

Dynamic Problem Encoding for Optimization

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Anne Auger
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Marc Schoenauer
Olivier Teytaud

*Einstein once spoke of the “unreasonable effectiveness of mathematics” in describing how the natural world works. Whether one is talking about basic physics, about the increasingly important environmental sciences, or the transmission of disease, **mathematics is never any more, or any less, than a way of thinking clearly.** As such, it always has been and always will be a valuable tool, but only valuable when it is part of a larger arsenal embracing analytic experiments and, above all, wide-ranging imagination.*

Lord Kay

Problem Statement: Search

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 and Objectives

Continuous Domain Search/Optimization

● Goal

- ▶ fast convergence toward 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)
 - ▶ parameter calibration
 - ▶ model calibration
- curve fitting, airfoils
controller, plants, images
biological, physical

● Difficulties

- ▶ exhaustive search is infeasible
- ▶ deterministic search is often not successful
- ▶ (naive) random search takes too long

Approach: stochastic search, Evolutionary Algorithms

Problem Formulation

A real world problem requires

- a representation; the encoding of problem parameters into $\mathbf{x} \in \mathcal{X} \subset \mathbb{R}^n$
- the definition of a objective function $f : \mathbf{x} \mapsto f(\mathbf{x})$ to be minimized

One might distinguish two approaches

Natural Encoding

Use a “natural” encoding and **design the optimizer** with respect to the problem e.g. use of specific “genetic operators”

frequently done in discrete domain

Concerned Encoding (Pure Black Box)

Use problem specific knowledge for encoding and use a “**generic**” optimizer

frequently done in continuous domain

Advantage: Sophisticated and well-validated optimizers can be used

How about *Adaptive Encoding*?

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

- ...

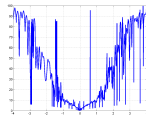
Goal : cope with any of these function properties

they are related to real-world problems

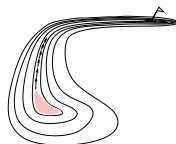
What Makes a Function Difficult to Solve?

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 5-D solvable example



a narrow ridge

How Can a Difficult Function Be Solved?

... therefore ...

The Problem	What can be done
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>

Stochastic Search

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

Initialize distribution parameters θ , set sample 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*

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

The Evolution Strategy

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 $\theta \leftarrow F_\theta(\theta, x_1, \dots, x_\lambda, f(x_1), \dots, f(x_\lambda))$

- P is a **multi-variate normal** distribution

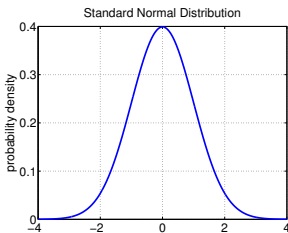
$$\mathcal{N}(\mathbf{m}_i, \sigma_i^2 \mathbf{C}_i) \sim \boxed{\mathbf{m}_i + \sigma_i \mathcal{N}(\mathbf{0}, \mathbf{C}_i)} \quad \text{for } i = 1, \dots, \lambda$$

- $\theta = \{\mathbf{m}_i, \mathbf{C}_i, \sigma_i\}_{i=1, \dots, \lambda} \in (\mathbb{R}^n \times \mathbb{R}^{n \times n} \times \mathbb{R}_+)^{\lambda}$
- $F_\theta = F_\theta(\theta, \mathbf{x}_{1:\lambda}, \dots, \mathbf{x}_{\mu:\lambda})$, where $\mu \leq \lambda$ and $\mathbf{x}_{i:\lambda}$ is the i -th best of the λ points

Why Normal Distributions?

