CMA-ES and Advanced Adaptation Mechanisms

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We are happy to answer questions at any time.

Topics

1. What makes an optimization problem difficult to solve?

2. How does the CMA-ES work?

- Normal Distribution, Rank-Based Recombination
- Step-Size Adaptation
- Covariance Matrix Adaptation

3. What can/should the users do for the CMA-ES to work effectively on their problem?

- Choice of problem formulation and encoding (not covered)
- Choice of initial solution and initial step-size
- Restarts, Increasing Population Size
- Restricted Covariance Matrix

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Problem Statement

Continuous Domain Search/Optimization

- Task: minimize an objective function (*fitness* function, *loss* function) in continuous domain

$$f : \mathcal{X} \subseteq \mathbb{R}^n \to \mathbb{R}, \qquad \boldsymbol{x} \mapsto f(\boldsymbol{x})$$

- Black Box scenario (direct search scenario)

  - gradients are not available or not useful
  - problem domain specific knowledge is used only within the black box, e.g. within an appropriate encoding
- Search costs: number of function evaluations

Problem Statement

Continuous Domain Search/Optimization

- Goal
  - fast convergence to the global optimum
  - solution $\boldsymbol{x}$ with small function value $f(\boldsymbol{x})$ with least search cost

    ... or to a robust solution $\boldsymbol{x}$

    there are two conflicting objectives
- Typical Examples
  - shape optimization (e.g. using CFD) — curve fitting, airfoils
  - model calibration — biological, physical
  - parameter calibration — controller, plants, images
- Difficulties
  - exhaustive search is infeasible
  - naive random search takes too long
  - deterministic search is not successful / takes too long

Approach: stochastic search, Evolutionary Algorithms

What Makes a Function Difficult to Solve?

Why stochastic search?

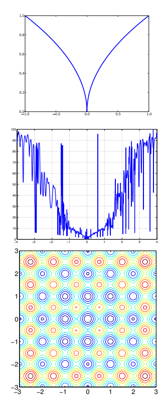
- non-linear, non-quadratic, non-convex

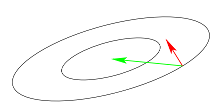
  on linear and quadratic functions much better search policies are available
- ruggedness

  non-smooth, discontinuous, multimodal, and/or noisy function
- dimensionality (size of search space)

  (considerably) larger than three
- non-separability

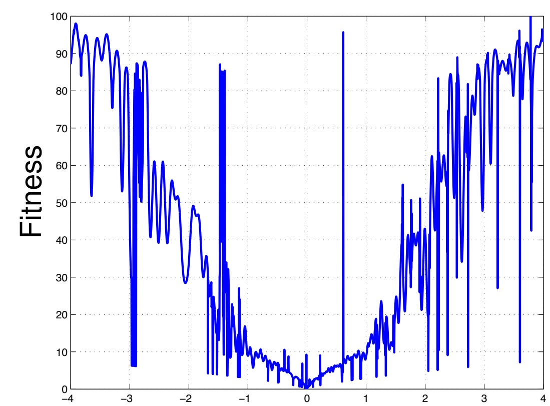
  dependencies between the objective variables
- ill-conditioning
- non-smooth level sets





Ruggedness

non-smooth, discontinuous, multimodal, and/or noisy



cut from a 5-D example, (easily) solvable with evolution strategies

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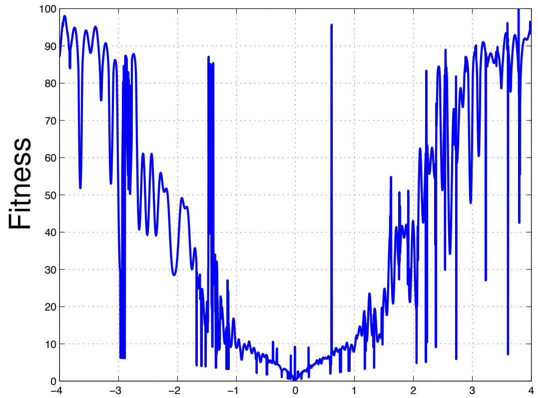


cut from a 5-D example, (easily) solvable with evolution strategies

Curse of Dimensionality

The term *Curse of dimensionality* (Richard Bellman) refers to problems caused by the rapid increase in volume associated with adding extra dimensions to a (mathematical) space.

Example: Consider placing 20 points equally spaced onto the interval $[0,1]$. Now consider the 10-dimensional space $[0,1]^{10}$. To get similar coverage in terms of distance between adjacent points requires $20^{10} \approx 10^{13}$ points. 20 points appear now as isolated points in a vast empty space.

Remark: distance measures break down in higher dimensionalities (the central limit theorem kicks in)

Consequence: a search policy that is valuable in small dimensions might be useless in moderate or large dimensional search spaces. Example: exhaustive search.

Separable Problems

Definition (Separable Problem)

A function f is separable if

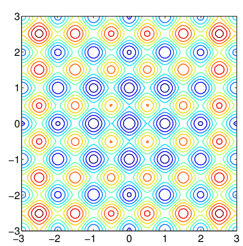
$$\arg\min_{(x_1,\ldots,x_n)} f(x_1,\ldots,x_n) = \left(\arg\min_{x_1} f(x_1,\ldots),\ldots,\arg\min_{x_n} f(\ldots,x_n)\right)$$

$\Rightarrow$ it follows that f can be optimized in a sequence of n independent 1-D optimization processes

Example: Additively decomposable functions

$$f(x_1,\ldots,x_n) = \sum_{i=1}^{n} f_i(x_i)$$

Rastrigin function



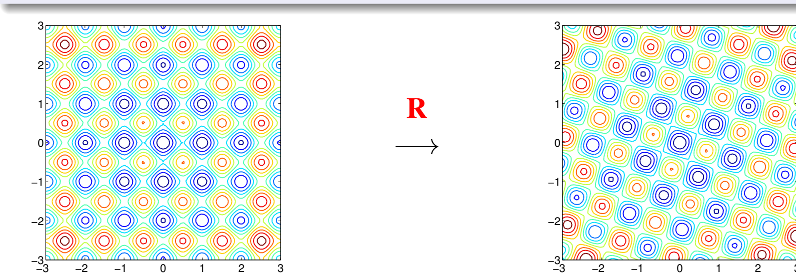
Non-Separable Problems

Building a non-separable problem from a separable one [1,2]

Rotating the coordinate system

- $f : \boldsymbol{x} \mapsto f(\boldsymbol{x})$ separable
- $f : \boldsymbol{x} \mapsto f(\mathbf{R}\boldsymbol{x})$ non-separable

$\mathbf{R}$ rotation matrix



[1] Hansen, Ostermeier, Gawelczyk (1995). On the adaptation of arbitrary normal mutation distributions in evolution strategies: The generating set adaptation. Sixth ICGA, pp. 57-64, Morgan Kaufmann

[2] Salomon (1996). "Reevaluating Genetic Algorithm Performance under Coordinate Rotation of Benchmark Functions; A survey of some theoretical and practical aspects of genetic algorithms." BioSystems, 39(3):263-278

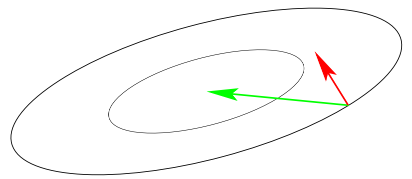
Ill-Conditioned Problems

Curvature of level sets

Consider the convex-quadratic function

$f(\boldsymbol{x}) = \frac{1}{2}(\boldsymbol{x}-\boldsymbol{x}^*)^T\boldsymbol{H}(\boldsymbol{x}-\boldsymbol{x}^*) = \frac{1}{2}\sum_i h_{i,i}\,(x_i-x_i^*)^2 + \frac{1}{2}\sum_{i\neq j} h_{i,j}\,(x_i-x_i^*)(x_j-x_j^*)$

$\boldsymbol{H}$ is Hessian matrix of f and symmetric positive definite



gradient direction $-f'(\boldsymbol{x})^{\mathrm{T}}$

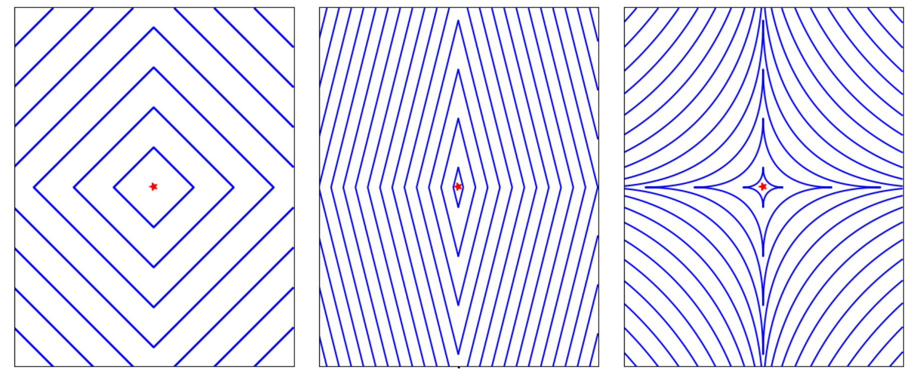
Newton direction $-\boldsymbol{H}^{-1}f'(\boldsymbol{x})^{\mathrm{T}}$

Ill-conditioning means squeezed level sets (high curvature). Condition number equals nine here. Condition numbers up to 10^{10} are not unusual in real world problems.

If $\boldsymbol{H} \approx \mathbf{I}$ (small condition number of $\boldsymbol{H}$) first order information (e.g. the gradient) is sufficient. Otherwise second order information (estimation of $\boldsymbol{H}^{-1}$) is necessary.

Non-smooth level sets (sharp ridges)

Similar difficulty **but worse** than ill-conditioning



1-norm | scaled 1-norm | 1/2-norm

opening angle is the crucial parameter

What Makes a Function Difficult to Solve?

. . . and what can be done

The Problem	Possible Approaches
Dimensionality	exploiting the problem structure separability, locality/neighborhood, encoding
Ill-conditioning	second order approach changes the neighborhood metric
Ruggedness and non-smooth level sets	non-local policy, large sampling width (step-size) as large as possible while preserving a reasonable convergence speed
	population-based method, stochastic, non-elitistic
	recombination operator serves as repair mechanism
	restarts

. . . metaphors

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Stochastic Search

A black box search template to minimize $f : \mathbb{R}^n \to \mathbb{R}$

Initialize distribution parameters $\boldsymbol{\theta}$, set population size $\lambda \in \mathbb{N}$
While not terminate

1. Sample distribution $P(\boldsymbol{x}|\boldsymbol{\theta}) \to \boldsymbol{x}_1, \dots, \boldsymbol{x}_\lambda \in \mathbb{R}^n$
2. Evaluate $\boldsymbol{x}_1, \dots, \boldsymbol{x}_\lambda$ on f
3. Update parameters $\boldsymbol{\theta} \leftarrow F_\theta(\boldsymbol{\theta}, \boldsymbol{x}_1, \dots, \boldsymbol{x}_\lambda, f(\boldsymbol{x}_1), \dots, f(\boldsymbol{x}_\lambda))$

Everything depends on the definition of P and F_θ

deterministic algorithms are covered as well

In many Evolutionary Algorithms the distribution P is implicitly defined via operators on a population, in particular, selection, recombination and mutation

Natural template for (incremental) *Estimation of Distribution Algorithms*

Evolution Strategies (ES) | A Search Template

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The CMA-ES

Input: $\boldsymbol{m} \in \mathbb{R}^n$; $\sigma \in \mathbb{R}_+$; $\lambda \in \mathbb{N}_{\geq 2}$, usually $\lambda \geq 5$, default $4 + \lfloor 3 \log n \rfloor$

Set $c_m = 1$; $c_1 \approx 2/n^2$; $c_\mu \approx \mu_w/n^2$; $c_c \approx 4/n$; $c_\sigma \approx 1/\sqrt{n}$; $d_\sigma \approx 1$; $w_{i=1\ldots\lambda}$ decreasing in i and $\sum_i^\mu w_i = 1$, $w_\mu > 0 \geq w_{\mu+1}$, $\mu_w^{-1} := \sum_{i=1}^\mu w_i^2 \approx 3/\lambda$

Initialize $\mathbf{C} = \mathbf{I}$, and $\boldsymbol{p}_c = \mathbf{0}$, $\boldsymbol{p}_\sigma = \mathbf{0}$

While not *terminate*

$\boldsymbol{x}_i = \boldsymbol{m} + \sigma \boldsymbol{y}_i$, where $\boldsymbol{y}_i \sim \mathcal{N}_i(\mathbf{0}, \mathbf{C})$ for $i = 1, \ldots, \lambda$ — sampling

$\boldsymbol{m} \leftarrow \boldsymbol{m} + c_m \sigma \boldsymbol{y}_w$, where $\boldsymbol{y}_w = \sum_{i=1}^\mu w_{\mathrm{rk}(i)} \boldsymbol{y}_i$ — update mean

$\boldsymbol{p}_\sigma \leftarrow (1 - c_\sigma)\, \boldsymbol{p}_\sigma + \sqrt{1 - (1 - c_\sigma)^2} \sqrt{\mu_w}\, \mathbf{C}^{-\frac{1}{2}} \boldsymbol{y}_w$ — path for σ

$\boldsymbol{p}_c \leftarrow (1 - c_c)\, \boldsymbol{p}_c + \mathbb{1}_{[0,2n]}\{\|\boldsymbol{p}_\sigma\|^2\} \sqrt{1 - (1 - c_c)^2} \sqrt{\mu_w}\, \boldsymbol{y}_w$ — path for $\mathbf{C}$

$\sigma \leftarrow \sigma \times \exp\left(\frac{c_\sigma}{d_\sigma}\left(\frac{\|\boldsymbol{p}_\sigma\|}{\mathsf{E}\|\mathcal{N}(\mathbf{0},\mathbf{I})\|} - 1\right)\right)$ — update of σ

$\mathbf{C} \leftarrow \mathbf{C} + c_\mu \sum_{i=1}^\lambda w_{\mathrm{rk}(i)} (\boldsymbol{y}_i \boldsymbol{y}_i^\mathsf{T} - \mathbf{C}) + c_1 (\boldsymbol{p}_c \boldsymbol{p}_c^\mathsf{T} - \mathbf{C})$ — update $\mathbf{C}$

Not covered: termination, restarts, useful output, search boundaries and encoding, corrections for: positive definiteness guaranty, $\boldsymbol{p}_c$ variance loss, c_σ and d_σ for large λ

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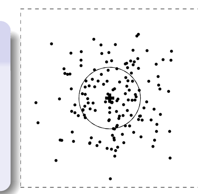
Evolution Strategies

New search points are sampled normally distributed

$$\boldsymbol{x}_i \sim \boldsymbol{m} + \sigma\, \mathcal{N}_i(\mathbf{0}, \mathbf{C}) \qquad \text{for } i = 1, \ldots, \lambda$$

as perturbations of $\boldsymbol{m}$, where $\boldsymbol{x}_i, \boldsymbol{m} \in \mathbb{R}^n$, $\sigma \in \mathbb{R}_+$, $\mathbf{C} \in \mathbb{R}^{n \times n}$



where

- the mean vector $\boldsymbol{m} \in \mathbb{R}^n$ represents the favorite solution
- the so-called step-size $\sigma \in \mathbb{R}_+$ controls the *step length*
- the covariance matrix $\mathbf{C} \in \mathbb{R}^{n \times n}$ determines the shape of the distribution ellipsoid

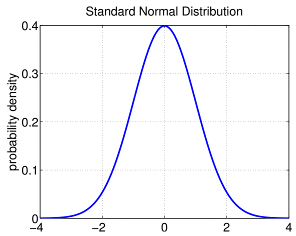
here, all new points are sampled with the same parameters

The question remains how to update $\boldsymbol{m}$, $\mathbf{C}$, and σ.

