

Tutorial—Evolution Strategies and Related Estimation of Distribution Algorithms

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Content

- 1 Problem Statement
 - Black Box Optimization and Its Difficulties
 - Non-Separable Problems
 - Ill-Conditioned Problems
- 2 Evolution Strategies and EDAs
 - A Search Template
 - The Normal Distribution
 - Invariance
- 3 Step-Size Control
 - Why Step-Size Control
 - One-Fifth Success Rule
 - Self-Adaptation
 - Path Length Control (CSA)
- 4 Covariance Matrix Adaptation
 - Covariance Matrix Rank-One Update
 - Cumulation—the Evolution Path
 - Covariance Matrix Rank- μ Update
 - Estimation of Distribution
- 5 Experiments
- 6 Summary

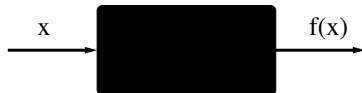
Problem Statement

Continuous Domain Search/Optimization

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

$$f : \mathcal{X} \subseteq \mathbb{R}^n \rightarrow \mathbb{R}, \quad \mathbf{x} \mapsto f(\mathbf{x})$$

- **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 x with **small function value** with **least search cost**

... or to a robust solution x

there are two conflicting objectives

- Typical Examples

- shape optimization (e.g. using CFD)
- model calibration
- parameter calibration

curve fitting, airfoils
biological, physical
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	↔	candidate solution decision variables design variables object variables
population	↔	set of candidate solutions
fitness function	↔	objective function loss function cost function
generation	↔	iteration

...function properties

Objective Function Properties

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

Additionally, f can be

- multimodal

there are eventually many local optima

- non-smooth

derivatives do not exist

- discontinuous

- ill-conditioned

- noisy

- ...

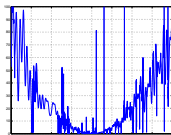
Goal : cope with any of these function properties

they are related to real-world problems

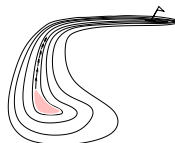
What Makes a Function Difficult to Solve?

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.

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

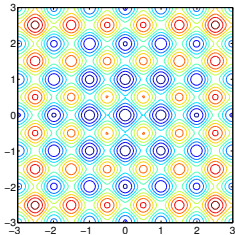
$$\arg \min_{(x_1, \dots, x_n)} f(x_1, \dots, x_n) = \left(\arg \min_{x_1} f(x_1, \dots), \dots, \arg \min_{x_n} f(\dots, x_n) \right)$$

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

Example: Additively decomposable functions

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

Rastrigin function



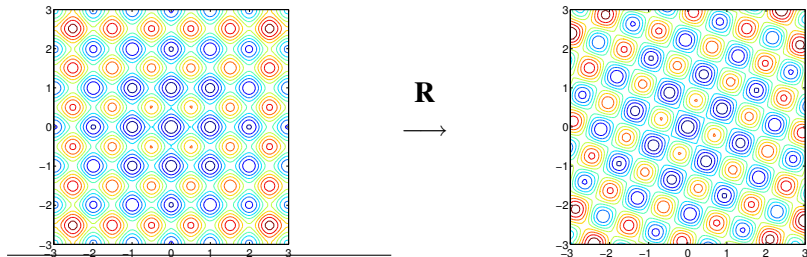
Non-Separable Problems

Building a non-separable problem from a separable one

Rotating the coordinate system

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

\mathbf{R} rotation matrix



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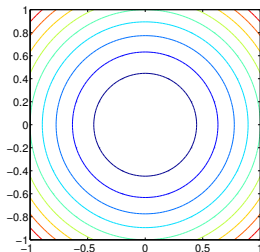
¹ Hansen, Ostermeier, Gawelczyk (1995). On the adaptation of arbitrary normal mutation distributions in evolution strategies: The generating set adaptation. Sixth ICGA, pp. 57-64, Morgan Kaufmann

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

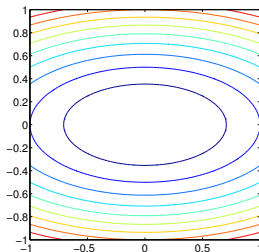
III-Conditioned Problems

If f is quadratic, $f : x \mapsto x^T H x$, ill-conditioned means a high condition number of Hessian Matrix H

ill-conditioned means “**squeezed**” lines of equal function value



Increased
 →
 condition
 number



consider the curvature of iso-fitness lines

What Makes a Function Difficult to Solve?

