Tutorial—Evolution Strategies and Covariance Matrix Adaptation

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Content

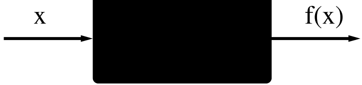
Problem Statement

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

    . . . or to a robust solution x
  - solution x with **small function value** with **least search cost**

    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

- Problems
  - exhaustive search is infeasible
  - naive random search takes too long
  - deterministic search is not successful / takes too long

Approach: stochastic search, Evolutionary Algorithms

Metaphors

Evolutionary Computation		Optimization
individual, offspring, parent	$\longleftrightarrow$	candidate solution
		decision variables
		design variables
		object variables
population	$\longleftrightarrow$	set of candidate solutions
fitness function	$\longleftrightarrow$	objective function
		loss function
		cost function
generation	$\longleftrightarrow$	iteration

. . . function properties

Objective Function Properties

We assume $f : \mathcal{X} \subset \mathbb{R}^n \to \mathbb{R}$ to be *non-linear, non-separable* and to have at least moderate dimensionality, say $n \not\ll 10$.
Additionally, f can be

- non-convex
- multimodal

  there are eventually many local optima
- non-smooth

  derivatives do not exist
- discontinuous
- ill-conditioned
- noisy
- ...

Goal : cope with any of these function properties
they are related to real-world problems

What Makes a Function Difficult to Solve?

Why stochastic search?

- ruggedness

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

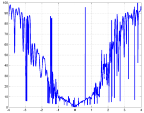
- dimensionality

  (considerably) larger than three

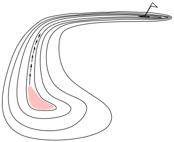
- non-separability

  dependencies between the objective variables

- ill-conditioning



cut from 3-D example, solvable with an evolution strategy



a narrow ridge

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 100 points onto a real interval, say $[0, 1]$. To get **similar coverage**, in terms of distance between adjacent points, of the 10-dimensional space $[0, 1]^{10}$ would require $100^{10} = 10^{20}$ points. A 100 points appear now as isolated points in a vast empty space.

Consequently, a **search policy** (e.g. exhaustive search) that is valuable in small dimensions **might be useless** in moderate or large dimensional search spaces.

Separable Problems

Definition (Separable Problem)

A function f is separable if

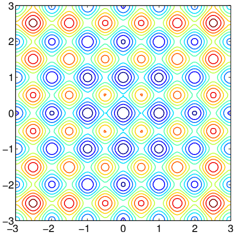
$$\arg\min_{(x_1,\ldots,x_n)} f(x_1,\ldots,x_n) = \left(\arg\min_{x_1} f(x_1,\ldots),\ldots,\arg\min_{x_n} f(\ldots,x_n)\right)$$

$\Rightarrow$ 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



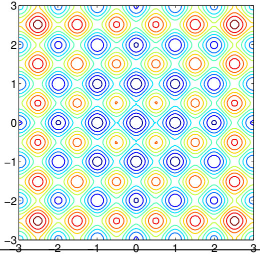
Non-Separable Problems

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

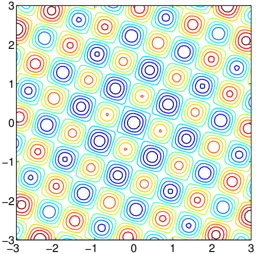
Rotating the coordinate system

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

R rotation matrix



$$\xrightarrow{\mathbf{R}}$$



[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

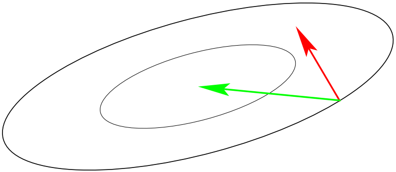
[2] Salomon (1996). "Reevaluating Genetic Algorithm Performance under Coordinate Rotation of Benchmark Functions; A survey of some theoretical and practical aspects of genetic algorithms." BioSystems, 39(3):263-278

Ill-Conditioned Problems

Curvature of level sets

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

$\boldsymbol{H}$ 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**.

What Makes a Function Difficult to Solve?

. . . and what can be done

The Problem	The Approach in ESs and continuous EDAs
Ruggedness	**non-local** policy, large sampling width (step-size) as large as possible while preserving a reasonable convergence speed
	stochastic, non-elitistic, **population-based** method recombination operator serves as repair mechanism
Dimensionality, Non-Separability	exploiting the problem structure locality, neighborhood, encoding
Ill-conditioning	second order approach changes the neighborhood metric

Stochastic Search

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

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

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

Everything depends on the definition of P and F_θ

deterministic algorithms are covered as well

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

Natural template for *Estimation of Distribution Algorithms*

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

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?

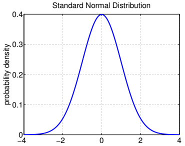
1. widely observed in nature, for example as phenotypic traits
2. only stable distribution with finite variance
   stable means the sum of normal variates is again normal,
   helpful in **design and analysis** of algorithms
3. most convenient way to generate **isotropic** search points
   the isotropic distribution does **not favor any direction**
   (unfoundedly), supports rotational invariance
4. maximum entropy distribution with finite variance
   the least possible assumptions on f in the distribution shape

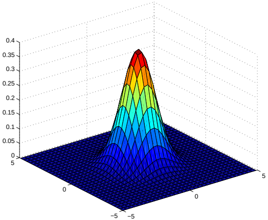
The Multi-Variate (n-Dimensional) Normal Distribution

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 $\mathbf{C}$.