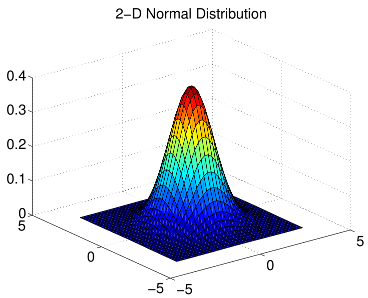
Why Normal Distributions?

1. widely observed in nature, for example as phenotypic traits
2. only stable distribution with finite variance
   stable means that the sum of normal variates is again normal:
   $$\mathcal{N}(\boldsymbol{x}, \mathbf{A}) + \mathcal{N}(\boldsymbol{y}, \mathbf{B}) \sim \mathcal{N}(\boldsymbol{x} + \boldsymbol{y}, \mathbf{A} + \mathbf{B})$$
   helpful in design and analysis of algorithms
   related to the *central limit theorem*
3. most convenient way to generate isotropic search points
   the isotropic distribution does not favor any direction, rotational invariant
4. maximum entropy distribution with finite variance
   the least possible assumptions on f in the distribution shape

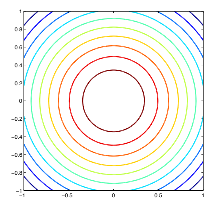
Normal Distribution



probability density of the 1-D standard normal distribution



probability density of a 2-D normal distribution

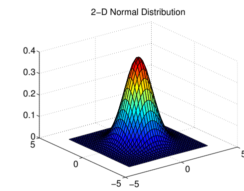


The Multi-Variate (n-Dimensional) Normal Distribution

Any multi-variate normal distribution $\mathcal{N}(\boldsymbol{m}, \mathbf{C})$ is uniquely determined by its mean value $\boldsymbol{m} \in \mathbb{R}^n$ and its symmetric positive definite $n \times n$ covariance matrix $\mathbf{C}$.

The mean value $\boldsymbol{m}$

- determines the displacement (translation)
- value with the largest density (modal value)
- the distribution is symmetric about the distribution mean

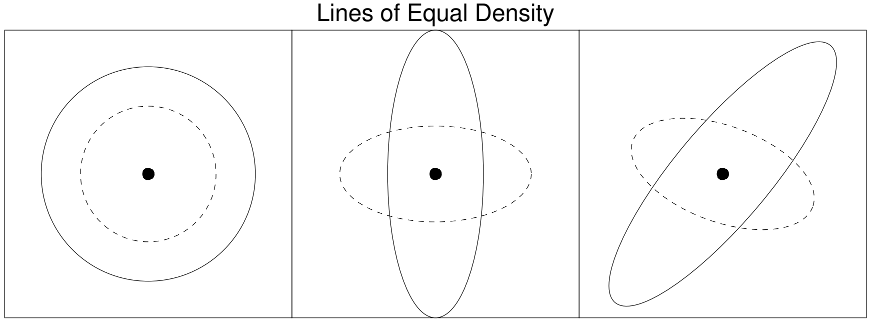


The covariance matrix $\mathbf{C}$

- determines the shape
- geometrical interpretation: any covariance matrix can be uniquely identified with the iso-density ellipsoid $\{\boldsymbol{x} \in \mathbb{R}^n \mid (\boldsymbol{x}-\boldsymbol{m})^{\mathrm{T}}\mathbf{C}^{-1}(\boldsymbol{x}-\boldsymbol{m}) = n\}$

. . . any covariance matrix can be uniquely identified with the iso-density ellipsoid $\{\boldsymbol{x} \in \mathbb{R}^n \mid (\boldsymbol{x}-\boldsymbol{m})^{\mathrm{T}}\mathbf{C}^{-1}(\boldsymbol{x}-\boldsymbol{m}) = n\}$

Lines of Equal Density



$\mathcal{N}(\boldsymbol{m}, \sigma^2\mathbf{I}) \sim \boldsymbol{m} + \sigma\mathcal{N}(\mathbf{0}, \mathbf{I})$	$\mathcal{N}(\boldsymbol{m}, \mathbf{D}^2) \sim \boldsymbol{m} + \mathbf{D}\mathcal{N}(\mathbf{0}, \mathbf{I})$	$\mathcal{N}(\boldsymbol{m}, \mathbf{C}) \sim \boldsymbol{m} + \mathbf{C}^{\frac{1}{2}}\mathcal{N}(\mathbf{0}, \mathbf{I})$
one degree of freedom σ	n degrees of freedom	$(n^2+n)/2$ degrees of freedom
components are independent standard normally distributed	components are independent, scaled	components are correlated

where $\mathbf{I}$ is the identity matrix (isotropic case) and $\mathbf{D}$ is a diagonal matrix (reasonable for separable problems) and $\mathbf{A} \times \mathcal{N}(\mathbf{0}, \mathbf{I}) \sim \mathcal{N}(\mathbf{0}, \mathbf{A}\mathbf{A}^{\mathrm{T}})$ holds for all $\mathbf{A}$.

Multivariate Normal Distribution and Eigenvalues

For any positive definite symmetric $\mathbf{C}$,

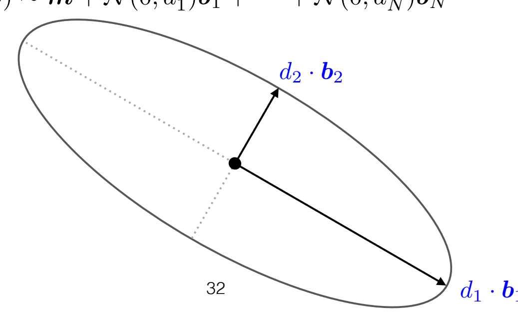
$$\mathbf{C} = d_1^2 \boldsymbol{b}_1 \boldsymbol{b}_1^{\mathrm{T}} + \cdots + d_N^2 \boldsymbol{b}_N \boldsymbol{b}_N^{\mathrm{T}}$$

d_i: square root of the eigenvalue of $\mathbf{C}$

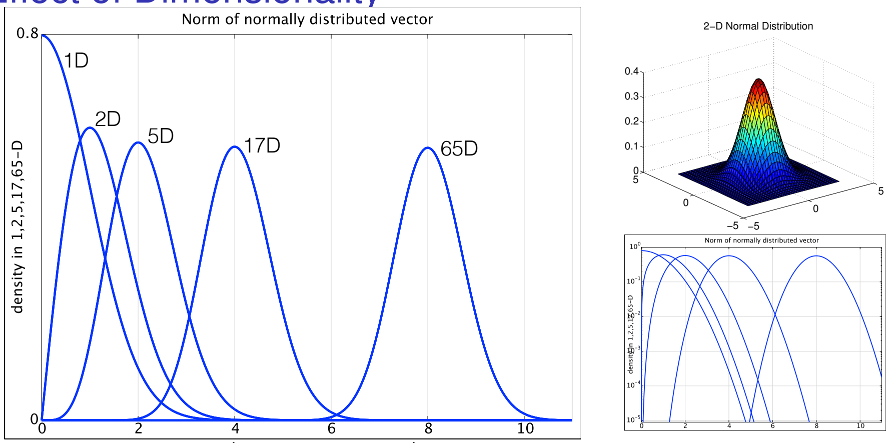
$\boldsymbol{b}_i$: eigenvector of $\mathbf{C}$, corresponding to d_i

The multivariate normal distribution $\mathcal{N}(\boldsymbol{m}, \mathbf{C})$

$$\mathcal{N}(\boldsymbol{m}, \mathbf{C}) \sim \boldsymbol{m} + \mathcal{N}(0, d_1^2)\boldsymbol{b}_1 + \cdots + \mathcal{N}(0, d_N^2)\boldsymbol{b}_N$$



Effect of Dimensionality



$\|\mathcal{N}(\mathbf{0},\mathbf{I})\| \longrightarrow \mathcal{N}\left(\sqrt{n-1/2}, 1/2\right)$ with modal value $\sqrt{n-1}$

yet: maximum entropy distribution

also consider a difference between two vectors:

$\|\mathcal{N}(\mathbf{0},\mathbf{I}) - \mathcal{N}(\mathbf{0},\mathbf{I})\| \sim \|\mathcal{N}(\mathbf{0},\mathbf{I}) + \mathcal{N}(\mathbf{0},\mathbf{I})\| \sim \sqrt{2}\|\mathcal{N}(\mathbf{0},\mathbf{I})\|$

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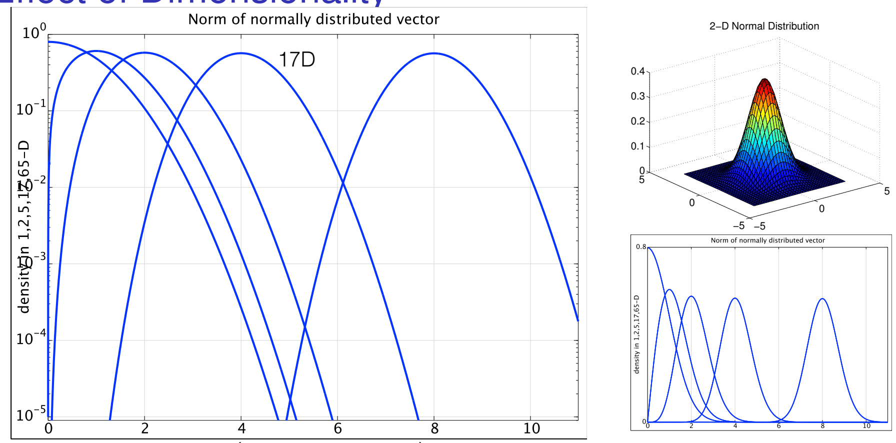

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yet: maximum entropy distribution

also consider a difference between two vectors:

$\|\mathcal{N}(\mathbf{0},\mathbf{I}) - \mathcal{N}(\mathbf{0},\mathbf{I})\| \sim \|\mathcal{N}(\mathbf{0},\mathbf{I}) + \mathcal{N}(\mathbf{0},\mathbf{I})\| \sim \sqrt{2}\|\mathcal{N}(\mathbf{0},\mathbf{I})\|$

The $(\mu/\mu, \lambda)$-ES, Update of the Distribution Mean

Non-elitist selection and intermediate (weighted) recombination

Given the i-th solution point $\boldsymbol{x}_i = \boldsymbol{m} + \sigma \underbrace{\mathcal{N}_i(\mathbf{0}, \mathbf{C})}_{=:\boldsymbol{y}_i} = \boldsymbol{m} + \sigma\, \boldsymbol{y}_i$

Let $\boldsymbol{x}_{i:\lambda}$ the i-th ranked solution point, such that $f(\boldsymbol{x}_{1:\lambda}) \leq \dots \leq f(\boldsymbol{x}_{\lambda:\lambda})$.

The new mean reads

$$\boldsymbol{m} \leftarrow \sum_{i=1}^{\mu} w_i\, \boldsymbol{x}_{i:\lambda} = \boldsymbol{m} + \sigma \underbrace{\sum_{i=1}^{\mu} w_i\, \boldsymbol{y}_{i:\lambda}}_{=:\boldsymbol{y}_w}$$

where

$$w_1 \geq \dots \geq w_\mu > 0, \quad \sum_{i=1}^{\mu} w_i = 1, \quad \frac{1}{\sum_{i=1}^{\mu} {w_i}^2} =: \mu_w \approx \frac{\lambda}{4}$$

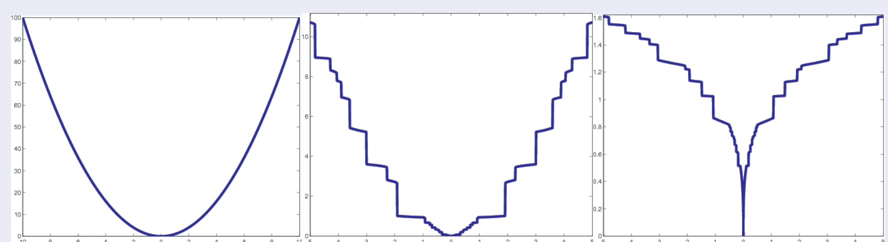
The best μ points are selected from the new solutions (non-elitistic) and weighted intermediate recombination is applied.