... and what can be done

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

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Stochastic Search

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

Initialize distribution parameters θ , set population size $\lambda \in \mathbb{N}$

While not terminate

- ① **Sample distribution** $P(x|\theta) \rightarrow x_1, \dots, x_\lambda \in \mathbb{R}^n$
- ② **Evaluate** x_1, \dots, x_λ on f
- ③ **Update parameters** $\theta \leftarrow F_\theta(\theta, x_1, \dots, x_\lambda, f(x_1), \dots, f(x_\lambda))$

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 and Normal Estimation of Distribution Algorithms

New search points are sampled normally distributed

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

as perturbations of \mathbf{m}

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

where

- the **mean** vector $\mathbf{m} \in \mathbb{R}^n$ 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

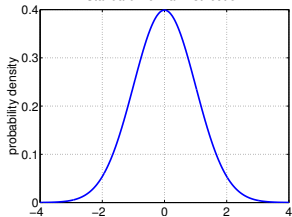
here, all new points are sampled with the same parameters

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

Normal Distribution

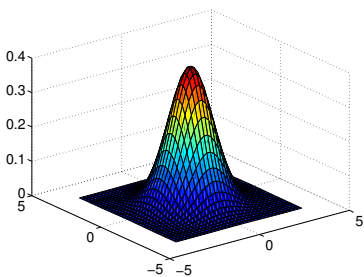
Isotropic Case

Standard Normal Distribution

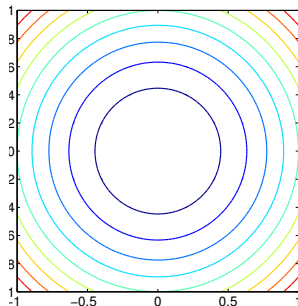


probability density of 1-D standard normal distribution

2-D Normal Distribution



2-D

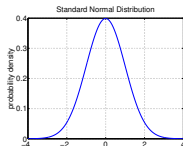


The Multi-Variate (n -Dimensional) Normal Distribution

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

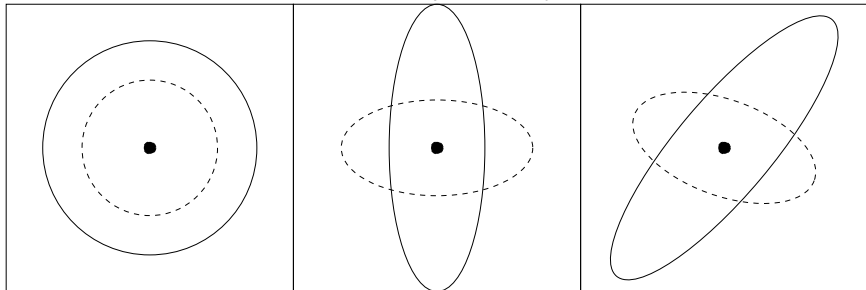
The **mean** value \mathbf{m}

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



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 $\{\mathbf{x} \in \mathbb{R}^n \mid \mathbf{x}^T \mathbf{C}^{-1} \mathbf{x} = 1\}$

Lines of Equal Density



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

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

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

Evolution Strategies

$(\mu \dagger \lambda)$ μ : # parents, λ : # offspring

+ selection in $\{\text{parents}\} \cup \{\text{offspring}\}$

, selection in $\{\text{offspring}\}$

$(1 + 1)$ -ES

Sample one offspring from parent m

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

If \mathbf{x} better than m select

$$m \leftarrow \mathbf{x}$$

... why?

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

Non-elitist selection and intermediate (weighted) recombination

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

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

The new mean reads

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

where

$$w_1 \geq \dots \geq w_{\mu} > 0, \quad \sum_{i=1}^{\mu} w_i = 1$$

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

Invariance

Motivation

- 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

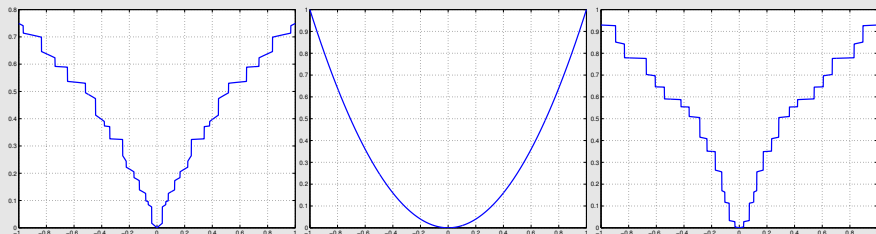
Invariance Under Strictly Monotonically Increasing Functions

Rank-based algorithms

Selection based on the rank:

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

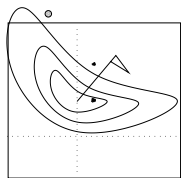
Update of all parameters uses only the rank