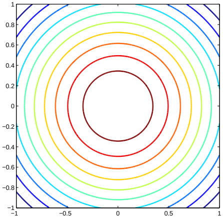
The **mean** value $\boldsymbol{m}$

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



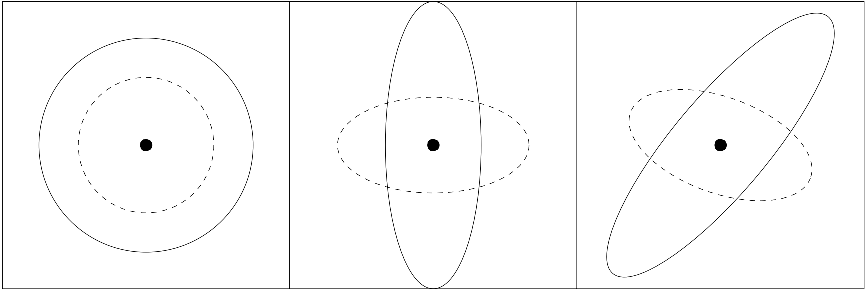


2-D



The **covariance matrix** $\mathbf{C}$ determines the shape. It has a valuable **geometrical interpretation**: any covariance matrix can be uniquely identified with the iso-density ellipsoid $\{\boldsymbol{x} \in \mathbb{R}^n \,|\, \boldsymbol{x}^{\mathrm{T}}\mathbf{C}^{-1}\boldsymbol{x} = 1\}$

Lines of Equal Density



$\mathcal{N}\left(\boldsymbol{m}, \sigma^2\mathbf{I}\right) \sim \boldsymbol{m} + \sigma\mathcal{N}(\mathbf{0}, \mathbf{I})$
one degree of freedom σ
components of $\mathcal{N}(\mathbf{0}, \mathbf{I})$ are independent standard normally distributed

$\mathcal{N}\left(\boldsymbol{m}, \mathbf{D}^2\right) \sim \boldsymbol{m} + \mathbf{D}\,\mathcal{N}(\mathbf{0}, \mathbf{I})$
n **degrees of freedom**
components are independent, scaled

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

Evolution Strategies

Terminology

$(\mu \overset{+}{,} \lambda)$-selection, μ: # parents, λ: # offspring

$(\mu + \lambda)$-ES: selection in $\{$parents$\} \cup \{$offspring$\}$
(μ, λ)-ES: selection in $\{$offspring$\}$

$(1 + 1)$-ES

Sample one offspring from parent $\boldsymbol{m}$

$$\boldsymbol{x} = \boldsymbol{m} + \sigma\,\mathcal{N}(\mathbf{0}, \mathbf{C})$$

If $\boldsymbol{x}$ better than $\boldsymbol{m}$ select

$$\boldsymbol{m} \leftarrow \boldsymbol{x}$$

. . . why?

The $(\mu/\mu, \lambda)$-ES

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 $f(\boldsymbol{x}_{1:\lambda}) \leq \cdots \leq f(\boldsymbol{x}_{\lambda:\lambda})$. 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

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

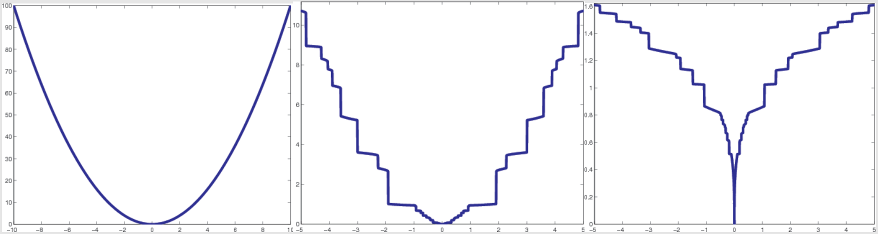
The best μ points are selected **from the new solutions** (non-elitistic) and **weighted intermediate recombination** is applied.

Invariance Under Monotonically Increasing Functions

Rank-based algorithms

Update of all parameters uses only the ranks

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



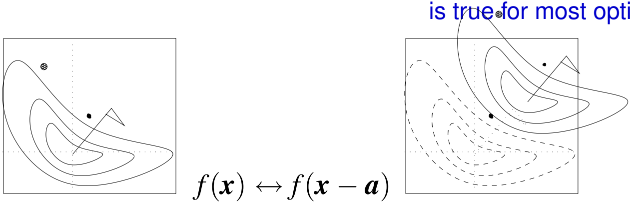
$$g(f(x_{1:\lambda})) \leq g(f(x_{2:\lambda})) \leq \ldots \leq g(f(x_{\lambda:\lambda})) \quad \forall g$$

g is strictly monotonically increasing
g preserves ranks

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_a

$$\begin{aligned} f: \quad & \boldsymbol{x} \mapsto f(\boldsymbol{x}), & \boldsymbol{x}^{(t=0)} &= \boldsymbol{x}_0 \\ f_a: \quad & \boldsymbol{x} \mapsto f(\boldsymbol{x}-\boldsymbol{a}), & \boldsymbol{x}^{(t=0)} &= \boldsymbol{x}_0 + \boldsymbol{a} \end{aligned}$$