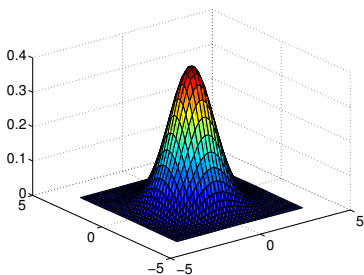
- ① widely observed in nature, for example as phenotypic traits
- ② only stable distribution with finite variance
 - stable means the *sum* of normal variates is also normal,
helpful in **design and analysis** of algorithms
- ③ most convenient way to generate **isotropic** search points
 - the isotropic 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

Normal Distribution



probability density of 1-D standard normal distribution

2-D Normal Distribution



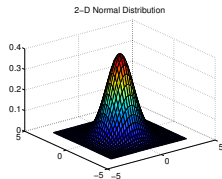
probability density of 2-D normal distribution

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} .

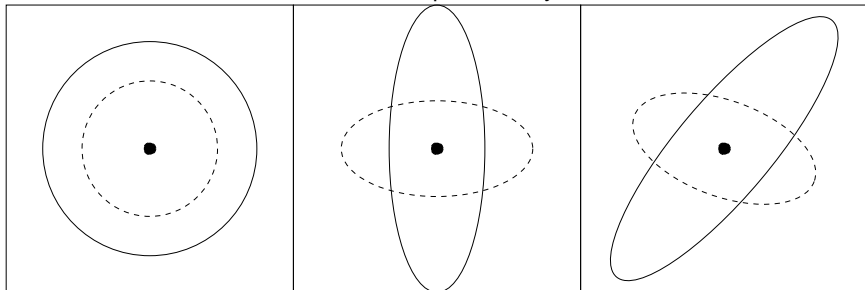
The **mean** value \mathbf{m}

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



The **covariance matrix** $\mathbf{C} \dots$

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

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

Sampling New Search Points

The governing equation for derandomized Evolution Strategies

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

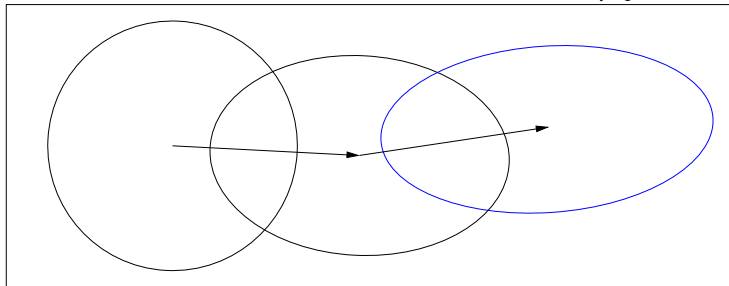
- the **mean** vector $\mathbf{m} \in \mathbb{R}^n$ represents the favorite solution
- the so-called **step-size** $\sigma \in \mathbb{R}_+$ controls the *step length*
- the **covariance matrix** $\mathbf{C} \in \mathbb{R}^{n \times n}$ determines the **shape** of the distribution ellipsoid

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

Covariance Matrix Adaptation

Rank-One Update

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



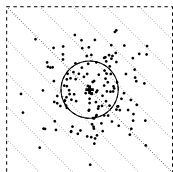
new distribution,

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

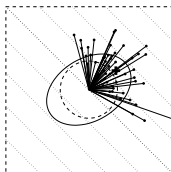
the ruling principle: the adaptation increases the probability of successful steps, \mathbf{y}_w , to appear again

Rank- μ Update

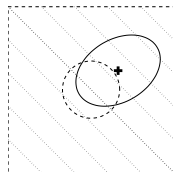
$$\begin{aligned}
 \mathbf{x}_i &= \mathbf{m} + \sigma \mathbf{y}_i, & \mathbf{y}_i &\sim \mathcal{N}_i(\mathbf{0}, \mathbf{C}), \\
 \mathbf{m} &\leftarrow \mathbf{m} + \sigma \mathbf{y}_w, & \mathbf{y}_w &= \sum_{i=1}^{\mu} w_i \mathbf{y}_{i:\lambda}
 \end{aligned}$$