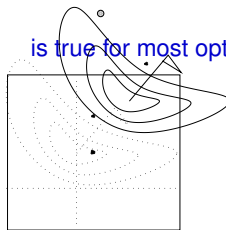
$$g(f(x_{1:\lambda})) \leq g(f(x_{2:\lambda})) \leq \dots \leq g(f(x_{\lambda:\lambda}))$$

Basic Invariance in Search Space

- translation invariance



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



is true for most optimization algorithms

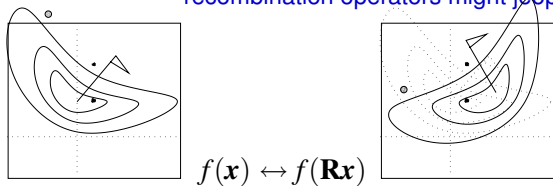
Identical behavior on f and f_a

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

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 $\mathbf{R}\mathbf{R}^T = \mathbf{I}$
 e.g. true for simple evolution strategies
 recombination operators might jeopardize rotational invariance



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

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

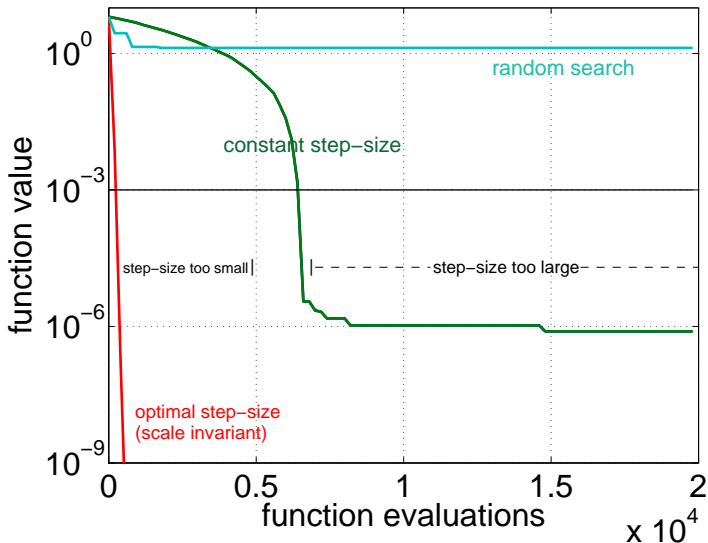
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3

³Salomon (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

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 - **One-Fifth Success Rule**
 - **Self-Adaptation**
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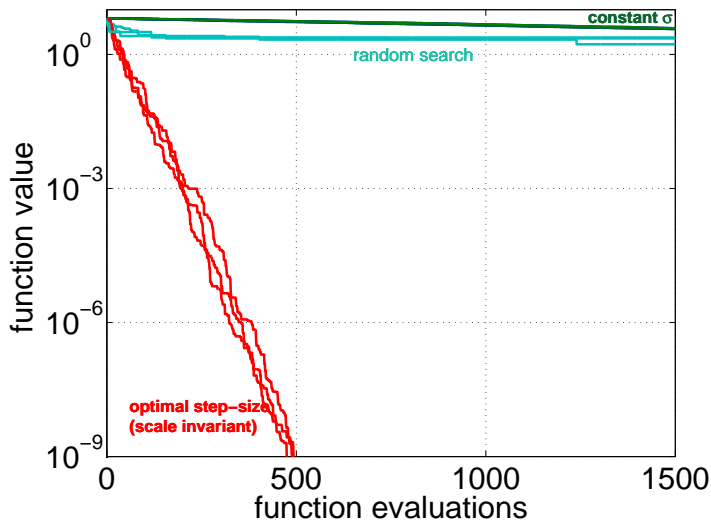
Why Step-Size Control?