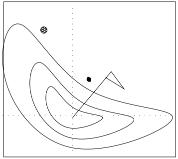
No difference can be observed w.r.t. the argument of f

Rotational Invariance in Search Space

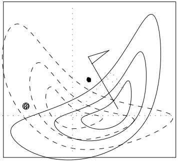
- invariance to an orthogonal transformation $\mathbf{R}$, where $\mathbf{R}\mathbf{R}^{\mathrm{T}} = \mathbf{I}$

e.g. true for simple evolution strategies

recombination operators might jeopardize rotational invariance



$f(\boldsymbol{x}) \leftrightarrow f(\mathbf{R}\boldsymbol{x})$



Identical behavior on f and $f_{\mathbf{R}}$

$$
\begin{aligned}
f: \quad & \boldsymbol{x} \mapsto f(\boldsymbol{x}), & \boldsymbol{x}^{(t=0)} &= \boldsymbol{x}_0 \\
f_{\mathbf{R}}: \quad & \boldsymbol{x} \mapsto f(\mathbf{R}\boldsymbol{x}), & \boldsymbol{x}^{(t=0)} &= \mathbf{R}^{-1}(\boldsymbol{x}_0)
\end{aligned}
$$

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

34

[3] Salomon (1996). "Reevaluating Genetic Algorithm Performance under Coordinate Rotation of Benchmark Functions; A

Invariance

Impact

The grand aim of all science is to cover the greatest number of empirical facts by logical deduction from the smallest number of hypotheses or axioms.
— Albert Einstein

- empirical performance results, for example
  - from benchmark functions
  - from solved real world problems

  are only useful if they do **generalize** to other problems

- **Invariance** is a strong **non-empirical** statement about the feasibility of generalization

  generalizing (identical) performance from a single function to a whole class of functions

consequently, invariance is important for the evaluation of search algorithms

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

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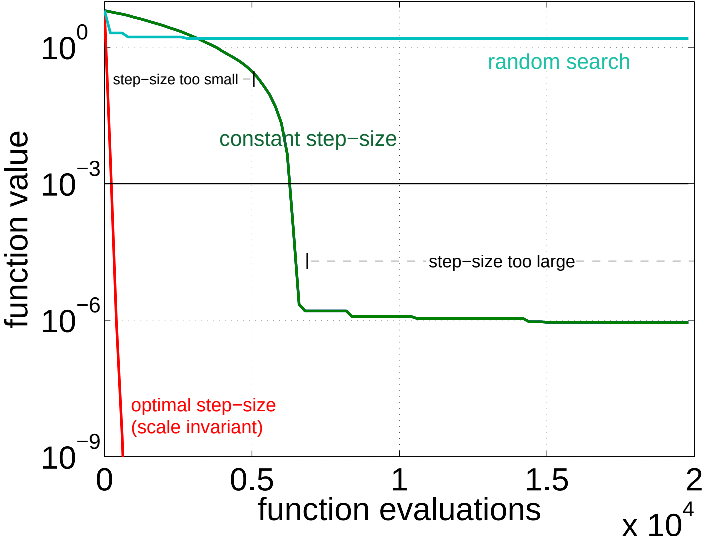
- the so-called step-size $\sigma \in \mathbb{R}_+$ controls the *step length*
- the covariance matrix $\mathbf{C} \in \mathbb{R}^{n \times n}$ determines the **shape** of the distribution ellipsoid

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

Why Step-Size Control?

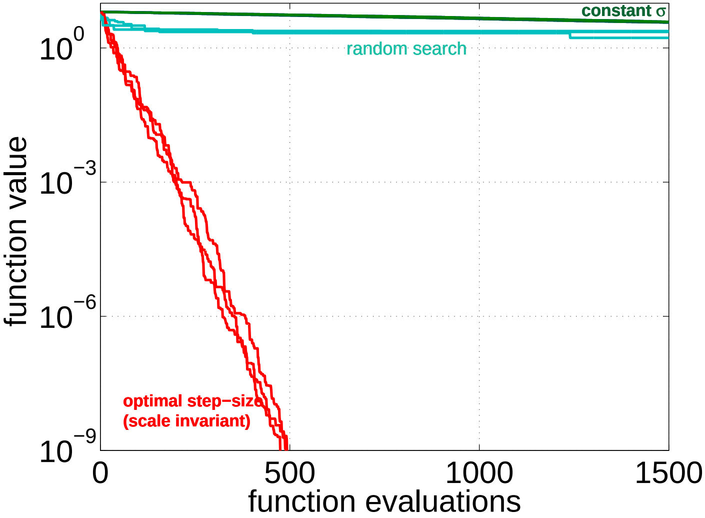


$\mathbf{C} = \mathbf{I}$

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

in $[-0.2, 0.8]^n$
for $n = 10$

Why Step-Size Control?