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



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



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

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

calculating \mathbf{C} from
 $\mu = 50$ points,
 $w_1 = \dots = w_\mu = \frac{1}{\mu}$

new distribution

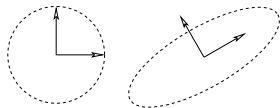
Remark: the old (sample) distribution shape has a great influence on the new distribution \rightarrow iterations needed

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

covariance matrix adaptation in the evolution strategy

- 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



- approximates the inverse Hessian on quadratic functions
overwhelming empirical evidence, proof is in progress

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

covariance matrix adaptation

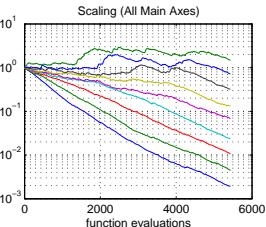
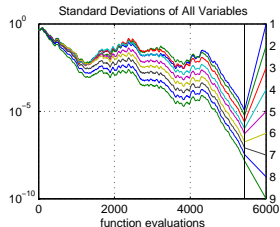
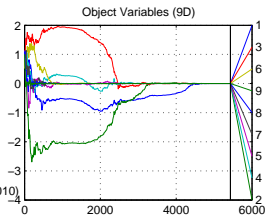
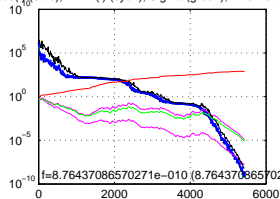
- is equivalent with an adaptive (general) linear encoding¹

¹Hansen 2000, Invariance, Self-Adaptation and Correlated Mutations in Evolution Strategies, PPSN VI

Experimentum Crucis (1)

f convex quadratic, separable

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

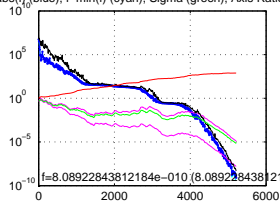


$$f(\mathbf{x}) = \sum_{i=1}^n 10^{\alpha \frac{i-1}{n-1}} x_i^2, \alpha = 6$$

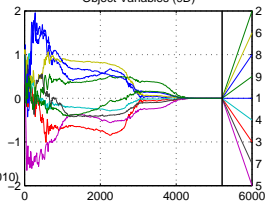
Experimentum Crucis (2)

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

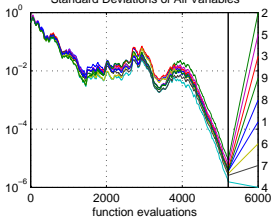
abs(f_0) (blue), f -min(f) (cyan), Sigma (green), Axis Ratio (red)



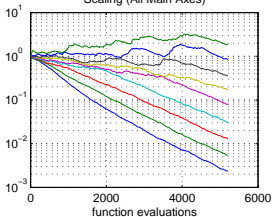
Object Variables (9D)



Standard Deviations of All Variables



Scaling (All Main Axes)



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

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

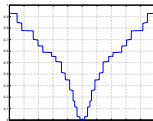
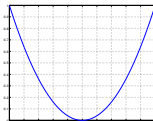
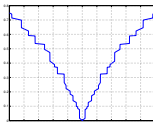
Invariance

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

Invariance is a *guaranty for generalization* of performance from a single function to a class of functions. Most important invariance properties of the Covariance Matrix Adaptation (CMA) Evolution Strategy (ES) are

- invariance to **order preserving transformations** in function space \longrightarrow
- Translation and **rotation invariance** in search space
to rigid transformations of the search space