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

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

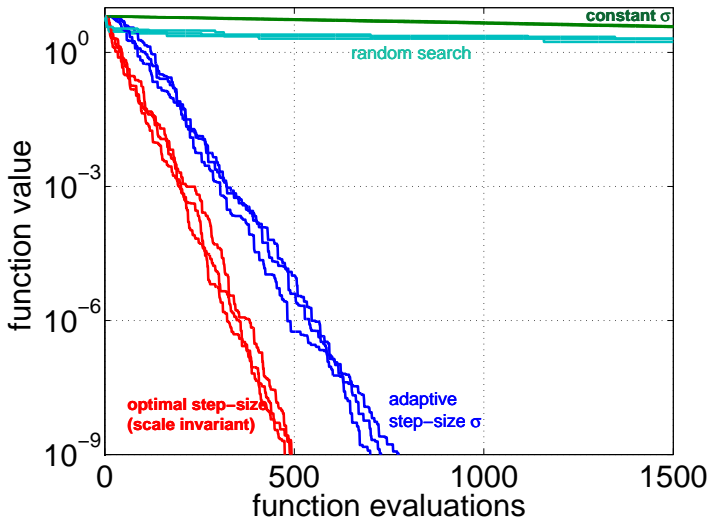
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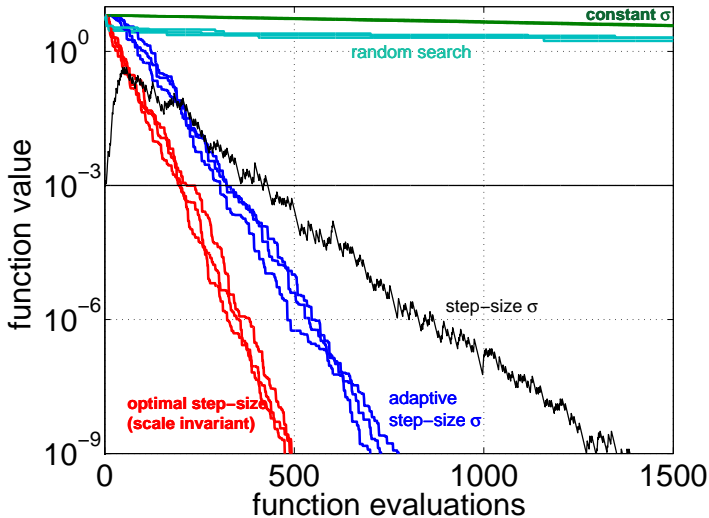
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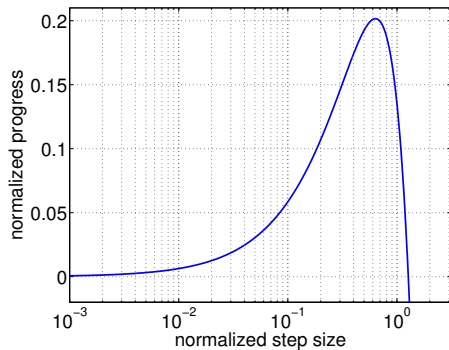
Why Step-Size Control?



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

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

Why Step-Size Control?



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^{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 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

^aRechenberg 1973, *Evolutionstrategie, Optimierung technischer Systeme nach Prinzipien der biologischen Evolution*,
Frommann-Holzboog

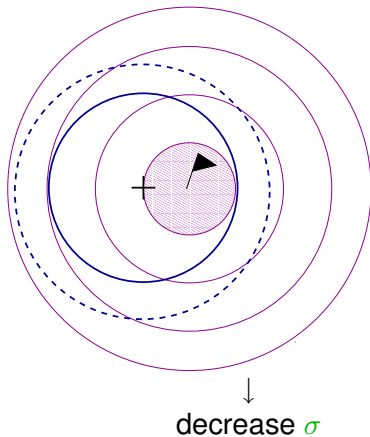
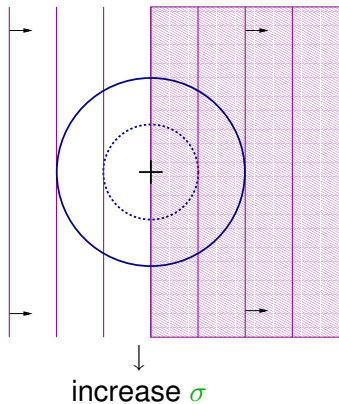
^bSchumer and Steiglitz 1968. Adaptive step size random search. *IEEE TAC*

^cSchwefel 1981, *Numerical Optimization of Computer Models*, Wiley

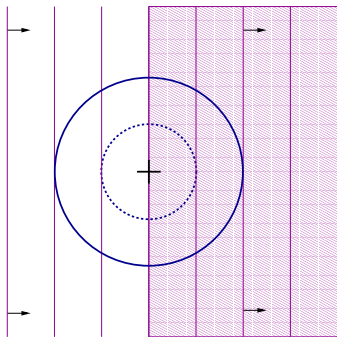
^dHansen & Ostermeier 2001, Completely Derandomized Self-Adaptation in Evolution Strategies, *Evol. Comput.* 9(2)

^eOstermeier *et al* 1994. Step-size adaptation based on non-local use of selection information. *PPSN IV*