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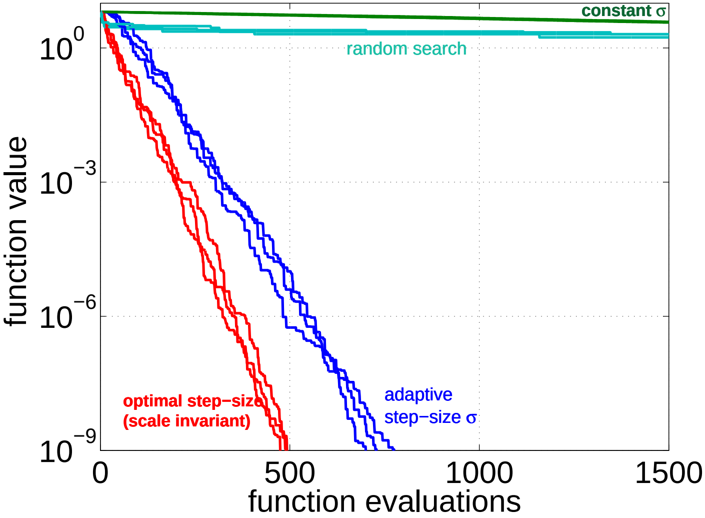

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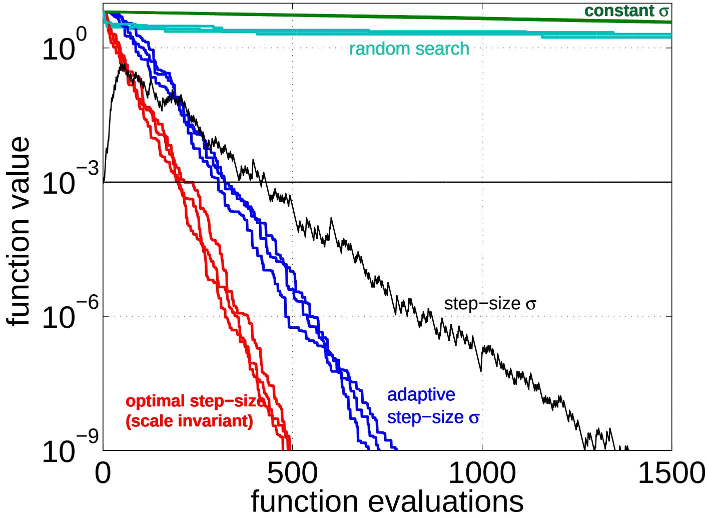

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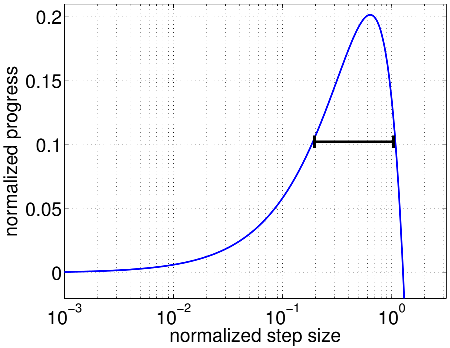
Why Step-Size Control?

The evolution window



evolution window for the step-size on the sphere function

evolution window refers to the step-size interval where reasonable performance is observed

Methods for Step-Size Control

- $1/5$-th success rule[a][b], 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 one, according to the objective function value, is selected

  simplified "global" self-adaptation

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

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

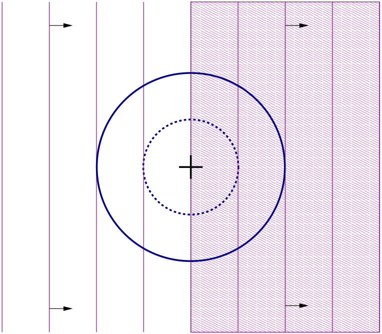
[b] Schumer and Steiglitz 1968. Adaptive step size random search. *IEEE TAC*

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

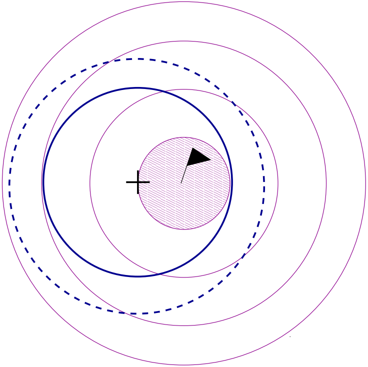
[d] Hansen & Ostermeier 2001, Completely Derandomized Self-Adaptation in Evolution Strategies, *Evol. Comput. 9(2)*

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

One-fifth success rule

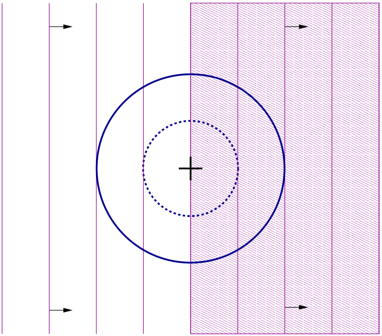


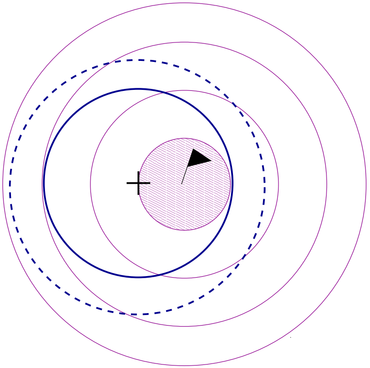
↓
increase σ



↓
decrease σ

One-fifth success rule





Probability of success (p_s)