Invariance Under Monotonically Increasing Functions

Rank-based algorithms

Update of all parameters uses only the ranks

$$f(x_{1:\lambda}) \leq f(x_{2:\lambda}) \leq \dots \leq f(x_{\lambda:\lambda})$$



$$g(f(x_{1:\lambda})) \leq g(f(x_{2:\lambda})) \leq \dots \leq g(f(x_{\lambda:\lambda})) \quad \forall g$$

g is strictly monotonically increasing
g preserves ranks

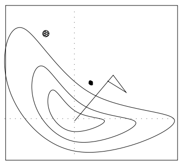
[3]

[3] Whitley 1989. The GENITOR algorithm and selection pressure: Why rank-based allocation of reproductive trials is best, ICGA

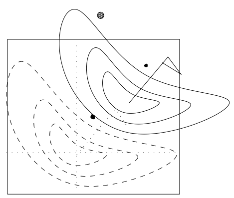
Basic Invariance in Search Space

- translation invariance

is true for most optimization algorithms



$f(\boldsymbol{x}) \leftrightarrow f(\boldsymbol{x}-\boldsymbol{a})$

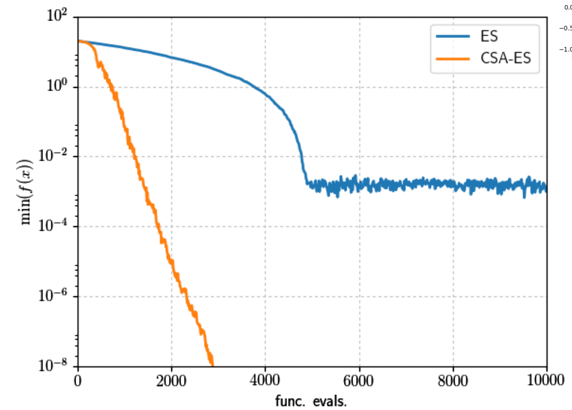


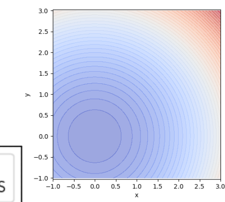
Identical behavior on f and $f_{\boldsymbol{a}}$

$$f: \quad \boldsymbol{x} \mapsto f(\boldsymbol{x}), \qquad \boldsymbol{x}^{(t=0)} = \boldsymbol{x}_0$$
$$f_{\boldsymbol{a}}: \quad \boldsymbol{x} \mapsto f(\boldsymbol{x}-\boldsymbol{a}), \quad \boldsymbol{x}^{(t=0)} = \boldsymbol{x}_0 + \boldsymbol{a}$$

No difference can be observed w.r.t. the argument of f

Summary





On 20D Sphere Function: $f(\mathbf{x}) = \sum_{i=1}^{N} [\mathbf{x}]_i^2$

- ES without adaptation can't approach the optimum ⇒ adaptation required

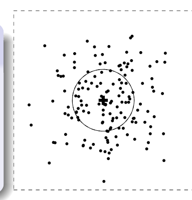
Evolution Strategies

Recalling

New search points are sampled normally distributed

$$\boldsymbol{x}_i \sim \boldsymbol{m} + \sigma \mathcal{N}_i(\mathbf{0}, \mathbf{C}) \qquad \text{for } i = 1, \ldots, \lambda$$

as perturbations of $\boldsymbol{m}$, where $\boldsymbol{x}_i, \boldsymbol{m} \in \mathbb{R}^n$, $\sigma \in \mathbb{R}_+$, $\mathbf{C} \in \mathbb{R}^{n\times n}$



where

- the mean vector $\boldsymbol{m} \in \mathbb{R}^n$ represents the favorite solution and $\boldsymbol{m} \leftarrow \sum_{i=1}^{\mu} w_i \boldsymbol{x}_{i:\lambda}$
- the so-called step-size $\sigma \in \mathbb{R}_+$ controls the *step length*
- the covariance matrix $\mathbf{C} \in \mathbb{R}^{n\times n}$ determines the shape of the distribution ellipsoid

The remaining question is how to update σ and $\mathbf{C}$.

Methods for Step-Size Control

- $1/5$-th success rule[ab], often applied with "+"-selection

  increase step-size if more than 20% of the new solutions are successful, decrease otherwise

- σ-self-adaptation[c], applied with ","-selection

  mutation is applied to the step-size and the better, according to the objective function value, is selected

  simplified "global" self-adaptation

- path length control[d] (Cumulative Step-size Adaptation, CSA)[e]

  self-adaptation derandomized and non-localized

[a] Rechenberg 1973, *Evolutionsstrategie, Optimierung technischer Systeme nach Prinzipien der biologischen Evolution*, Frommann-Holzboog

[b] Schumer and Steiglitz 1968. Adaptive step size random search. *IEEE TAC*

[c] Schwefel 1981, *Numerical Optimization of Computer Models*, Wiley

[d] Hansen & Ostermeier 2001, Completely Derandomized Self-Adaptation in Evolution Strategies, *Evol. Comput. 9(2)*

[e] Ostermeier *et al* 1994, Step-size adaptation based on non-local use of selection information, *PPSN IV*

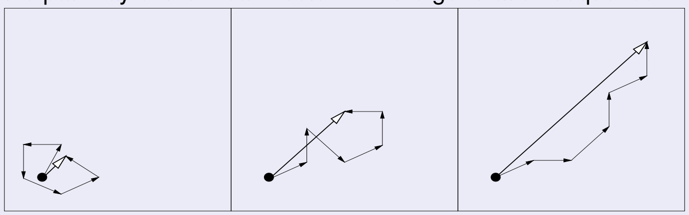
Path Length Control (CSA)

The Concept of Cumulative Step-Size Adaptation

$$x_i = m + \sigma y_i$$
$$m \leftarrow m + \sigma y_w$$

Measure the length of the *evolution path*

the pathway of the mean vector m in the generation sequence



⇓ decrease σ ⇓ increase σ

loosely speaking steps are

- perpendicular under random selection (in expectation)
- perpendicular in the desired situation (to be most efficient)

Path Length Control (CSA)

The Equations

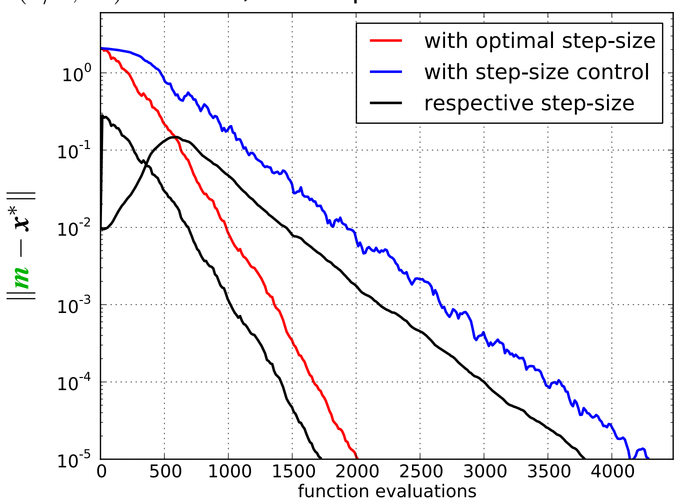
Initialize $m \in \mathbb{R}^n$, $\sigma \in \mathbb{R}_+$, evolution path $p_\sigma = \mathbf{0}$,
set $c_\sigma \approx 4/n$, $d_\sigma \approx 1$.

$$m \leftarrow m + \sigma y_w \quad \text{where } y_w = \sum_{i=1}^{\mu} w_i y_{i:\lambda} \qquad \text{update mean}$$

$$p_\sigma \leftarrow (1 - c_\sigma) p_\sigma + \underbrace{\sqrt{1 - (1 - c_\sigma)^2}}_{\text{accounts for } 1-c_\sigma} \underbrace{\sqrt{\mu_w}}_{\text{accounts for } w_i} y_w$$

$$\sigma \leftarrow \sigma \times \underbrace{\exp\left(\frac{c_\sigma}{d_\sigma}\left(\frac{\|p_\sigma\|}{\mathsf{E}\|\mathcal{N}(\mathbf{0},\mathbf{I})\|} - 1\right)\right)}_{>1 \iff \|p_\sigma\| \text{ is greater than its expectation}} \qquad \text{update step-size}$$

$(5/5, 10)$-CSA-ES, default parameters



$$f(x) = \sum_{i=1}^{n} x_i^2$$

in $[-0.2, 0.8]^n$
for $n = 30$

Two-Point Step-Size Adaptation (TPA)

- Sample a pair of symmetric points along the previous mean shift

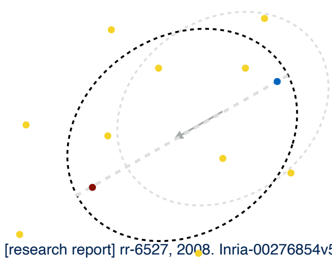
$$x_{1/2} = m^{(g)} \pm \sigma^{(g)} \frac{\|\mathcal{N}(\mathbf{0},\mathbf{I})\|}{\|m^{(g)} - m^{(g-1)}\|_{\mathbf{C}^{(g)}}} (m^{(g)} - m^{(g-1)}) \qquad \|x\|_{\mathbf{C}} := x^{\mathrm{T}}\mathbf{C}^{-1}x$$

- Compare the ranking of x_1 and x_2 among λ current populations

$$s^{(g+1)} = (1 - c_s)s^{(g)} + c_s \underbrace{\frac{\text{rank}(x_2) - \text{rank}(x_1)}{\lambda - 1}}_{>0 \text{ if the previous step still produces a promising solution}}$$

- Update the step-size

$$\sigma^{(g+1)} = \sigma^{(g)} \exp\left(\frac{s^{(g+1)}}{d_\sigma}\right)$$



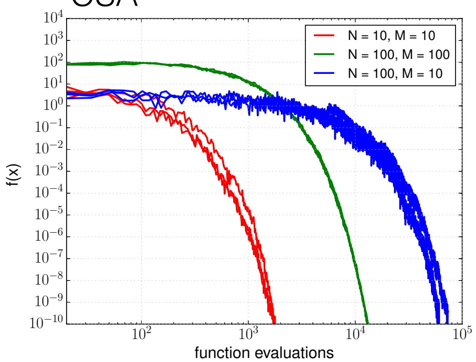
[Hansen, 2008] Hansen, N. (2008). CMA-ES with two-point step-size adaptation. [research report] rr-6527, 2008. Inria-00276854v5.
[Hansen et al., 2014] Hansen, N., Atamna, A., and Auger, A. (2014). How to assess step-size adaptation mechanisms in randomised search. In Parallel Problem Solving from Nature–PPSN XIII, pages 60–69. Springer.

On Sphere with Low Effective Dimension

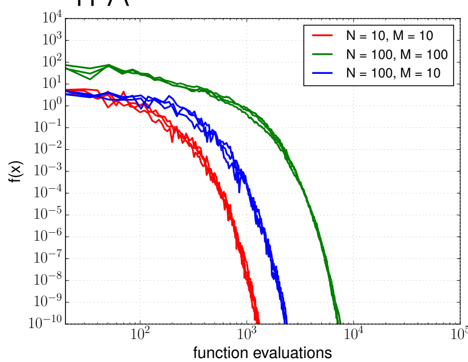
On a function with low effective dimension

- $f(\boldsymbol{x}) = \sum_{i=1}^{M} [\boldsymbol{x}]_i^2, \quad \boldsymbol{x} \in \mathbb{R}^N, \quad M \leq N.$
- $N - M$ variables do not affect the function value

CSA



TPA



Alternatives: Success-Based Step-Size Control

comparing the fitness distributions of current and previous iterations

Generalizations of $1/5$th-success-rule for non-elitist and multi-recombinant ES

- Median Success Rule [Ait Elhara et al., 2013]
- Population Success Rule [Loshchilov, 2014]

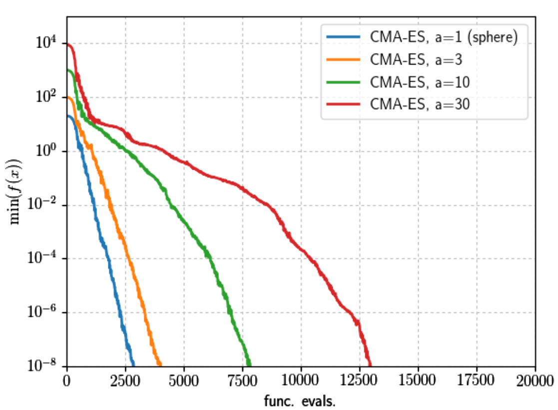
controls a *success probability*

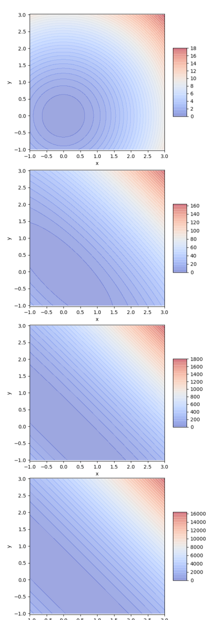
An advantage over CSA and TPA: Cheap Computation

- It depends only on λ.
- cf. CSA and TPA require a computation of $C^{-1/2}\boldsymbol{x}$ and $C^{-1}\boldsymbol{x}$, respectively.

[Ait Elhara et al., 2013] Ait Elhara, O., Auger, A., and Hansen, N. (2013). A median success rule for non- elitist evolution strategies: Study of feasibility. In Proc. of the GECCO, pages 415–422.
[Loshchilov, 2014] Loshchilov, I. (2014). A computationally efficient limited memory cma-es for large scale optimization. In Proc. of the GECCO, pages 397–404.