One-fifth success rule

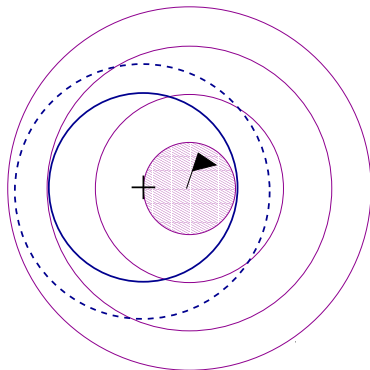


One-fifth success rule



Proba of success (p_s)

$1/2$



Proba of success (p_s)

“too small”

One-fifth success rule

Let p_s : # of successful offspring / 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

$$p_{\text{target}} = 1/5$$

IF *offspring better parent*

$$p_s = 1$$

ELSE

$$p_s = 0$$

Self-adaptation

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

MUTATE for $i = 1, \dots, \lambda$

step-size

parent

$$\sigma_i \leftarrow \sigma \exp(\tau N(0, 1))$$

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

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)

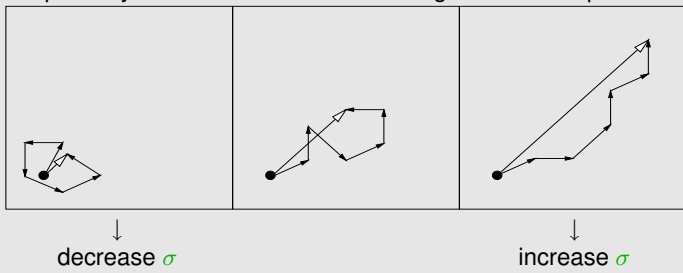
The Concept

$$x_i = m + \sigma y_i$$

$$m \leftarrow m + \sigma y_w$$

Measure the length of the *evolution path*

the pathway of the mean vector m in the generation sequence



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

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

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

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

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Evolution Strategies and Normal Estimation of Distribution Algorithms

New search points are sampled normally distributed

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

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

where

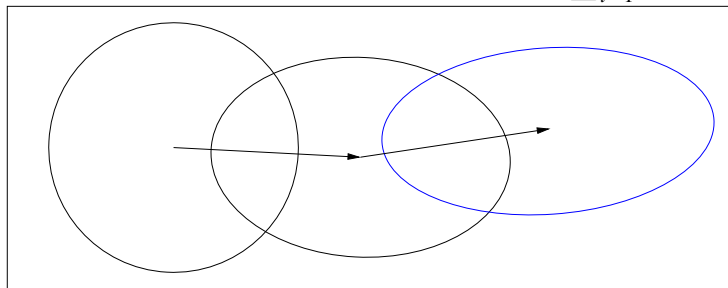
- the **mean** vector $\mathbf{m} \in \mathbb{R}^n$ represents the favorite solution
- the so-called **step-size** $\sigma \in \mathbb{R}_+$ controls the *step length*
- the **covariance matrix** $\mathbf{C} \in \mathbb{R}^{n \times n}$ determines the **shape** of the distribution ellipsoid

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

Covariance Matrix Adaptation

Rank-One Update

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



new distribution,

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

the ruling principle: the adaptation increases the probability of successful steps, \mathbf{y}_w , to appear again

... equations

Covariance Matrix Adaptation

Rank-One Update

Initialize $\mathbf{m} \in \mathbb{R}^n$, and $\mathbf{C} = \mathbf{I}$, set $\sigma = 1$, learning rate $c_{\text{cov}} \approx 2/n^2$

While not terminate

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

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

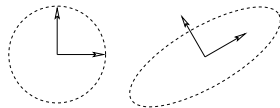
$$\mathbf{C} \leftarrow (1 - c_{\text{cov}})\mathbf{C} + c_{\text{cov}} \underbrace{\mu_w \mathbf{y}_w \mathbf{y}_w^T}_{\text{rank-one}} \quad \text{where } \mu_w = \frac{1}{\sum_{i=1}^{\mu} w_i^2} \geq 1$$

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

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 \mathbf{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** 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

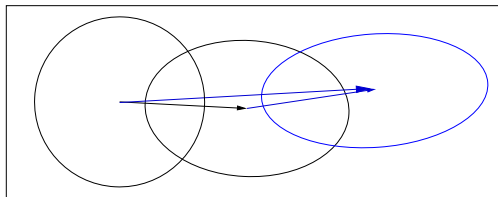
- 1 Problem Statement
- 2 Evolution Strategies and EDAs
- 3 Step-Size Control
- 4 Covariance Matrix Adaptation**
 - Covariance Matrix Rank-One Update
 - Cumulation—the Evolution Path
 - Covariance Matrix Rank- μ Update
 - Estimation of Distribution
- 5 Experiments
- 6 Summary

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 m .