$1/2$

$1/5$

Probability of success (p_s)

"too small"

One-fifth success rule

p_s: # of successful offspring / # offspring (per generation)

$$\sigma \leftarrow \sigma \times \exp\left(\frac{1}{3} \times \frac{p_s - p_{\text{target}}}{1 - p_{\text{target}}}\right)$$

Increase σ if $p_s > p_{\text{target}}$
Decrease σ if $p_s < p_{\text{target}}$

$(1+1)$-ES

$p_{target} = 1/5$

IF *offspring better parent*

$p_s = 1$, $\sigma \leftarrow \sigma \times \exp(1/3)$

ELSE

$p_s = 0$, $\sigma \leftarrow \sigma / \exp(1/3)^{1/4}$

Self-adaptation

in a $(1, \lambda)$-ES

MUTATE `for` $i = 1, \ldots \lambda$

step-size $\sigma_i \leftarrow \sigma \exp(\tau N_i(0, 1))$

parent $x_i \leftarrow x + \sigma_i \mathcal{N}_i(0, \mathbf{I})$

EVALUATE

SELECT

Best offspring x_* with its step-size σ_*

Rationale

Unadapted step-size won't produce successive good individuals

"The step-size are adjusted by the evolution itself"

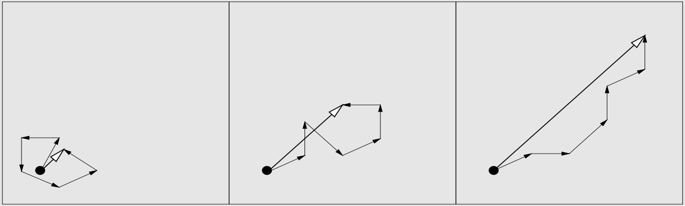
Path Length Control (CSA)

The Concept of Cumulative Step-Size Adaptation

$$\begin{aligned} \boldsymbol{x}_i &= \boldsymbol{m} + \sigma\, \boldsymbol{y}_i \\ \boldsymbol{m} &\leftarrow \boldsymbol{m} + \sigma \boldsymbol{y}_w \end{aligned}$$

Measure the length of the *evolution path*

the pathway of the mean vector $\boldsymbol{m}$ in the generation sequence



$\Downarrow$ decrease σ

$\Downarrow$ 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)

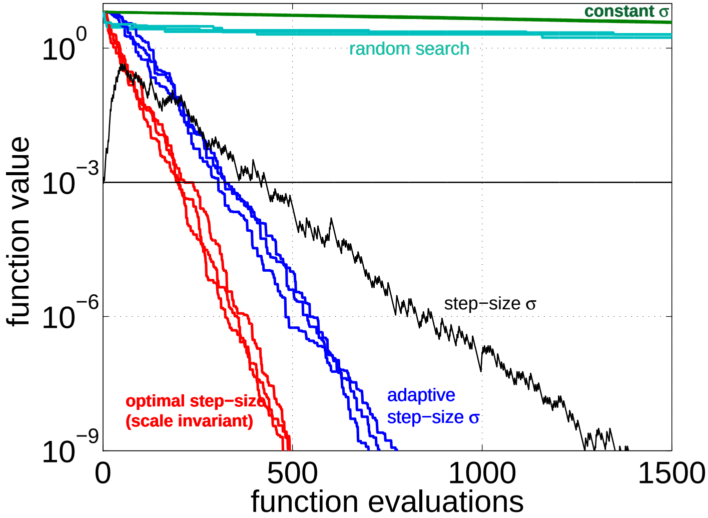
The Equations

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

$$\boldsymbol{m} \leftarrow \boldsymbol{m} + \sigma \boldsymbol{y}_w \quad \text{where } \boldsymbol{y}_w = \sum_{i=1}^{\mu} w_i \boldsymbol{y}_{i:\lambda} \qquad \text{update mean}$$

$$\boldsymbol{p}_\sigma \leftarrow (1 - c_\sigma)\, \boldsymbol{p}_\sigma + \underbrace{\sqrt{1 - (1 - c_\sigma)^2}}_{\text{accounts for } 1-c_\sigma} \quad \underbrace{\sqrt{\mu_w}}_{\text{accounts for } w_i} \quad \boldsymbol{y}_w$$

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



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

in $[-0.2, 0.8]^n$
for $n = 10$

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

where

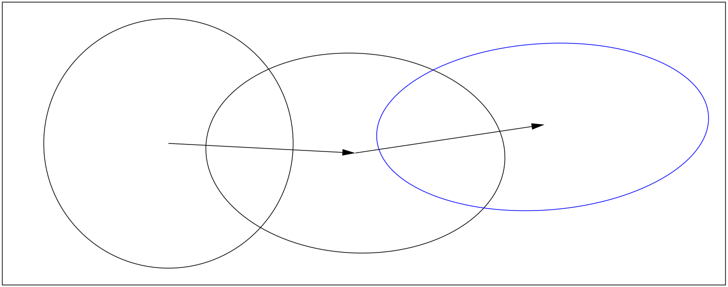
- the mean vector $\boldsymbol{m} \in \mathbb{R}^n$ represents the favorite solution
- the so-called step-size $\sigma \in \mathbb{R}_+$ controls the *step length*
- the covariance matrix $\mathbf{C} \in \mathbb{R}^{n \times n}$ determines the **shape** of the distribution ellipsoid