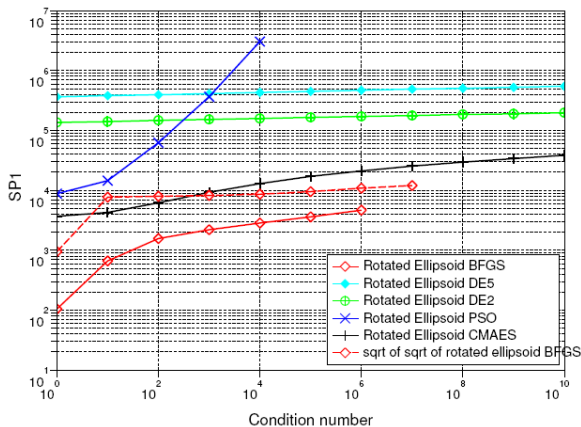


... empirical validation

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 $1e+07$



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

$f(x) = g(x^T \mathbf{H}x)$ with
 g identity (BFGS, red) or
 $g(\cdot) = (\cdot)^{1/4}$ (BFGS, red dashed) or
 g order-preserving = strictly increasing (all other)

BFGS: quasi-Newton method

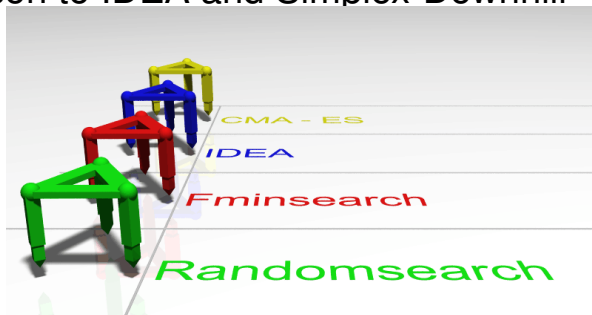
PSO: Particle Swarm Optimization

DE: Differential Evolution

CMA-ES —

... population size, invariance

Comparison to IDEA and Simplex-Downhill



CMA-ES: Covariance Matrix Adaptation Evolution Strategy²

IDEA: Iterated Density-Estimation Evolutionary Algorithm³

Fminsearch: Nelder-Mead simplex downhill method⁴

Randomsearch: pure Monte-Carlo sampling

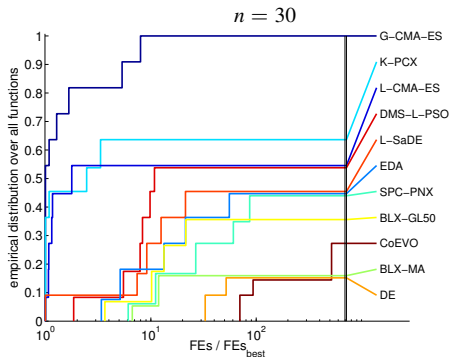
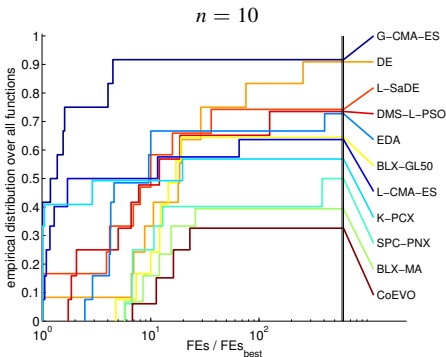
Peter Dürri and Andreas Pfister 2004. Optimization of Walking Gaits for a Three Legged Walking Robot,
Diploma Thesis, Institut für Mechanische Systeme, ETH Zurich

²Hansen (2001) Completely Derandomized Self-Adaptation in Evolution Strategies. *Evolutionary Computation Journal*

³Hansen, (2002) Evolutionary Algorithms for the Black-Box Optimization of Functions of Continuous Parameters. *Evolutionary Computation*

CEC 2005 Real Parameter Optimization Session

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

The Covariance Matrix Adaptation Evolution Strategy

In a Nutshell

- ① Multivariate normal distribution to generate new search points
follows the maximum entropy principle
- ② Selection only based on the ranking of the f -values, weighted recombination
using only the ranking of f -values preserves invariance
- ③ *Covariance matrix adaptation (CMA)* **increases the probability** to repeat **successful steps**
learning all pairwise dependencies
⇒ conducts an incremental PCA
⇒ new (rotated) problem representation
- ④ An **evolution path** (a trajectory) is exploited in two places
 - ▶ enhances the covariance matrix (rank-one) adaptation
yields sometimes linear time complexity
 - ▶ controls the **step-size** (step length)
aims at conjugate perpendicularity