An exponentially weighted sum of steps y_w is used

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

The recursive construction of the evolution path (cumulation):

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

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

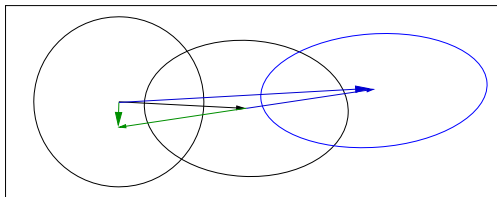
- *exponential smoothing* in time series, forecasting
- exponentially weighted *moving average*
- *iterate averaging* in stochastic approximation
- *momentum* in the back-propagation algorithm for ANNs
- ...

...why?

Cumulation

Utilizing the Evolution Path

We used $\mathbf{y}_w \mathbf{y}_w^T$ for updating \mathbf{C} . Because $\mathbf{y}_w \mathbf{y}_w^T = -\mathbf{y}_w (-\mathbf{y}_w)^T$ the sign of \mathbf{y}_w is neglected. The sign information is (re-)introduced by using the *evolution path*.



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

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

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

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

^aHansen, 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

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

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 matrix

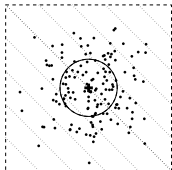
$$\mathbf{C}_{\mu} = \sum_{i=1}^{\mu} w_i \mathbf{y}_{i:\lambda} \mathbf{y}_{i:\lambda}^T$$

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

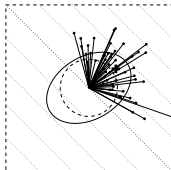
The rank- μ update then reads

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

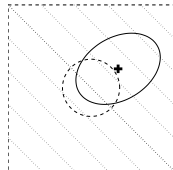
where $c_{\text{cov}} \approx \mu_w/n^2$ and $c_{\text{cov}} \leq 1$.



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



$$\begin{aligned} \mathbf{C}_\mu &= \frac{1}{\mu} \sum y_{i:\lambda} y_{i:\lambda}^T \\ \mathbf{C} &\leftarrow \frac{1}{(1-\lambda)} \mathbf{C} + \lambda \mathbf{C}_\mu \end{aligned}$$



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

new distribution

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

calculating \mathbf{C} where
 $\mu = 50$,
 $w_1 = \dots = w_\mu = \frac{1}{\mu}$,
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 $\mathcal{O}(n)$ ⁴
given $\mu_w \propto \lambda \propto n$

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

say $\lambda \geq 3n + 10$

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...

⁴Hansen, 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

- 1 Problem Statement
- 2 Evolution Strategies and EDAs
- 3 Step-Size Control
- 4 Covariance Matrix Adaptation**
 - Covariance Matrix Rank-One Update
 - Cumulation—the Evolution Path
 - Covariance Matrix Rank- μ Update
 - Estimation of Distribution
- 5 Experiments
- 6 Summary

Estimation of Distribution Algorithms

- Estimate a distribution that (re-)samples the parental population.
- All parameters of the distribution θ are estimated from the given population.

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

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

While not terminate

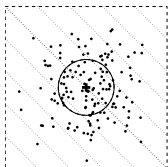
$$\mathbf{x}_i = \mathbf{m} + \mathbf{y}_i, \quad \mathbf{y}_i \sim \mathcal{N}_i(\mathbf{0}, \mathbf{C}), \quad \text{for } i = 1, \dots, \lambda$$

$$\mathbf{C} \leftarrow \sum_{i=1}^{\mu} (\mathbf{x}_{i:\lambda} - \mathbf{m})(\mathbf{x}_{i:\lambda} - \mathbf{m})^T$$

$$\mathbf{m} \leftarrow \sum_{i=1}^{\mu} \mathbf{x}_{i:\lambda}$$

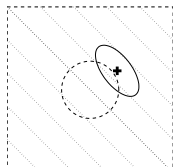
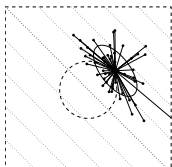
Larrañaga and Lozano 2002. *Estimation of Distribution Algorithms*

Estimation of Multivariate Normal Algorithm EMNA_{global} versus rank- μ CMA⁵



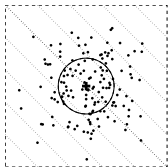
$$x_i = m_{\text{old}} + y_i, \quad y_i \sim \mathcal{N}(0, \mathbf{C})$$