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

Covariance Matrix Adaptation

Rank-One Update

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



new distribution,

$\mathbf{C} \leftarrow 0.8 \times \mathbf{C} + 0.2 \times \boldsymbol{y}_w \boldsymbol{y}_w^{\mathrm{T}}$

the ruling principle: the adaptation **increases the likelyhood of successful steps**, $\boldsymbol{y}_w$, to appear again

. . . equations

Covariance Matrix Adaptation

Rank-One Update

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

$$
\begin{aligned}
\boldsymbol{x}_i &= \boldsymbol{m} + \sigma\, \boldsymbol{y}_i, \qquad \boldsymbol{y}_i \sim \mathcal{N}_i(\mathbf{0}, \mathbf{C}), \\
\boldsymbol{m} &\leftarrow \boldsymbol{m} + \sigma \boldsymbol{y}_w \qquad \text{where } \boldsymbol{y}_w = \sum_{i=1}^{\mu} w_i\, \boldsymbol{y}_{i:\lambda} \\
\mathbf{C} &\leftarrow (1 - c_{\mathrm{cov}})\mathbf{C} + c_{\mathrm{cov}} \mu_w \underbrace{\boldsymbol{y}_w \boldsymbol{y}_w^{\mathrm{T}}}_{\text{rank-one}} \qquad \text{where } \mu_w = \frac{1}{\sum_{i=1}^{\mu} {w_i}^2} \geq 1
\end{aligned}
$$

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

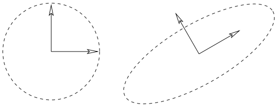
covariance matrix adaptation

- learns all **pairwise dependencies** between variables

  off-diagonal entries in the covariance matrix reflect the dependencies

- conducts a **principle component analysis** (PCA) of steps $\boldsymbol{y}_w$, sequentially in time and space

  eigenvectors of the covariance matrix $\mathbf{C}$ are the principle components / the principle axes of the mutation ellipsoid, rotational invariant



- learns a new, **rotated problem representation** and a **new metric** (Mahalanobis)

  components are independent (only) in the new representation

  rotational invariant

- approximates the inverse Hessian on quadratic functions

  overwhelming empirical evidence, proof is in progress

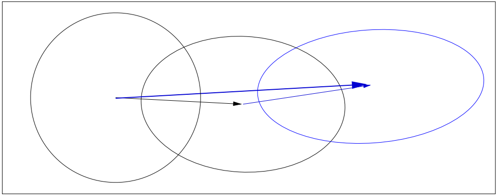
…cumulation, rank-μ

Cumulation

The Evolution Path

Evolution Path

Conceptually, the evolution path is the 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

$$\boldsymbol{p}_\mathrm{c} \propto \sum_{i=0}^{g} \underbrace{(1-c_\mathbf{c})^{g-i}}_{\substack{\text{exponentially}\\ \text{fading weights}}} \boldsymbol{y}_w^{(i)}$$

The recursive construction of the evolution path (cumulation):

$$\boldsymbol{p}_\mathrm{c} \quad \leftarrow \quad \underbrace{(1-c_\mathbf{c})}_{\text{decay factor}} \boldsymbol{p}_\mathrm{c} + \underbrace{\sqrt{1-(1-c_\mathbf{c})^2}\sqrt{\mu_w}}_{\text{normalization factor}} \underbrace{\boldsymbol{y}_w}_{\text{input} = \frac{\boldsymbol{m}-\boldsymbol{m}_\mathrm{old}}{\sigma}}$$

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

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

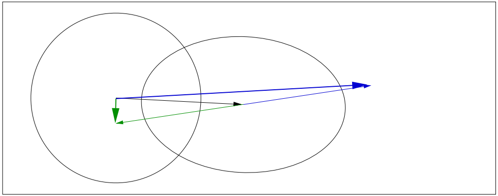
- *exponential smoothing* in time series, forecasting
- exponentially weighted *mooving average*
- *iterate averaging* in stochastic approximation
- *momentum* in the back-propagation algorithm for ANNs
- ...

... why?

Cumulation

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 is (re-)introduced by using the *evolution path*.

$$\boldsymbol{p}_{\mathrm{c}} \leftarrow \underbrace{(1 - c_{\mathbf{c}})}_{\text{decay factor}} \boldsymbol{p}_{\mathrm{c}} + \underbrace{\sqrt{1 - (1 - c_{\mathbf{c}})^2} \sqrt{\mu_w}}_{\text{normalization factor}} \boldsymbol{y}_w$$

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

where $\mu_w = \frac{1}{\sum {w_i}^2}$, $c_{\mathbf{c}} \ll 1$.