Step-Size Control Is Not Enough





On 20D TwoAxes Function: $f(\mathbf{x}) = \sum_{i=1}^{N/2} [\mathbf{Rx}]_i^2 + a^2 \sum_{i=N/2+1}^{N} [\mathbf{Rx}]_i^2$, $\mathbf{R}$: orthogonal

- convergence speed of CSA-ES becomes lower as the function becomes ill conditioned (a^2 becomes greater) ⇒ covariance matrix adaptation required

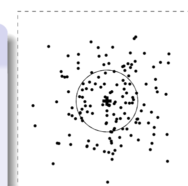
Evolution Strategies

Recalling

New search points are sampled normally distributed

$$\boldsymbol{x}_i \sim \boldsymbol{m} + \sigma \mathcal{N}_i(\mathbf{0}, \mathbf{C}) \qquad \text{for } i = 1, \dots, \lambda$$

as perturbations of $\boldsymbol{m}$, where $\boldsymbol{x}_i, \boldsymbol{m} \in \mathbb{R}^n$, $\sigma \in \mathbb{R}_+$, $\mathbf{C} \in \mathbb{R}^{n \times n}$



where

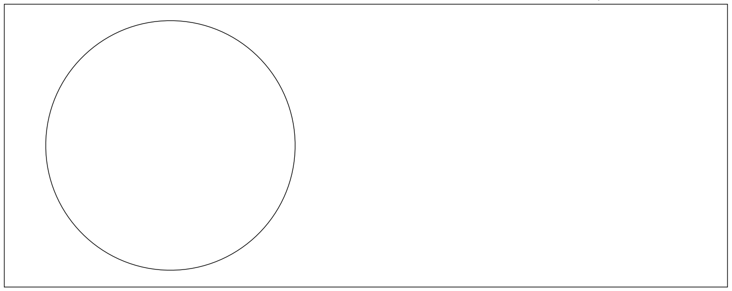
- the mean vector $\boldsymbol{m} \in \mathbb{R}^n$ represents the favorite solution
- the so-called step-size $\sigma \in \mathbb{R}_+$ controls the *step length*
- the covariance matrix $\mathbf{C} \in \mathbb{R}^{n \times n}$ determines the shape of the distribution ellipsoid

The remaining question is how to update $\mathbf{C}$.

Covariance Matrix Adaptation

Rank-One Update

$$\boldsymbol{m} \leftarrow \boldsymbol{m} + \sigma \boldsymbol{y}_w, \quad \boldsymbol{y}_w = \sum_{i=1}^{\mu} w_i \boldsymbol{y}_{i:\lambda}, \quad \boldsymbol{y}_i \sim \mathcal{N}_i(\boldsymbol{0}, \mathbf{C})$$



initial distribution, $\mathbf{C} = \mathbf{I}$

Covariance Matrix Adaptation

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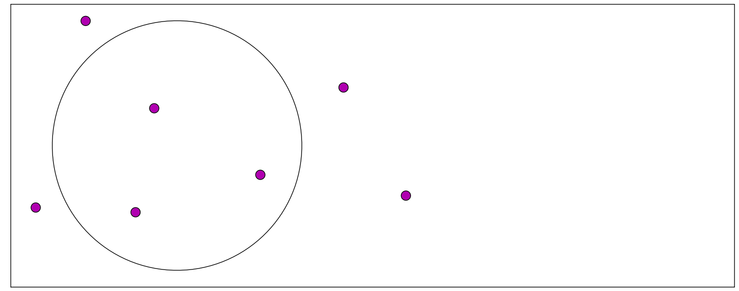

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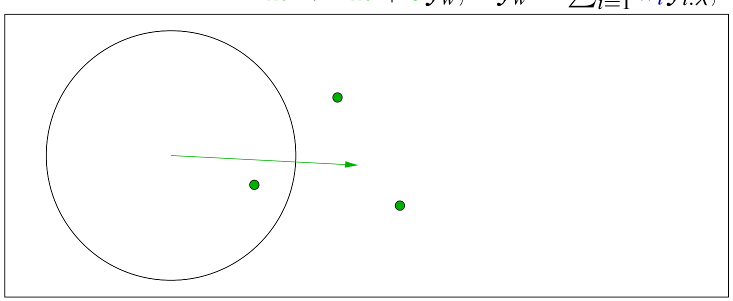
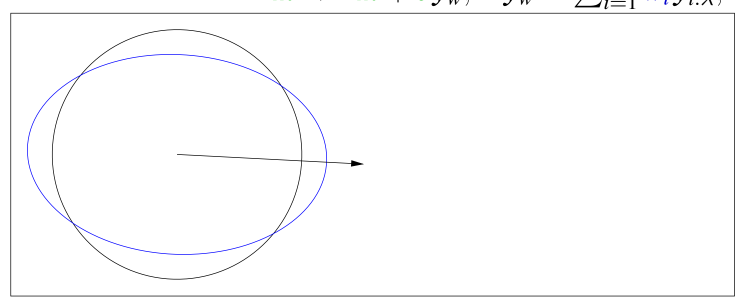


$\boldsymbol{y}_w$, movement of the population mean $\boldsymbol{m}$ (disregarding σ)

Covariance Matrix Adaptation

Rank-One Update

$$\boldsymbol{m} \leftarrow \boldsymbol{m} + \sigma \boldsymbol{y}_w, \quad \boldsymbol{y}_w = \sum_{i=1}^{\mu} w_i \boldsymbol{y}_{i:\lambda}, \quad \boldsymbol{y}_i \sim \mathcal{N}_i(\boldsymbol{0}, \mathbf{C})$$

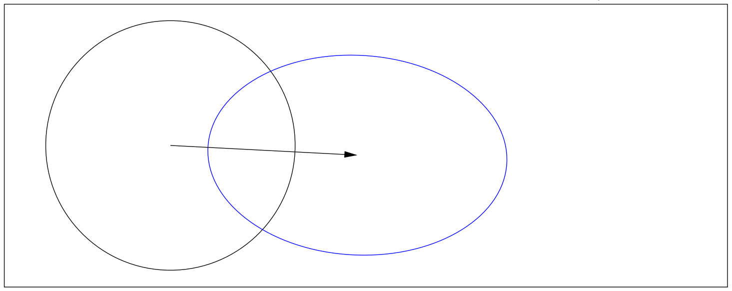


mixture of distribution $\mathbf{C}$ and step $\boldsymbol{y}_w$,
$\mathbf{C} \leftarrow 0.8 \times \mathbf{C} + 0.2 \times \boldsymbol{y}_w \boldsymbol{y}_w^{\mathrm{T}}$

Covariance Matrix Adaptation

Rank-One Update

$$\boldsymbol{m} \leftarrow \boldsymbol{m} + \sigma \boldsymbol{y}_w, \quad \boldsymbol{y}_w = \sum_{i=1}^{\mu} w_i \boldsymbol{y}_{i:\lambda}, \quad \boldsymbol{y}_i \sim \mathcal{N}_i(\mathbf{0}, \mathbf{C})$$



new distribution (disregarding σ)

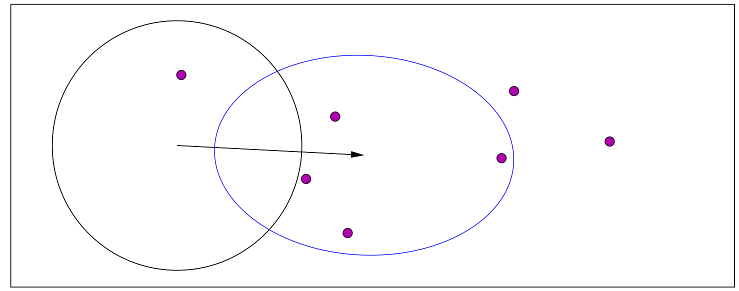
. . . equations

Covariance Matrix Adaptation (CMA) | Covariance Matrix Rank-One Update

Covariance Matrix Adaptation

Rank-One Update

$$\boldsymbol{m} \leftarrow \boldsymbol{m} + \sigma \boldsymbol{y}_w, \quad \boldsymbol{y}_w = \sum_{i=1}^{\mu} w_i \boldsymbol{y}_{i:\lambda}, \quad \boldsymbol{y}_i \sim \mathcal{N}_i(\mathbf{0}, \mathbf{C})$$



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Covariance Matrix Adaptation (CMA) | Covariance Matrix Rank-One Update

Covariance Matrix Adaptation

Rank-One Update

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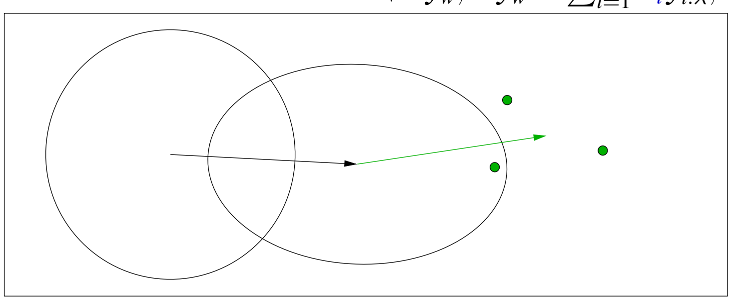

movement of the population mean $\boldsymbol{m}$

. . . equations

Covariance Matrix Adaptation (CMA) | Covariance Matrix Rank-One Update

Covariance Matrix Adaptation

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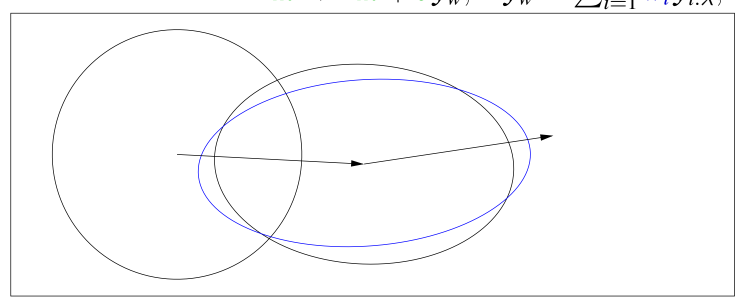


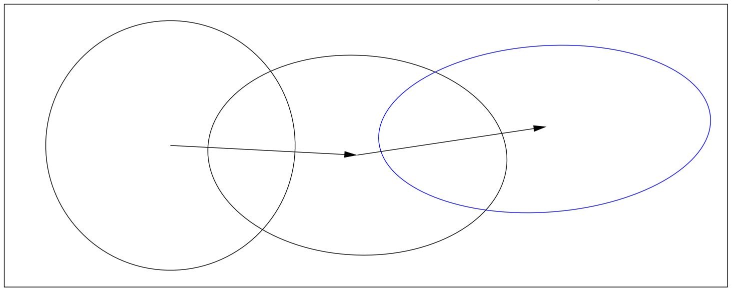
mixture of distribution $\mathbf{C}$ and step $\boldsymbol{y}_w$,
$\mathbf{C} \leftarrow 0.8 \times \mathbf{C} + 0.2 \times \boldsymbol{y}_w \boldsymbol{y}_w^{\mathrm{T}}$

. . . equations

Covariance Matrix Adaptation

Rank-One Update

$$m \leftarrow m + \sigma y_w, \quad y_w = \sum_{i=1}^{\mu} w_i y_{i:\lambda}, \quad y_i \sim \mathcal{N}_i(\mathbf{0}, \mathbf{C})$$



new distribution,
$\mathbf{C} \leftarrow 0.8 \times \mathbf{C} + 0.2 \times y_w y_w^{\mathrm{T}}$
the ruling principle: the adaptation increases the likelihood of successful steps, y_w, to appear again
another viewpoint: the adaptation follows a natural gradient approximation of the expected fitness

. . . equations

Covariance Matrix Adaptation

Rank-One Update

Initialize $m \in \mathbb{R}^n$, and $\mathbf{C} = \mathbf{I}$, set $\sigma = 1$, learning rate $c_{\mathrm{cov}} \approx 2/n^2$
While not terminate

$$x_i = m + \sigma y_i, \quad y_i \sim \mathcal{N}_i(\mathbf{0}, \mathbf{C}),$$

$$m \leftarrow m + \sigma y_w \quad \text{where } y_w = \sum_{i=1}^{\mu} w_i y_{i:\lambda}$$

$$\mathbf{C} \leftarrow (1 - c_{\mathrm{cov}})\mathbf{C} + c_{\mathrm{cov}} \mu_w \underbrace{y_w y_w^{\mathrm{T}}}_{\text{rank-one}} \quad \text{where } \mu_w = \frac{1}{\sum_{i=1}^{\mu} w_i^2} \geq 1$$

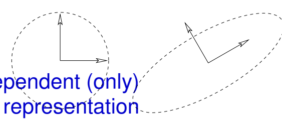
The rank-one update has been found independently in several domains[6] [7] [8] [9]

[6] Kjellström&Taxén 1981. Stochastic Optimization in System Design, IEEE TCS
[7] Hansen&Ostermeier 1996. Adapting arbitrary normal mutation distributions in evolution strategies: The covariance matrix adaptation, ICEC
[8] Ljung 1999. System Identification: Theory for the User
[9] Haario et al 2001. An adaptive Metropolis algorithm, JSTOR

$$\mathbf{C} \leftarrow (1 - c_{\mathrm{cov}})\mathbf{C} + c_{\mathrm{cov}} \mu_w y_w y_w^{\mathrm{T}}$$

covariance matrix adaptation

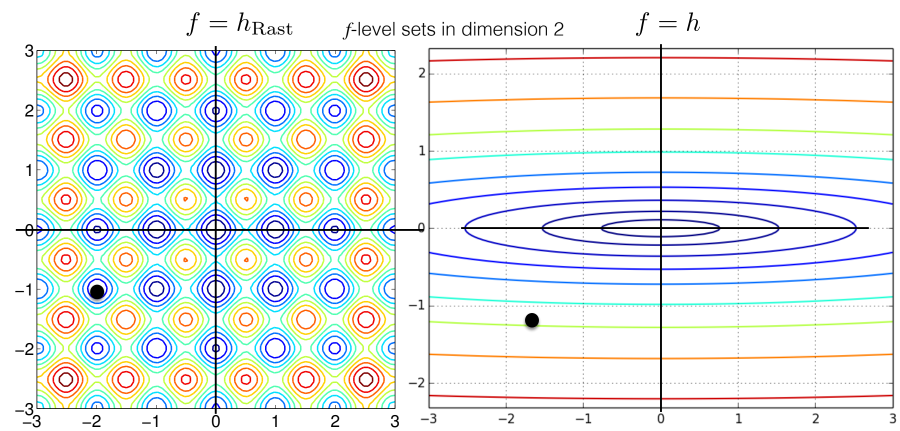
- learns all pairwise dependencies between variables
  off-diagonal entries in the covariance matrix reflect the dependencies
- conducts a principle component analysis (PCA) of steps y_w, sequentially in time and space
  eigenvectors of the covariance matrix $\mathbf{C}$ are the principle components / the principle axes of the mutation ellipsoid
- learns a new rotated problem representation
  components are independent (only) in the new representation