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



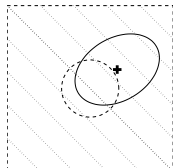
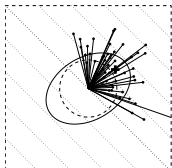
$$m_{\text{new}} = m_{\text{old}} + \frac{1}{\mu} \sum y_{i:\lambda}$$

EMNA_{global}
conducts a
PCA of
points



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

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



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

rank- μ CMA
conducts a
PCA of
steps

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

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

new distribution

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

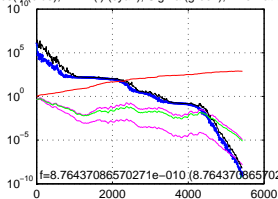
⁵ Hansen, N. (2006). The CMA Evolution Strategy: A Comparing Review. In J.A. Lozano, P. Larranga, I. Inza and E. Bengoetxea (Eds.). Towards a new evolutionary computation. Advances in estimation of distribution algorithms. pp. 75-102

- 1 Problem Statement
- 2 Evolution Strategies and EDAs
- 3 Step-Size Control
- 4 Covariance Matrix Adaptation
- 5 Experiments**
- 6 Summary

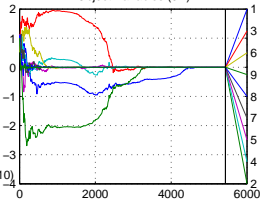
Experimentum Crucis (1)

f convex quadratic, separable

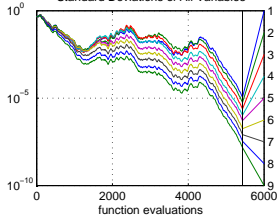
abs(f_0) (blue), $f - \min(f)$ (cyan), Sigma (green), Axis Ratio (red)



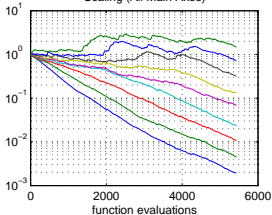
Object Variables (9D)



Standard Deviations of All Variables



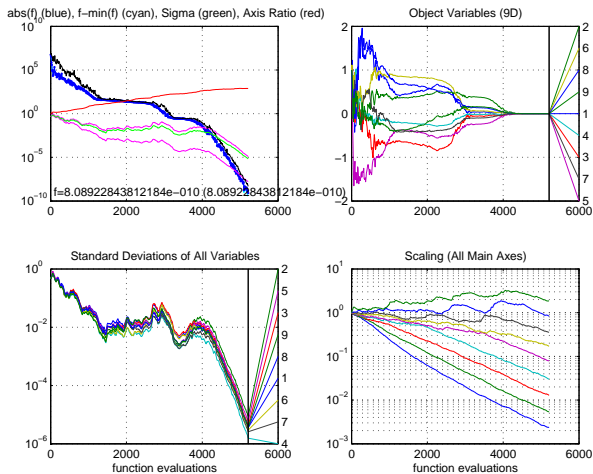
Scaling (All Main Axes)



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

Experimentum Crucis (2)

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



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

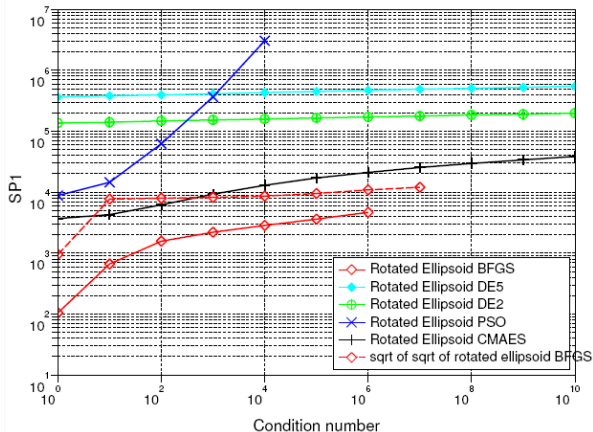
$$f(\mathbf{x}) = g(\mathbf{x}^T \mathbf{H} \mathbf{x}), \quad g : \mathbb{R} \rightarrow \mathbb{R} \text{ strictly monotonic}$$

... internal parameters

Comparison to BFGS, PSO and DE

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

Ellipsoid dimension 20, 21 trials, tolerance $1e-09$, eval max $1e+07$



$f(\mathbf{x}) = g(\mathbf{x}^T \mathbf{H} \mathbf{x})$ with
 g identity (BFGS, red) or
 $g(\cdot) = (\cdot)^{1/4}$ (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}

... population size, invariance

CEC 2005

Comparison of 11 Evolutionary Algorithms

- Task: black-box optimization of **25 benchmark functions** and submission of results to the *Congress of Evolutionary Computation*
- **Performance measure:** cost (number of function evaluations) to reach the target function value, where the maximum number of

function evaluations was $FE_{\max} = \begin{cases} 10^5 & \text{for } n = 10 \\ 3 \times 10^5 & \text{for } n = 30 \end{cases}$

Remark: the setting of FE_{\max} has a remarkable influence on the results, if the target function value can be reached only for a (slightly) larger number of function evaluations with a high probability.