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** $\mathcal{O}(n^2)$ **to** $\mathcal{O}(n)$.[a]

[a] 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

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

... rank μ update

Rank-μ Update

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

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 matrix

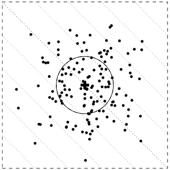
$$\mathbf{C}_\mu = \sum_{i=1}^{\mu} w_i\, \boldsymbol{y}_{i:\lambda} \boldsymbol{y}_{i:\lambda}^{\mathrm{T}}$$

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

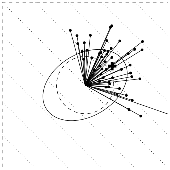
The rank-μ update then reads

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

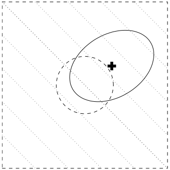
where $c_{\mathrm{cov}} \approx \mu_w / n^2$ and $c_{\mathrm{cov}} \leq 1$.



$\boldsymbol{x}_i = \boldsymbol{m} + \sigma\, \boldsymbol{y}_i, \quad \boldsymbol{y}_i \sim \mathcal{N}(\mathbf{0}, \mathbf{C})$



$$\mathbf{C}_\mu = \frac{1}{\mu} \sum \boldsymbol{y}_{i:\lambda} \boldsymbol{y}_{i:\lambda}^{\mathrm{T}}$$
$$\mathbf{C} \leftarrow (1-1) \times \mathbf{C} + 1 \times \mathbf{C}_\mu$$



$\boldsymbol{m}_{\text{new}} \leftarrow \boldsymbol{m} + \frac{1}{\mu} \sum \boldsymbol{y}_{i:\lambda}$

new distribution

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 $c_{\text{cov}} = 1$

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 $\mathcal{O}(n)$ [5]

  given $\mu_w \propto \lambda \propto n$

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

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

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...

[5] 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

Estimation of Distribution Algorithms

- Estimate a distribution that (re-)samples the parental population.
- All parameters of the distribution $\boldsymbol{\theta}$ are estimated from the given population.

Example: EMNA (Estimation of Multi-variate Normal Algorithm)

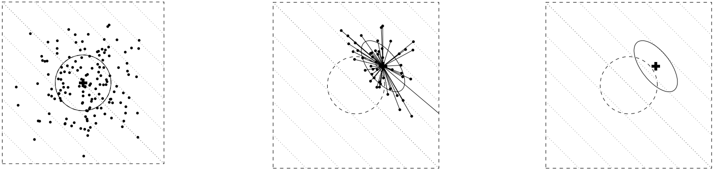
Initialize $\boldsymbol{m} \in \mathbb{R}^n$, and $\mathbf{C} = \mathbf{I}$

While not terminate

$$\begin{aligned} \boldsymbol{x}_i &= \boldsymbol{m} + \boldsymbol{y}_i, \qquad \boldsymbol{y}_i \sim \mathcal{N}_i(\mathbf{0}, \mathbf{C}), \qquad \text{for } i = 1, \ldots, \lambda \\ \boldsymbol{m} &\leftarrow \frac{1}{\mu} \sum_{i=1}^{\mu} \boldsymbol{x}_{i:\lambda} \\ \mathbf{C} &\leftarrow \sum_{i=1}^{\mu} (\boldsymbol{x}_{i:\lambda} - \boldsymbol{m})(\boldsymbol{x}_{i:\lambda} - \boldsymbol{m})^{\mathrm{T}} \end{aligned}$$

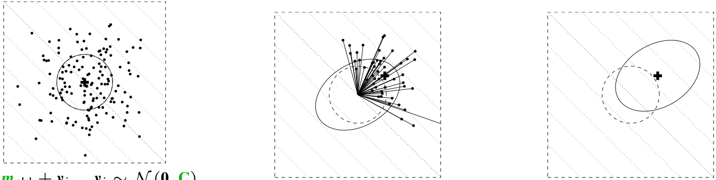
Larrañaga and Lozano 2002. *Estimation of Distribution Algorithms*

Estimation of Multivariate Normal Algorithm EMNA$_{\text{global}}$ versus rank-μ CMA[6]



$\boldsymbol{x}_i = \boldsymbol{m}_{\text{old}} + \boldsymbol{y}_i, \quad \boldsymbol{y}_i \sim \mathcal{N}(\boldsymbol{0}, \mathbf{C})$ $\qquad$ $\mathbf{C} \leftarrow \frac{1}{\mu} \sum (x_{i:\lambda} - \boldsymbol{m}_{\text{new}})(x_{i:\lambda} - \boldsymbol{m}_{\text{new}})^{\mathrm{T}}$ $\qquad$ $\boldsymbol{m}_{\text{new}} = \boldsymbol{m}_{\text{old}} + \frac{1}{\mu} \sum \boldsymbol{y}_{i:\lambda}$