- learns a new (Mahalanobis) metric
  variable metric method
- approximates the inverse Hessian on quadratic functions
  transformation into the sphere function
- for $\mu = 1$: conducts a natural gradient ascent on the distribution $\mathcal{N}$
  entirely independent of the given coordinate system

. . . cumulation, rank-μ

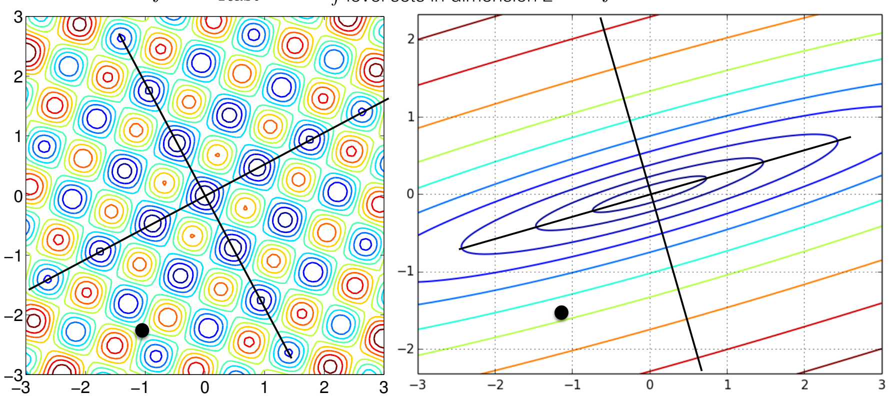
Invariance Under Rigid Search Space Transformation



for example, invariance under search space rotation
(separable ⇔ non-separable)

Invariance Under Rigid Search Space Transformation

$f = h_{\text{Rast}} \circ R$ f-level sets in dimension 2 $f = h \circ R$



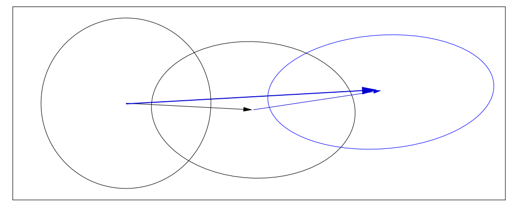
for example, invariance under search space rotation
(separable ⇔ non-separable)

Cumulation

The Evolution Path

Evolution Path

Conceptually, the evolution path is the search path the strategy takes over a number of generation steps. It can be expressed as a sum of consecutive *steps* of the mean $\boldsymbol{m}$.



An exponentially weighted sum of steps $\boldsymbol{y}_w$ is used

$$p_c \propto \sum_{i=0}^{g} \underbrace{(1-c_c)^{g-i}}_{\text{exponentially fading weights}} \boldsymbol{y}_w^{(i)}$$

The recursive construction of the evolution path (cumulation):

$$p_c \leftarrow \underbrace{(1-c_c)}_{\text{decay factor}} p_c + \underbrace{\sqrt{1-(1-c_c)^2}\sqrt{\mu_w}}_{\text{normalization factor}} \underbrace{\boldsymbol{y}_w}_{\text{input} = \frac{m - m_{\text{old}}}{\sigma}}$$

where $\mu_w = \frac{1}{\sum w_i^2}$, $c_c \ll 1$. History information is accumulated in the evolution path.

Cumulation

The Evolution Path

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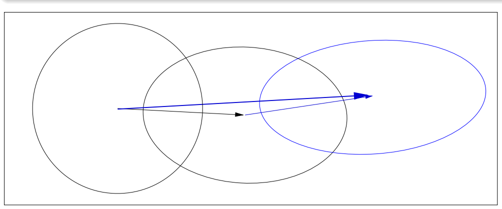

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The recursive construction of the evolution path (cumulation):

$$p_c \leftarrow \underbrace{(1-c_c)}_{\text{decay factor}} p_c + \underbrace{\sqrt{1-(1-c_c)^2}\sqrt{\mu_w}}_{\text{normalization factor}} \underbrace{\boldsymbol{y}_w}_{\text{input} = \frac{m - m_{\text{old}}}{\sigma}}$$

where $\mu_w = \frac{1}{\sum w_i^2}$, $c_c \ll 1$. History information is accumulated in the evolution path.

"Cumulation" is a widely used technique and also know as

- *exponential smoothing* in time series, forecasting
- exponentially weighted *mooving average*
- *iterate averaging* in stochastic approximation
- *momentum* in the back-propagation algorithm for ANNs
- ...

"Cumulation" conducts a *low-pass* filtering, but there is more to it...

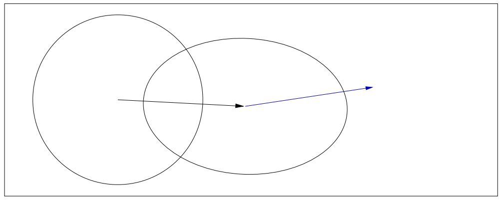
...why?

Cumulation

$\mathbf{C} \leftarrow (1 - c_{\text{cov}})\mathbf{C} + c_{\text{cov}}\mu_w \boldsymbol{y}_w \boldsymbol{y}_w^{\mathrm{T}}$

Utilizing the Evolution Path

We used $\boldsymbol{y}_w\boldsymbol{y}_w^{\mathrm{T}}$ for updating $\mathbf{C}$. Because $\boldsymbol{y}_w\boldsymbol{y}_w^{\mathrm{T}} = -\boldsymbol{y}_w(-\boldsymbol{y}_w)^{\mathrm{T}}$ the sign of $\boldsymbol{y}_w$ is lost.



The sign information (signifying correlation *between* steps) is (re-)introduced by using the *evolution path*.

$$p_c \leftarrow \underbrace{(1-c_c)}_{\text{decay factor}} p_c + \underbrace{\sqrt{1-(1-c_c)^2}\sqrt{\mu_w}}_{\text{normalization factor}} \boldsymbol{y}_w$$

$$\mathbf{C} \leftarrow (1-c_{\text{cov}})\mathbf{C} + c_{\text{cov}} \underbrace{p_c {p_c}^{\mathrm{T}}}_{\text{rank-one}}$$

where $\mu_w = \frac{1}{\sum w_i^2}$, $c_{\text{cov}} \ll c_c \ll 1$ such that $1/c_c$ is the "backward time horizon".

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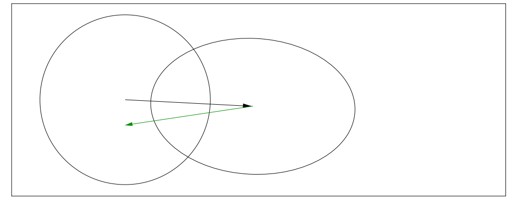

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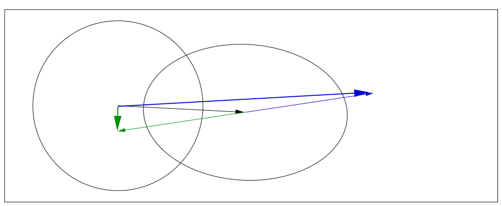

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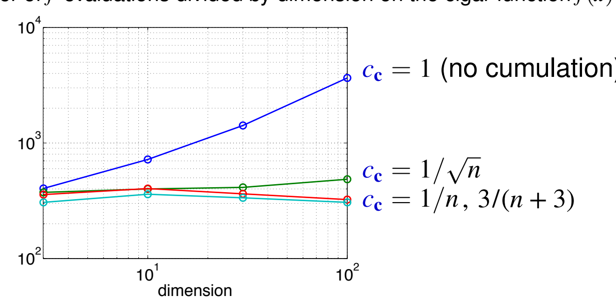
Using an evolution path for the rank-one update of the covariance matrix reduces the number of function evaluations to adapt to a straight ridge from about $\mathcal{O}(n^2)$ to $\mathcal{O}(n)$.[a]

[a] Hansen & Auger 2013. Principled design of continuous stochastic search: From theory to practice.

Number of f-evaluations divided by dimension on the cigar function $f(\boldsymbol{x}) = x_1^2 + 10^6 \sum_{i=2}^{n} x_i^2$



The overall model complexity is n^2 but important parts of the model can be learned in time of order n

Rank-μ Update

$$\begin{aligned} x_i &= m + \sigma y_i, & y_i &\sim \mathcal{N}_i(\mathbf{0}, \mathbf{C}), \\ m &\leftarrow m + \sigma y_w & y_w &= \textstyle\sum_{i=1}^{\mu} w_i y_{i:\lambda} \end{aligned}$$

The rank-μ update extends the update rule for large population sizes λ using $\mu > 1$ vectors to update $\mathbf{C}$ at each generation step.

The weighted empirical covariance matrix

$$\mathbf{C}_\mu = \sum_{i=1}^{\mu} w_i y_{i:\lambda} y_{i:\lambda}^{\mathrm{T}}$$

computes a weighted mean of the outer products of the best μ steps and has rank $\min(\mu, n)$ with probability one.

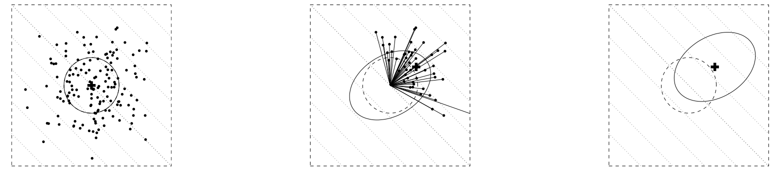
with $\mu = \lambda$ weights can be negative [10]

The rank-μ update then reads

$$\mathbf{C} \leftarrow (1 - c_{\mathrm{cov}})\,\mathbf{C} + c_{\mathrm{cov}}\,\mathbf{C}_\mu$$

where $c_{\mathrm{cov}} \approx \mu_w / n^2$ and $c_{\mathrm{cov}} \le 1$.

[10] Jastrebski and Arnold (2006). Improving evolution strategies through active covariance matrix adaptation. CEC.



$x_i = m + \sigma y_i, \quad y_i \sim \mathcal{N}(\mathbf{0}, \mathbf{C})$

$\mathbf{C}_\mu = \frac{1}{\mu}\sum y_{i:\lambda} y_{i:\lambda}^{\mathrm{T}}$

$\mathbf{C} \leftarrow (1-1)\times\mathbf{C} + 1 \times \mathbf{C}_\mu$

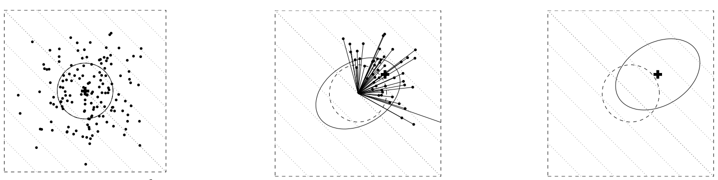
$m_{\text{new}} \leftarrow m + \frac{1}{\mu}\sum y_{i:\lambda}$

sampling of $\lambda = 150$ solutions where $\mathbf{C} = \mathbf{I}$ and $\sigma = 1$

calculating $\mathbf{C}$ where $\mu = 50$, $w_1 = \cdots = w_\mu = \frac{1}{\mu}$, and $c_{\mathrm{cov}} = 1$

new distribution

Rank-μ CMA versus Estimation of Multivariate Normal Algorithm $\text{EMNA}_{\text{global}}$ [11]

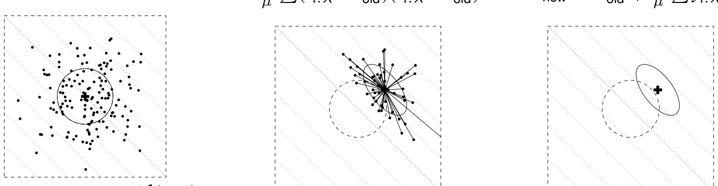


$x_i = m_{\text{old}} + y_i, \quad y_i \sim \mathcal{N}(\mathbf{0}, \mathbf{C})$

$\mathbf{C} \leftarrow \frac{1}{\mu}\sum (x_{i:\lambda} - m_{\text{old}})(x_{i:\lambda} - m_{\text{old}})^{\mathrm{T}}$

$m_{\text{new}} = m_{\text{old}} + \frac{1}{\mu}\sum y_{i:\lambda}$

rank-μ CMA conducts a PCA of steps



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$\mathbf{C} \leftarrow \frac{1}{\mu}\sum (x_{i:\lambda} - m_{\text{new}})(x_{i:\lambda} - m_{\text{new}})^{\mathrm{T}}$

$m_{\text{new}} = m_{\text{old}} + \frac{1}{\mu}\sum y_{i:\lambda}$

$\text{EMNA}_{\text{global}}$ conducts a PCA of points

sampling of $\lambda = 150$ solutions (dots)

calculating $\mathbf{C}$ from $\mu = 50$ solutions

new distribution

m_{new} is the minimizer for the variances when calculating $\mathbf{C}$

[11] Hansen, N. (2006). The CMA Evolution Strategy: A Comparing Review. In J.A. Lozano, P. Larranga, I. Inza and E. Bengoetxea (Eds.). Towards a new evolutionary computation. Advances in estimation of distribution algorithms. pp. 75-102

The rank-μ update

- increases the possible learning rate in large populations
  roughly from $2/n^2$ to μ_w/n^2
- can reduce the number of necessary generations roughly from $\mathcal{O}(n^2)$ to $\mathcal{O}(n)$ (12)
  given $\mu_w \propto \lambda \propto n$

Therefore the rank-μ update is the primary mechanism whenever a large population size is used

say $\lambda \ge 3\,n + 10$

The rank-one update

- uses the evolution path and reduces the number of necessary function evaluations to learn straight ridges from $\mathcal{O}(n^2)$ to $\mathcal{O}(n)$.