Where $FES \geq FE_{\max}$ the result must be taken with great care.

- **The competitors** included Differential Evolution (DE), Particle Swarm Optimization (PSO), real-coded GAs, Estimation of Distribution Algorithm (EDA), and hybrid methods combined e.g. with quasi-Newton BFGS.

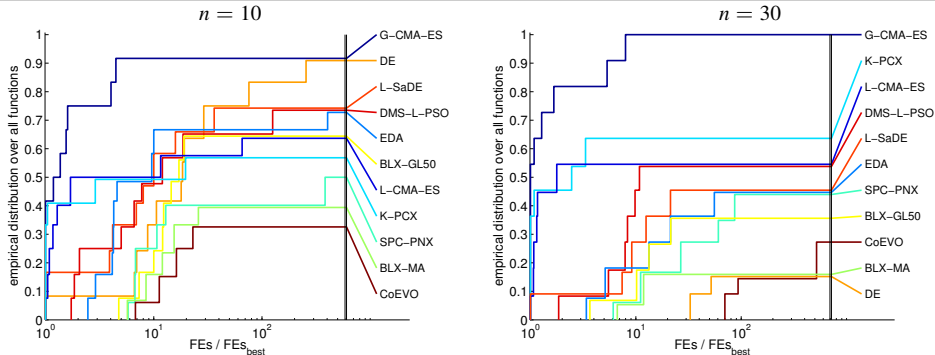
References to Algorithms

BLX-GL50	García-Martínez and Lozano (Hybrid Real-Coded...)
BLX-MA	Molina et al. (Adaptive Local Search...)
CoEVO	Pošík (Real-Parameter Optimization...)
DE	Rönkkönen et al. (Real-Parameter Optimization...)
DMS-L-PSO	Liang and Suganthan (Dynamic Multi-Swarm...)
EDA	Yuan and Gallagher (Experimental Results...)
G-CMA-ES	Auger and Hansen (A Restart CMA...)
K-PCX	Sinha et al. (A Population-Based,...)
L-CMA-ES	Auger and Hansen (Performance Evaluation...)
L-SaDE	Qin and Suganthan (Self-Adaptive Differential...)
SPC-PNX	Ballester et al. (Real-Parameter Optimization...)

In: CEC 2005 IEEE Congress on Evolutionary Computation, Proceedings

Summarized Results

Empirical Distribution of Normalized Success Performance



$FEs = \text{mean}(\#fevals) \times \frac{\#all\ runs\ (25)}{\#successful\ runs}$, where $\#fevals$ includes only successful runs.

Shown: **empirical distribution function** of the Success Performance FEs divided by FEs of the best algorithm on the respective function.

Results of all functions are used where at least one algorithm was successful at least once, i.e. where the target function value was reached in at least one experiment (out of 11×25 experiments).

Small values for FEs and therefore large (cumulative frequency) values in the graphs are preferable.

- 1 Problem Statement
- 2 Evolution Strategies and EDAs
- 3 Step-Size Control
- 4 Covariance Matrix Adaptation
- 5 Experiments
- 6 Summary**

Summary

The Problem	The Approach in ESs
Ruggedness	<p>non-local policy, large sampling width (step-size) as large as possible while preserving a reasonable convergence speed</p> <p>stochastic, non-elitistic, population-based method recombination operator serves as repair mechanism</p>
Dimensionality, Non-Separability	exploiting the problem structure, learn correlations (CMA)
Ill-conditioning	change the metric — CMA

Main Features of Evolution Strategies

- ① Rank-based selection: same performance on $g(f(\mathbf{x}))$ for any g
 $g : \mathbb{R} \rightarrow \mathbb{R}$ strictly monotonic (order preserving)

- ② Step-size control: converge log-linearly on the sphere

- ③ Covariance matrix adaptation: reduce any convex quadratic function

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

to the sphere model

$$f(\mathbf{x}) = \mathbf{x}^T \mathbf{x}$$

lines of equal density align with lines of equal fitness $\mathbf{C} \propto \mathbf{H}^{-1}$
 without use of derivatives