteria
  - N_{f_e} to convergence
  - The accuracy after 10^5 N_{f_e}
  - We aim to design an algorithm with the ability to adaptively develop more promising. Therefore we take the latter.

Experiments Design

- The algorithms are designed based on the assumption of increasing diversity and extracting implicit information.
- As a consequence, we demonstrate 2 comparisons to verify the assumption.
  1. Comparing original CMA-ES and 2-layer CMA-ES
  2. Comparing 2-layer CMA-ES and MAB-based CMA-ES
- Finally, a comparison between MAB-based CMA-ES and rECGA with SoD is demonstrated. The motivation is to verify if our algorithm provides comparable results in the field of discretization.

Comparison

- For original CMA-ES, the λ is set to 20 and σ is initialized to 1.
- For 2-layer CMA-ES, the λ and σ is as above.
- For 2-layer CMA-ES, the initial population size is set to 450 and inner CMA-ES executes for 1000 generations.

	CMA-ES	2-Layer CMA-ES
U	–	–
B	–	1
E	–	2
H	2	4
Total	2	7

Table: Best accuracy comparison

	CMA-ES	2-Layer CMA-ES
U	1	–
B	2	1
E	–	2
H	3	5
Total	6	8

Table: Median accuracy comparison

Comparison

- 2-layer CMA-ES is set as above.
- MAB-based CMA-ES sets t of inner CMA-ES to be 30 and t of outer CMA-ES to be 1. Other settings are identical 2-layer CMA-ES.

	2-Layer CMA-ES	MAB-basd CMA-ES
U	–	–
B	–	–
E	1	1
H	2	3
Total	3	4

Table: Best accuracy comparison

	2-Layer CMA-ES	MAB-basd CMA-ES
U	–	1
B	–	4
E	–	2
H	2	8
Total	2	15

Table: Median accuracy comparison

- SoD sets parameter as follows
  - Population size = 250
  - crossover probability = 0.975, tournament size = 8
  - $\gamma = 0.5, \epsilon = 0.998$
  - For every 5 generations a local optimizer is adopted.

	MAB-basd CMA-ES	rECGA+ SoD
U	5	0
B	5	1
E	0	2
H	4	4
Total	14	15

Table: Best accuracy comparison

	MAB-basd CMA-ES	rECGA+ SoD
U	5	0
B	5	1
E	0	2
H	8	4
Total	14	7

Table: Median accuracy comparison

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