Rank-one update and rank-μ update can be combined

...all equations

[12] Hansen, Müller, and Koumoutsakos 2003. Reducing the Time Complexity of the Derandomized Evolution Strategy with Covariance Matrix Adaptation (CMA-ES). *Evolutionary Computation, 11(1)*, pp. 1-18

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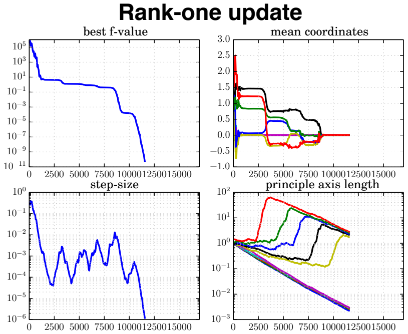
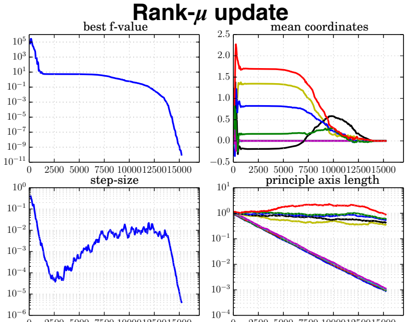
Rank-one update



Hybrid (combined) update

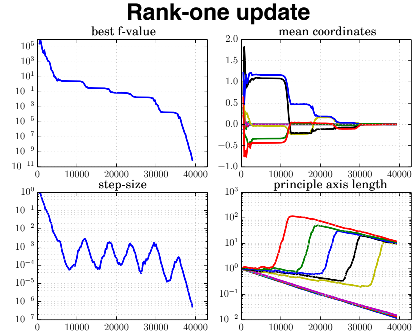
Rank-μ update



$$f_{\text{TwoAxes}}(x) = \sum_{i=1}^{5} x_i^2 + 10^6 \sum_{i=6}^{10} x_i^2$$

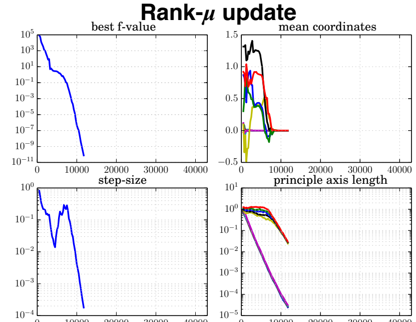
$\lambda = 10$ (default for $N = 10$)

Rank-one update



Hybrid (combined) update

Rank-μ update



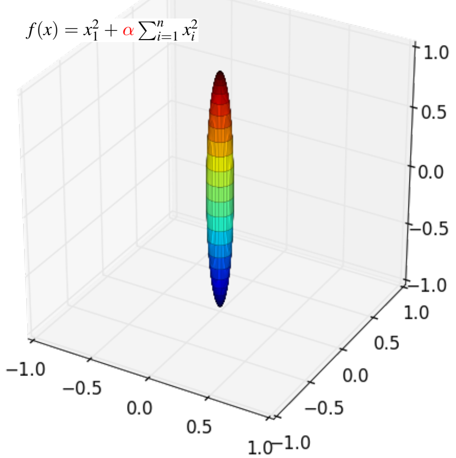
$$f_{\text{TwoAxes}}(x) = \sum_{i=1}^{5} x_i^2 + 10^6 \sum_{i=6}^{10} x_i^2$$

$\lambda = 50$

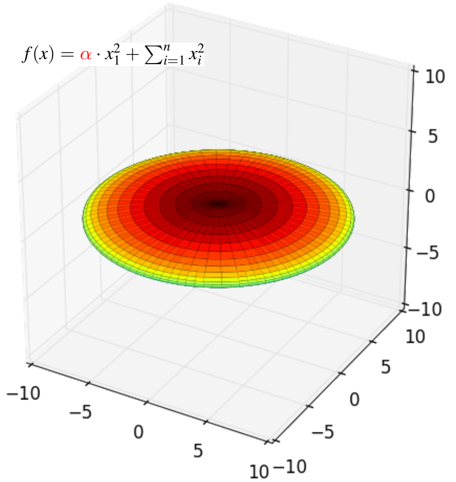
Different Types of Ill-Conditioning

(α: Axes Ratio = 10)

Cigar Type:
1 long axis = n-1 short axes



Discus Type:
1 short axis = n-1 long axes



Active Update

utilize negative weights [Jastrebski and Arnold, 2006]

Active Update (rewriting)

decreasing the variances in unpromising directions

$$C \leftarrow C + c_1 p_c p_c^T + c_\mu \sum_{i=1}^{\lfloor \lambda/2 \rfloor} w_i y_{i:\lambda} y_{i:\lambda}^T - c_\mu \sum_{i=\lambda-\lfloor \lambda/2 \rfloor+1}^{\lambda} |w_i| y_{i:\lambda} y_{i:\lambda}^T$$

increasing the variances in promising directions

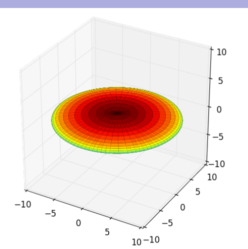
- increases the variance in the directions of p_c and promising steps $y_{i:\lambda}$ ($i \leq \lfloor \lambda/2 \rfloor$)
- decrease the variance in the directions of unpromising steps $y_{i:\lambda}$ ($i \geq \lambda - \lfloor \lambda/2 \rfloor + 1$)
- keep the variance in the subspace orthogonal to the above

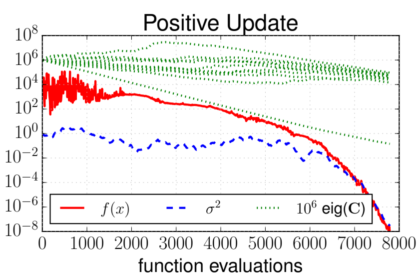
[Jastrebski and Arnold, 2006] Jastrebski, G. and Arnold, D. V. (2006). Improving Evolution Strategies through Active Covariance Matrix Adaptation. In 2006 IEEE Congress on Evolutionary Computation, pages 9719–9726.

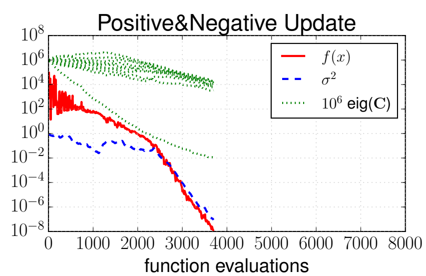
On 10D Discus Function

10D Discus Function (axis ratio: $\alpha = 10^3$)

$$f(x) = \alpha^2 \cdot x_1^2 + \sum_{i=1}^n x_i^2$$







- Positive: wait for the smallest eig(C) decreasing
- Active: decrease the smallest eig(C) actively

Summary

Active Covariance Matrix Adaptation + Cumulation

$$C \leftarrow (1 - c_1 - c_\mu + c_\mu^-) C + c_1 p_c p_c^T + c_\mu \sum_{i=1}^{\lfloor \lambda/2 \rfloor} w_i y_{i:\lambda} y_{i:\lambda}^T - c_\mu^- \sum_{i=\lambda-\lfloor \lambda/2 \rfloor+1}^{\lambda} |w_i| y_{i:\lambda} y_{i:\lambda}^T$$

- $-|w_i| < 0$ (for $i \geq \lambda - \lfloor \lambda/2 \rfloor + 1$): negative weight assigned to $y_{i:\lambda}$, $\sum_{i=\lambda-\mu}^{\lambda} |w_i| = 1$.
- $c_\mu^- > 0$: learning rate for the active update

These components complement each other

- cumulation: excels to learn a long axis, but inefficient for a large λ
- rank-μ update: efficient for a large λ
- active update: effective to learn short axes

An important yet solvable issue of active update

- The positive definiteness of C will be violated if c_μ^- is not small enough
- The positive definiteness can be guaranteed w.p.1 by controlling $c_\mu^- w_i$

Input: $m \in \mathbb{R}^n$; $\sigma \in \mathbb{R}_+$; $\lambda \in \mathbb{N}_{\geq 2}$, usually $\lambda \geq 5$, default $4 + \lfloor 3 \log n \rfloor$

Set $c_m = 1$; $c_1 \approx 2/n^2$; $c_\mu \approx \mu_w/n^2$; $c_c \approx 4/n$; $c_\sigma \approx 1/\sqrt{n}$; $d_\sigma \approx 1$; $w_{i=1\ldots\lambda}$ decreasing in i and $\sum_i^\mu w_i = 1$, $w_\mu > 0 \geq w_{\mu+1}$, $\mu_w^{-1} := \sum_{i=1}^\mu w_i^2 \approx 3/\lambda$

Initialize $\mathbf{C} = \mathbf{I}$, and $\boldsymbol{p}_c = \mathbf{0}$, $\boldsymbol{p}_\sigma = \mathbf{0}$

While not *terminate*

$\boldsymbol{x}_i = \boldsymbol{m} + \sigma \boldsymbol{y}_i$, where $\boldsymbol{y}_i \sim \mathcal{N}_i(\mathbf{0}, \mathbf{C})$ for $i = 1, \ldots, \lambda$ — sampling

$\boldsymbol{m} \leftarrow \boldsymbol{m} + c_m \sigma \boldsymbol{y}_w$, where $\boldsymbol{y}_w = \sum_{i=1}^\mu w_{\mathrm{rk}(i)}\, \boldsymbol{y}_i$ — update mean

$\boldsymbol{p}_\sigma \leftarrow (1 - c_\sigma)\, \boldsymbol{p}_\sigma + \sqrt{1 - (1 - c_\sigma)^2}\sqrt{\mu_w}\, \mathbf{C}^{-\frac{1}{2}} \boldsymbol{y}_w$ — path for σ

$\boldsymbol{p}_c \leftarrow (1 - c_c)\, \boldsymbol{p}_c + \mathbb{1}_{[0,2n]}\{\|\boldsymbol{p}_\sigma\|^2\} \sqrt{1 - (1 - c_c)^2}\sqrt{\mu_w}\, \boldsymbol{y}_w$ — path for $\mathbf{C}$

$\sigma \leftarrow \sigma \times \exp\left(\frac{c_\sigma}{d_\sigma}\left(\frac{\|\boldsymbol{p}_\sigma\|}{\mathsf{E}\|\mathcal{N}(\mathbf{0},\mathbf{I})\|} - 1\right)\right)$ — update of σ

$\mathbf{C} \leftarrow \mathbf{C} + c_\mu \sum_{i=1}^\lambda w_{\mathrm{rk}(i)} (\boldsymbol{y}_i \boldsymbol{y}_i^\mathsf{T} - \mathbf{C}) + c_1 (\boldsymbol{p}_c \boldsymbol{p}_c^\mathsf{T} - \mathbf{C})$ — update $\mathbf{C}$

Not covered: termination, restarts, useful output, search boundaries and encoding, corrections for: positive definiteness guaranty, $\boldsymbol{p}_c$ variance loss, c_σ and d_σ for large λ

Topics

1. What makes the problem difficult to solve?

2. How does the CMA-ES work?

- Normal Distribution, Rank-Based Recombination
- Step-Size Adaptation
- Covariance Matrix Adaptation

3. What can/should the users do for the CMA-ES to work effectively on their problem?

- Choice of problem formulation and encoding (not covered)
- Choice of initial solution and initial step-size
- Restarts, Increasing Population Size
- Restricted Covariance Matrix

Default Parameter Values

CMA-ES + (B)IPOP Restart Strategy = Quasi-Parameter Free Optimizer

The following parameters were identified in carefully chosen experimental set ups.

- related to selection and recombination
  - λ: offspring number, new solutions sampled, population size
  - μ: parent number, solutions involved in mean update
  - w_i: recombination weights
- related to $\boldsymbol{C}$-update
  - $1 - c_c$: decay rate for the evolution path, cumulation factor
  - c_1: learning rate for rank-one update of $\boldsymbol{C}$
  - c_μ: learning rate for rank-μ update of $\boldsymbol{C}$
- related to σ-update
  - $1 - c_\sigma$: decay rate of the evolution path
  - d_σ: damping for σ-change

The default values depends only on the dimension. They do in the first place not depend on the objective function.

Parameters to be set depending on the problem

Initialization and termination conditions

The following should be set or implemented depending on the problem.

- related to the initial search distribution
  - $\boldsymbol{m}^{(0)}$: initial mean vector
  - $\sigma^{(0)}$ (or $\sqrt{\boldsymbol{C}_{i,i}^{(0)}}$): initial (coordinate-wise) standard deviation
- related to stopping conditions
  - max. func. evals.
  - max. iterations
  - function value tolerance
  - min. axis length
  - stagnation

Practical Hints:

- start with an initial guess $\boldsymbol{m}^{(0)}$ with a relatively small step-size $\sigma^{(0)}$ to *locally* improve the current guess;
- then increase the step-size, e.g., by factor of 10, to *globally* search for a better solution.

Python CMA-ES Implementation

https://github.com/CMA-ES/pycma

pycma

A Python implementation of CMA-ES and a few related numerical optimization tools.

The Covariance Matrix Adaptation Evolution Strategy (CMA-ES) is a stochastic derivative-free numerical optimization algorithm for difficult (non-convex, ill-conditioned, multi-modal, rugged, noisy) optimization problems in continuous search spaces.

Useful links:

- A quick start guide with a few usage examples
- The API Documentation
- Hints for how to use this (kind of) optimization module in practice

Installation of the latest release

Type

```
python -m pip install cma
```

in a system shell to install the *latest release* from the Python Package Index (PyPI). The release link also provides more installation hints and a quick start guide.