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



$\boldsymbol{x}_i = \boldsymbol{m}_{\text{old}} + \boldsymbol{y}_i, \quad \boldsymbol{y}_i \sim \mathcal{N}(\boldsymbol{0}, \mathbf{C})$ $\qquad$ $\mathbf{C} \leftarrow \frac{1}{\mu} \sum (x_{i:\lambda} - \boldsymbol{m}_{\text{old}})(x_{i:\lambda} - \boldsymbol{m}_{\text{old}})^{\mathrm{T}}$ $\qquad$ $\boldsymbol{m}_{\text{new}} = \boldsymbol{m}_{\text{old}} + \frac{1}{\mu} \sum \boldsymbol{y}_{i:\lambda}$

rank-μ CMA conducts a PCA **of steps**

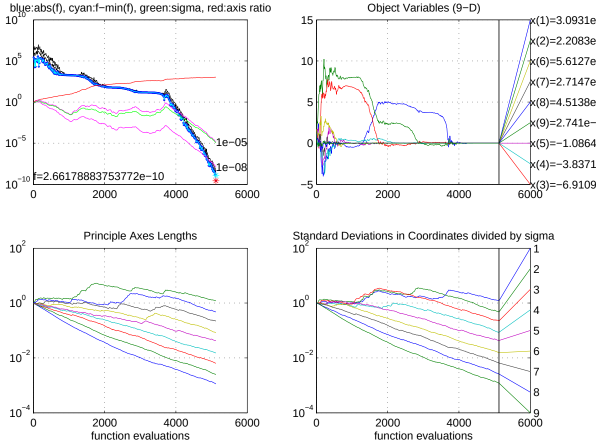
sampling of $\lambda = 150$ solutions (dots) $\qquad$ calculating $\mathbf{C}$ from $\mu = 50$ solutions $\qquad$ new distribution

The CMA-update yields a larger variance in particular in gradient direction, because $\boldsymbol{m}_{\text{new}}$ is the minimizer for the variances when calculating $\mathbf{C}$

[6] 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

Experimentum Crucis (1)

f convex quadratic, separable

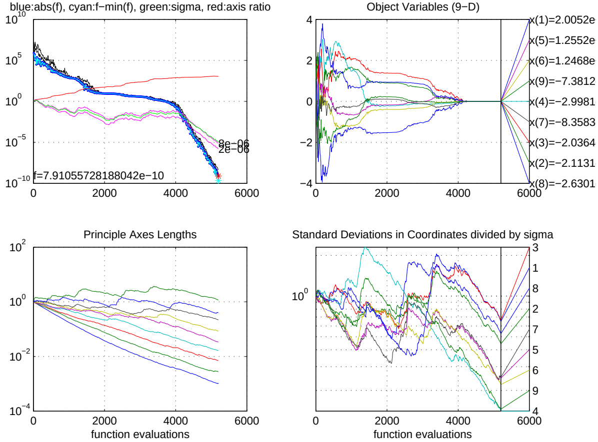


$$f(\boldsymbol{x}) = \sum_{i=1}^{n} 10^{\alpha \frac{i-1}{n-1}} x_i^2, \alpha = 6$$

. . . non-separable

Experimentum Crucis (2)

f convex quadratic, as before but non-separable (rotated)



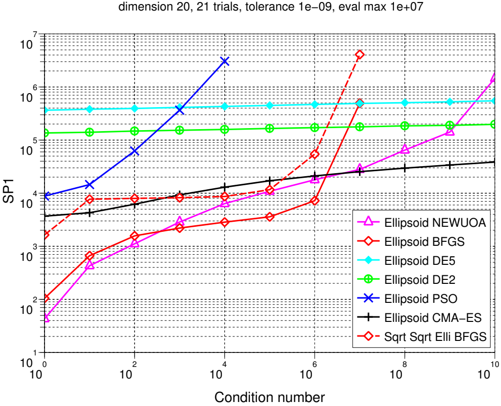
$\mathbf{C} \propto \boldsymbol{H}^{-1}$ **for all** $g, \mathbf{H}$

$f(\boldsymbol{x}) = g\left(\boldsymbol{x}^{\mathrm{T}}\mathbf{H}\boldsymbol{x}\right)$, $g : \mathbb{R} \to \mathbb{R}$ stricly monotonic

...internal parameters

Comparison to BFGS, NEWUOA, PSO and DE

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



BFGS (Broyden et al 1970)
NEWUAO (Powell 2004)
DE (Storn & Price 1996)
DE (Storn & Price 1996)
PSO (Kennedy & Eberhart 1995)

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

g identity (BFGS, *red*) or
$g(.) = (.)^{1/4}$ (BFGS, *red dashed*) or

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

SP1 = average number of objective function evaluations to reach the target function value of 10^{-9}

...CEC 2005

Three Main Features of Evolution Strategies

1. **Rank-based selection**: same performance on $g(f(\boldsymbol{x}))$ for any g

   $g : \mathbb{R} \to \mathbb{R}$ stricly monotonic (order preserving)

2. **Step-size control**: converge log-linearly on the sphere function and many others

3. **Covariance matrix adaptation**: reduce any convex quadratic function

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

   to the sphere function

   $$f(\boldsymbol{x}) = \boldsymbol{x}^{\mathrm{T}}\boldsymbol{x}$$

   without use of derivatives

   lines of equal density align with lines of equal fitness $\mathbf{C} \propto \boldsymbol{H}^{-1}$

Source code for CMA-ES in C, Java, Matlab, Octave, Scilab, Python is available at
`http://www.lri.fr/~hansen/cmaes_inmatlab.html`