Python CMA-ES Demo

https://github.com/CMA-ES/pycma

Optimizing 10D Rosenbrock Function

In [1]:

```
import cma                      # import
opts = cma.CMAOptions()         # CMA Options
opts['ftarget'] = 1e-4          # - function value target
opts['maxfevals'] = 1e6         # - max. function evaluations
cma.fmin(cma.ff.rosen,          # Minimize Rosenbrock function
         x0=[0.0] * 10,        # - x0 = [0,..., 0]
         sigma0=0.1,                # - sigma0 = 0.1
         options=opts)              # - other options
```

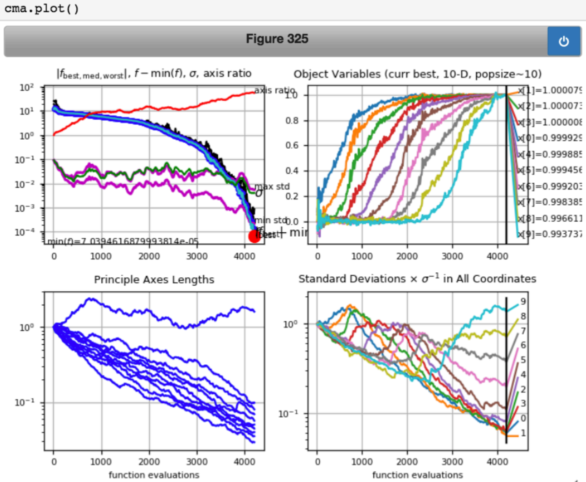
```
(5_w,10)-aCMA-ES (mu_w=3.2,w_1=45%) in dimension 10 (seed=909490, Mon Ap
r 16 13:39:57 2018)
Iterat #Fevals   function value  axis ratio  sigma  min&max std  t[m:s]
    1     10 1.169928472214858e+01 1.0e+00 9.12e-02  9e-02  9e-02 0:00.0
    2     20 1.363303277917634e+01 1.1e+00 8.33e-02  8e-02  8e-02 0:00.0
    3     30 1.232089008099892e+01 1.2e+00 7.55e-02  7e-02  8e-02 0:00.0
  100   1000 5.724977739870999e+00 9.1e+00 1.65e-02  7e-03  2e-02 0:00.1
  200   2000 2.550841127554589e+00 1.5e+01 3.97e-02  1e-02  4e-02 0:00.2
  300   3000 3.674986141687857e-01 1.5e+01 2.76e-02  3e-03  2e-02 0:00.4
  400   4000 1.266345464781239e-03 5.0e+01 1.18e-02  8e-04  2e-02 0:00.5
  420   4200 7.039461687999381e-05 5.5e+01 4.04e-03  2e-04  5e-03 0:00.5
termination on ftarget=0.0001 (Mon Apr 16 13:39:58 2018)
final/bestever f-value = 2.804423e-05 2.804423e-05
incumbent solution: [ 0.9998542   0.99996219  0.9999681   1.00000445  0.
99998977  0.99968537
  0.99954974  0.99918266 ...]
std deviations: [ 0.00023937  0.00022203  0.00024836  0.00024782  0.0003
1258  0.00043481
  0.00078261  0.0014964  ...]
```


Python CMA-ES Demo

https://github.com/CMA-ES/pycma

Optimizing 10D Rosenbrock Function

```
cma.plot()
```



Multimodality

Two approaches for multimodal functions: Try again with

- a larger population size
- a smaller initial step-size (and random initial mean vector)

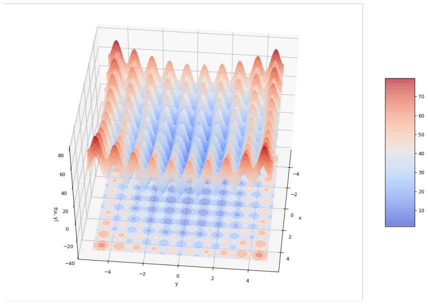
Multimodality

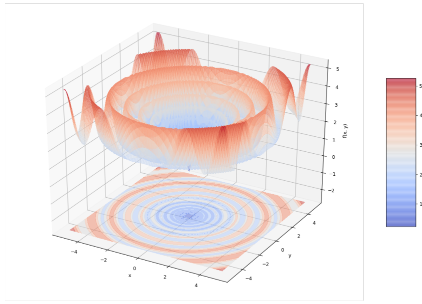
Approaches for multimodal functions: Try again with

- the final solution as initial solution (non-elitist) and small step-size
- a larger population size
- a different initial mean vector (and a smaller initial step-size)

A restart with a **large population size** helps if the objective function has a well global structure

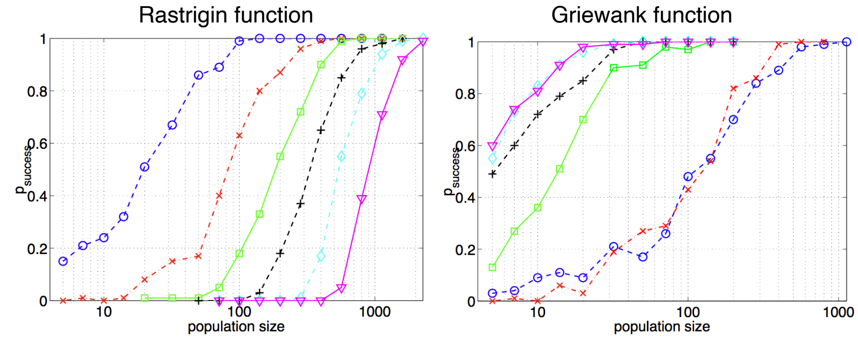
- functions such as Schaffer, Rastrigin, BBOB function 15~19
- loosely, unimodal global structure + deterministic noise





Multimodality

Hansen and Kern. Evaluating the CMA Evolution Strategy on Multimodal Test Functions, PPSN 2004.



(a) (b)

Fig. 1. Success rate to reach $f_{\text{stop}} = 10^{-10}$ versus population size for (a) Rastrigin function (b) Griewank function for dimensions $n = 2$ ('−−◯−−'), $n = 5$ ('−·−×−·−'), $n = 10$ ('—□—'), $n = 20$ ('−−+−−'), $n = 40$ ('−·−◇−·−'), and $n = 80$ ('—▽—').

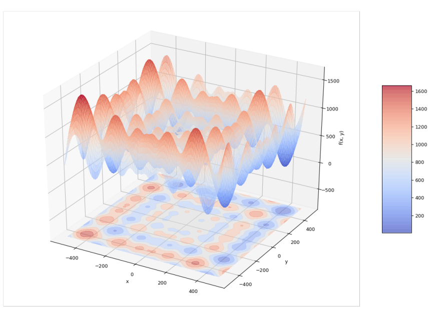
Multimodality

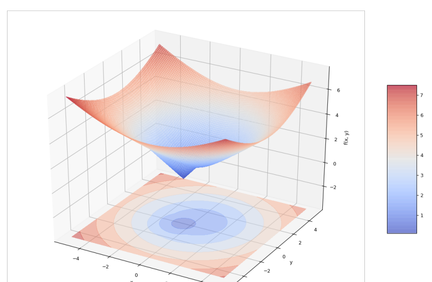
Approaches for multimodal functions: Try again with

- the final solution as initial solution (non-elitist) and small step-size
- a larger population size
- a different initial mean vector (and a smaller initial step-size)

A restart with a **small initial step-size** helps if the objective function has a weak global structure

- functions such as Schwefel, Bi-Sphere, BBOB function 20~24





a large population size has a negative effect

Restart Strategy

It makes the CMA-ES parameter free

IPOP: Restart with increasing the population size

- start with the default population size
- double the population size after each trial (parameter sweep)
- may be considered as gold standard for automated restarts

BIPOP: IPOP regime + Local search regime

- IPOP regime: restart with increasing population size
- Local search regime: restart with a smaller step-size and a smaller population size than the IPOP regime

Topics

1. What makes the problem difficult to solve?

2. How does the CMA-ES work?

- Normal Distribution, Rank-Based Recombination
- Step-Size Adaptation
- Covariance Matrix Adaptation

3. What can/should the users do for the CMA-ES to work effectively on their problem?

- Choice of problem formulation and encoding (not covered)
- Choice of initial solution and initial step-size
- Restarts, Increasing Population Size
- Restricted Covariance Matrix

Motivation of the Restricted Covariance Matrix

Bottlenecks of the CMA-ES on high dimensional problems

1. $\mathcal{O}(N^2)$ Time and Space Complexities
   - to store and update $C \in \mathbb{R}^{N \times N}$
   - to compute the eigen decomposition of C
2. $\mathcal{O}(1/N^2)$ Learning Rates for C-Update
   - $c_\mu \approx \mu_w / N^2$
   - $c_1 \approx 2/N^2$

Exploit prior knowledge on the problem structure such as separability

⇒ decrease the degrees of freedom of the covariance matrix for
- less time and space complexities
- a higher learning rates that potentially accelerate the adaptation

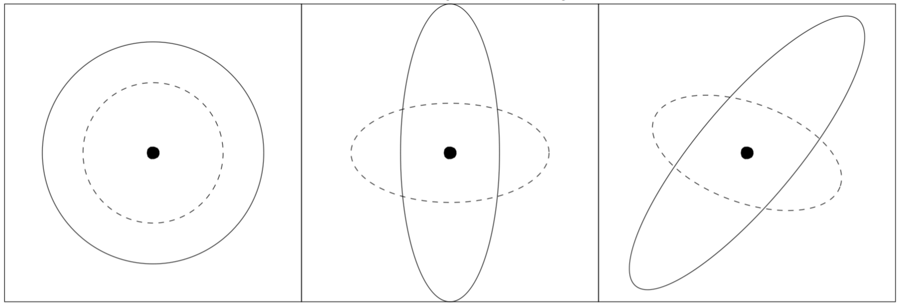
Variants with Restricted Covariance Matrix

CMA-ES Variants with Restricted Covariance Matrices

- Sep-CMA [Ros and Hansen, 2008]
  - $C = \mathbf{D}$. $\mathbf{D}$: Diagonal
- VD-CMA [Akimoto et al., 2014]
  - $C = \mathbf{D}(\mathbf{I} + v v^{\mathrm{T}})\mathbf{D}$. $\mathbf{D}$: Diagonal, $v \in \mathbb{R}^N$.
- LM-CMA [Loshchilov, 2014]
  - $C = \mathbf{I} + \sum_{i=1}^{k} v_i v_i^{\mathrm{T}}$. $v_i \in \mathbb{R}^N$.
- VkD-CMA [Akimoto and Hansen, 2016]
  - $C = \mathbf{D}(\mathbf{I} + \sum_{i=1}^{k} v_i v_i^{\mathrm{T}})\mathbf{D}$. $v_i \in \mathbb{R}^N$.

[Ros and Hansen, 2008] Ros, R. and Hansen, N. (2008). A simple modification in CMA-ES achieving linear time and space complexity. In Parallel Problem Solving from Nature - PPSN X, pages 296–305. Springer.
[Akimoto et al., 2014] Akimoto, Y., Auger, A., and Hansen, N. (2014). Comparison-based natural gradient optimization in high dimension. In Proceedings of Genetic and Evolutionary Computation Conference, pages 373–380, Vancouver, BC, Canada.
[Loshchilov, 2014] Loshchilov, I. (2014). A computationally efficient limited memory cma-es for large scale optimization. In Proceedings of Genetic and Evolutionary Computation Conference, pages 397–404.
[Akimoto and Hansen, 2016] Akimoto, Y. and Hansen, N. (2016). Projection-based restricted covariance matrix adaptation for high dimension. In Genetic and Evolutionary Computation Conference, GECCO 2016, Denver, Colorado, USA, July 20-24, 2016, page (accepted). ACM.

Separable CMA (Sep-CMA)



$\mathcal{N}(m, \sigma^2 \mathbf{I}) \sim m + \sigma \mathcal{N}(\mathbf{0}, \mathbf{I})$ — one degree of freedom σ

$\mathcal{N}(m, \mathbf{D}^2) \sim m + \mathbf{D}\mathcal{N}(\mathbf{0}, \mathbf{I})$ — n degrees of freedom

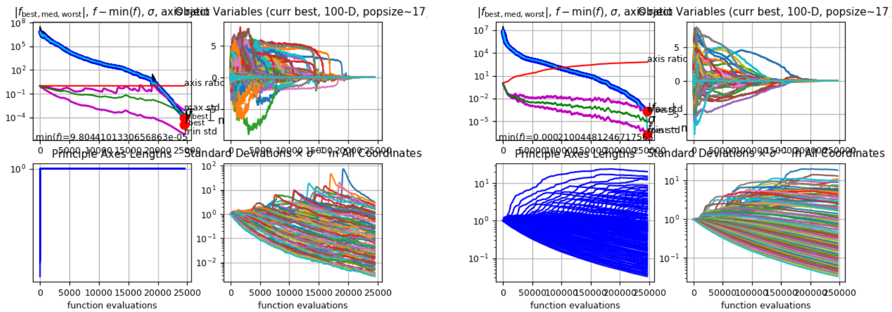
$\mathcal{N}(m, \mathbf{C}) \sim m + \mathbf{C}^{\frac{1}{2}}\mathcal{N}(\mathbf{0}, \mathbf{I})$ — $(n^2 + n)/2$ degrees of freedom

CMA $$C_{\mathrm{cma}}^{(t+1)} = C^{(t)} + c_1 \left(p_c p_c^{\mathrm{T}} - C^{(t)} \right) + c_\mu \sum_{i=1}^{\mu} w_i \left((x_i - m^{(t)})(x_i - m^{(t)})^{\mathrm{T}} - C^{(t)} \right)$$

SEP $$[C_{\mathrm{sep}}^{(t+1)}]_{k,k} = [C^{(t)}]_{k,k} + c_1 \left([p_c]_k^2 - [C^{(t)}]_{k,k} \right) + c_\mu \sum_{i=1}^{\mu} w_i \left([x_i - m^{(t)}]_k^2 - [C^{(t)}]_{k,k} \right)$$

(c_1, c_μ) → (N + 2)/3 times greater than CMA

Demo: On 100D Separable Ellipsoid Function



Separable-CMA CMA

- CMA needed 10 times more FEs + more CPU time
- However, Sep-CMA won't be able to solve rotated ellipsoid function as efficiently as it solves separable ellipsoid

Summary and Final Remarks

Main Characteristics of (CMA) Evolution Strategies

1. Multivariate normal distribution to generate new search points
   follows the maximum entropy principle
2. Rank-based selection
   implies invariance, same performance on $g(f(\boldsymbol{x}))$ for any increasing g
   more invariance properties are featured
3. Step-size control facilitates fast (log-linear) convergence and possibly linear scaling with the dimension
   in CMA-ES based on an evolution path (a non-local trajectory)
4. *Covariance matrix adaptation (CMA)* increases the likelihood of previously successful steps and can improve performance by orders of magnitude
   the update follows the natural gradient
   $\mathbf{C} \propto \boldsymbol{H}^{-1} \iff$ adapts a variable metric
   $\iff$ new (rotated) problem representation
   $\Longrightarrow f : \boldsymbol{x} \mapsto g(\boldsymbol{x}^\mathrm{T}\boldsymbol{H}\boldsymbol{x})$ reduces to $\boldsymbol{x} \mapsto \boldsymbol{x}^\mathrm{T}\boldsymbol{x}$

Limitations

of CMA Evolution Strategies

- internal CPU-time: $10^{-8}n^2$ seconds per function evaluation on a 2GHz PC, tweaks are available
  1 000 000 f-evaluations in 100-D take 100 seconds *internal* CPU-time
  variants with restricted covariance matrix such as Sep-CMA
- better methods are presumably available in case of
  - partly separable problems
  - specific problems, for example with cheap gradients
    specific methods
  - small dimension $(n \ll 10)$
    for example Nelder-Mead
  - small running times (number of f-evaluations $< 100n$)
    model-based methods

Thank you

Source code for CMA-ES in C, C++, Java, Matlab, Octave, Python, R, Scilab
and
Practical hints for problem formulation, variable encoding, parameter setting
are available (or linked to) at
http://cma.gforge.inria.fr/cmaes_sourcecode_page.html

Natural Gradient Descend

- Consider $\arg\min_{\boldsymbol{\theta}} \mathrm{E}(f(\boldsymbol{x})|\boldsymbol{\theta})$ under the sampling distribution $\boldsymbol{x} \sim p(.|\boldsymbol{\theta})$
  we could improve $\mathrm{E}(f(\boldsymbol{x})|\boldsymbol{\theta})$ by following the gradient $\nabla_{\boldsymbol{\theta}}\mathrm{E}(f(\boldsymbol{x})|\boldsymbol{\theta})$:
  $$\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \eta\nabla_{\boldsymbol{\theta}}\mathrm{E}(f(\boldsymbol{x})|\boldsymbol{\theta}), \qquad \eta > 0$$
  $\nabla_{\boldsymbol{\theta}}$ depends on the parameterization of the distribution, therefore
- Consider the natural gradient of the expected transformed fitness
  $$\widetilde{\nabla}_{\boldsymbol{\theta}}\,\mathrm{E}(w \circ P_f(f(\boldsymbol{x}))|\boldsymbol{\theta}) = F_{\boldsymbol{\theta}}^{-1}\nabla_{\boldsymbol{\theta}}\mathrm{E}(w \circ P_f(f(\boldsymbol{x}))|\boldsymbol{\theta}) = \mathrm{E}(w \circ P_f(f(\boldsymbol{x}))F_{\boldsymbol{\theta}}^{-1}\nabla_{\boldsymbol{\theta}} \ln p(\boldsymbol{x}|\boldsymbol{\theta}))$$
  using the Fisher information matrix $F_{\boldsymbol{\theta}} = \left(\left(E\frac{\partial^2 \log p(x|\boldsymbol{\theta})}{\partial\boldsymbol{\theta}_i\partial\boldsymbol{\theta}_j}\right)\right)_{ij}$ of the density p.
  The natural gradient is invariant under re-parameterization of the distribution.
- A Monte-Carlo approximation reads
  $$\widetilde{\nabla}_{\boldsymbol{\theta}}\,\widehat{\mathrm{E}}(\widehat{w}(f(\boldsymbol{x}))|\boldsymbol{\theta}) = \sum_{i=1}^{\lambda} w_i\,F_{\boldsymbol{\theta}}^{-1}\nabla_{\boldsymbol{\theta}} \ln p(\boldsymbol{x}_{i:\lambda}|\boldsymbol{\theta}), \quad w_i = \widehat{w}(f(\boldsymbol{x}_{i:\lambda})|\boldsymbol{\theta})$$

CMA-ES = Natural Evolution Strategy + Cumulation

Natural gradient descend using the MC approximation and the normal distribution

- Rewriting the update of the distribution mean
  $$\boldsymbol{m}_{\text{new}} \leftarrow \sum_{i=1}^{\mu} w_i \boldsymbol{x}_{i:\lambda} = \boldsymbol{m} + \underbrace{\sum_{i=1}^{\mu} w_i(\boldsymbol{x}_{i:\lambda} - \boldsymbol{m})}_{\text{natural gradient for mean } \frac{\tilde{\partial}}{\partial \boldsymbol{m}}\widehat{\mathrm{E}}(w \circ P_f(f(\boldsymbol{x}))|\boldsymbol{m}, \mathbf{C})}$$
- Rewriting the update of the covariance matrix[13]
  $$\mathbf{C}_{\text{new}} \leftarrow \mathbf{C} + c_1(\overbrace{\boldsymbol{p}_c\boldsymbol{p}_c^{\mathrm{T}}}^{\text{rank one}} - \mathbf{C}) + \underbrace{\frac{c_\mu}{\sigma^2}\sum_{i=1}^{\mu} w_i\left(\overbrace{(\boldsymbol{x}_{i:\lambda} - \boldsymbol{m})(\boldsymbol{x}_{i:\lambda} - \boldsymbol{m})^{\mathrm{T}}}^{\text{rank-}\mu} - \sigma^2\mathbf{C}\right)}_{\text{natural gradient for covariance matrix } \frac{\tilde{\partial}}{\partial \mathbf{C}}\widehat{\mathrm{E}}(w \circ P_f(f(\boldsymbol{x}))|\boldsymbol{m}, \mathbf{C})}$$

[13] Akimoto et.al. (2010): Bidirectional Relation between CMA Evolution Strategies and Natural Evolution Strategies, PPSN XI

Maximum Likelihood Update

The new distribution mean $\boldsymbol{m}$ maximizes the log-likelihood

$$\boldsymbol{m}_{\text{new}} = \arg\max_{\boldsymbol{m}} \sum_{i=1}^{\mu} w_i \log p_{\mathcal{N}}(\boldsymbol{x}_{i:\lambda}|\boldsymbol{m})$$

independently of the given covariance matrix

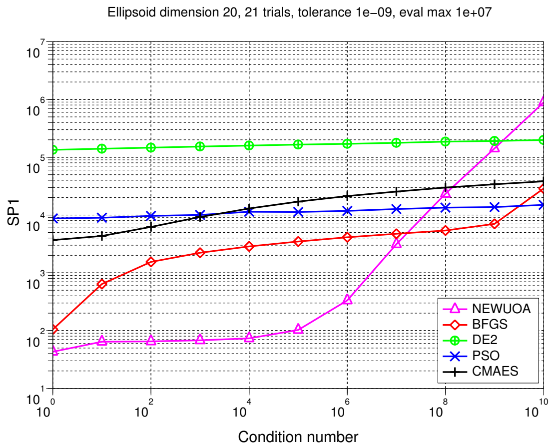
The rank-μ update matrix $\mathbf{C}_\mu$ maximizes the log-likelihood

$$\mathbf{C}_\mu = \arg\max_{\mathbf{C}} \sum_{i=1}^{\mu} w_i \log p_{\mathcal{N}}\left(\frac{\boldsymbol{x}_{i:\lambda} - \boldsymbol{m}_{\text{old}}}{\sigma}\middle|\boldsymbol{m}_{\text{old}}, \mathbf{C}\right)$$

$\log p_{\mathcal{N}}(\boldsymbol{x}|\boldsymbol{m}, \mathbf{C}) = -\frac{1}{2}\log\det(2\pi\mathbf{C}) - \frac{1}{2}(\boldsymbol{x} - \boldsymbol{m})^{\mathrm{T}}\mathbf{C}^{-1}(\boldsymbol{x} - \boldsymbol{m})$
$p_{\mathcal{N}}$ is the density of the multi-variate normal distribution

Comparison to BFGS, NEWUOA, PSO and DE

f convex quadratic, separable with varying condition number α



BFGS (Broyden et al 1970)
NEWUAO (Powell 2004)
DE (Storn & Price 1996)
PSO (Kennedy & Eberhart 1995)
CMA-ES (Hansen & Ostermeier 2001)

$f(\boldsymbol{x}) = g(\boldsymbol{x}^{\mathrm{T}}\mathbf{H}\boldsymbol{x})$ with

$\boldsymbol{H}$ diagonal

g identity (for BFGS and NEWUOA)

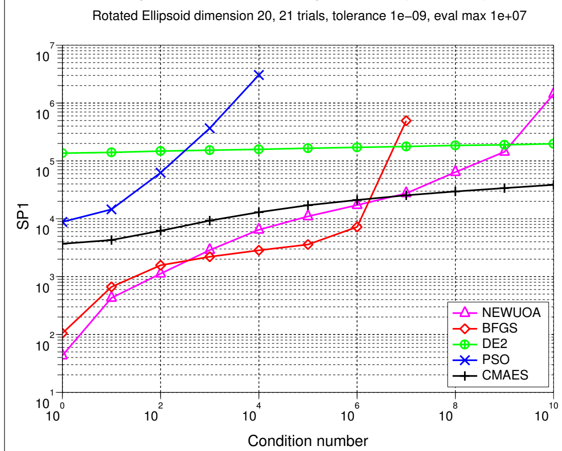
g any order-preserving = strictly increasing function (for all other)

SP1 = average number of objective function evaluations[14] to reach the target function value of $g^{-1}(10^{-9})$

[14] Auger et.al. (2009): Experimental comparisons of derivative free optimization algorithms, SEA

Comparison to BFGS, NEWUOA, PSO and DE

f convex quadratic, non-separable (rotated) with varying condition number α



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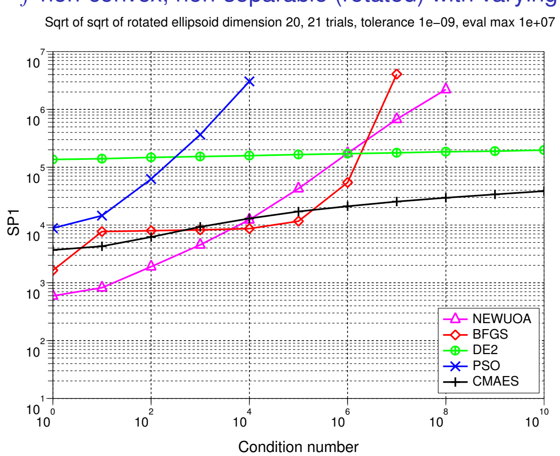
[15] Auger et.al. (2009): Experimental comparisons of derivative free optimization algorithms, SEA

Comparison to BFGS, NEWUOA, PSO and DE

f non-convex, non-separable (rotated) with varying condition number α



BFGS (Broyden et al 1970)
NEWUAO (Powell 2004)
DE (Storn & Price 1996)
PSO (Kennedy & Eberhart 1995)
CMA-ES (Hansen & Ostermeier 2001)

$f(\boldsymbol{x}) = g(\boldsymbol{x}^{\mathrm{T}}\mathbf{H}\boldsymbol{x})$ with

$\boldsymbol{H}$ full

$g : x \mapsto x^{1/4}$ (for BFGS and NEWUOA)

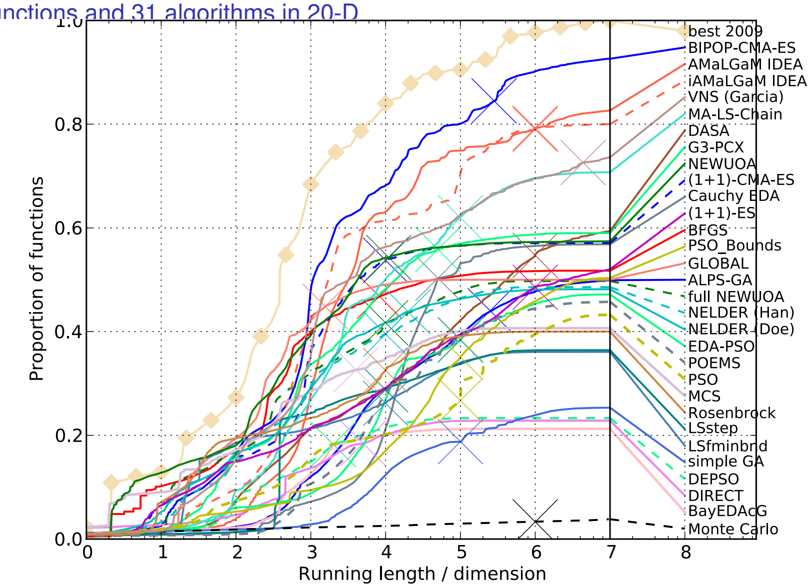
g any order-preserving = strictly increasing function (for all other)

SP1 = average number of objective function evaluations[16] to reach the target function value of $g^{-1}(10^{-9})$

[16] Auger et.al. (2009): Experimental comparisons of derivative free optimization algorithms, SEA

Comparison during BBOB at GECCO 2009

24 functions and 31 algorithms in 20-D



Comparison during BBOB at GECCO 2010

24 functions and 20+ algorithms in 20-D