Linear Encoding and the Covariance Matrix

Equivalence between change in encoding and transformation of the mutation operator

Let $\mathbf{x}_B, \mathbf{x}_A \in \mathbb{R}^n$ be **two genotypes** encoding the same phenotype

$$\mathbf{y} = \mathbf{A} \mathbf{x}_A = \mathbf{B} \mathbf{x}_B$$

The **effect of the different encodings** becomes evident, when the genotype is changed (adding $\mathcal{N}(\mathbf{0}, \mathbf{C})$).

$$\begin{aligned} \mathbf{y}_{\text{new}} &= \mathbf{B}(\mathbf{x}_B + \mathcal{N}(\mathbf{0}, \mathbf{C})) = \mathbf{B} \mathbf{x}_B + \mathbf{B} \mathcal{N}(\mathbf{0}, \mathbf{C}) \\ &= \mathbf{A} \mathbf{x}_A + \mathbf{A} \mathbf{A}^{-1} \mathbf{B} \mathcal{N}(\mathbf{0}, \mathbf{C}) \\ &= \mathbf{A} (\mathbf{x}_A + \mathbf{A}^{-1} \mathbf{B} \mathcal{N}(\mathbf{0}, \mathbf{C})) \\ \mathbf{y}_{\text{new}} &= \mathbf{A} (\mathbf{x}_A + \mathbf{A}^{-1} \mathbf{B} \mathcal{N}(\mathbf{0}, \mathbf{C})) \end{aligned}$$

Using a new encoding \mathbf{B} means using a different covariance matrix

Adaptive Encoding

Definition (Adaptive Encoding)

Given a search algorithm, \mathcal{A} in state s , an encoding, T_B and an update, \mathcal{U} , then the iteration step

$$s \leftarrow T_B \circ \mathcal{A} \circ T_B^{-1}(s) \quad (1)$$

$$\mathbf{B} \leftarrow \mathcal{U}(\mathbf{B}, s) \quad (2)$$

defines an *adaptive encoding* where $T_B \circ \mathcal{A} \circ T_B^{-1}(s) = T_B(\mathcal{A}(T_B^{-1}(s)))$.

Remark (Evaluation of Solutions)

In order to make use of Eq. (1), \mathcal{A} has to operate on $f \circ \mathbf{B}$.

Adaptive Encoding

Example: Adaptive Encoding of CSA-ES

AE_{CMA}-CSA-ES

```

1 initialize  $m \in \mathbb{R}^n$  (distribution mean),  $p_\sigma = \mathbf{0}$  (evolution path),  $\sigma > 0$  (step-size)
2 initialize  $B = B^\circ = I$  (encoding matrices)
3 repeat
4    $m \leftarrow B^{-1}m$ 
5    $p_\sigma \leftarrow B^{\circ T}p_\sigma$ 
6   begin
7      $x_i = m + \sigma \mathcal{N}_i(0, I)$ , for  $i = 1, \dots, \lambda$ 
8      $f_i = f \circ B(x_i) = f(Bx_i)$ , for  $i = 1, \dots, \lambda$  // encode to evaluate
9      $m^- = m$ 
10     $m \leftarrow \sum_{i=1}^{\mu} w_i x_{i(f)}$ 
11     $p_\sigma \leftarrow (1 - c_\sigma)p_\sigma + \sqrt{c_\sigma(2 - c_\sigma)\mu_w} \frac{1}{\sigma}(m - m^-)$ 
12     $\sigma \leftarrow \sigma \exp\left(\frac{c_\sigma}{d_\sigma} \left(\frac{\|p_\sigma\|}{E\|\mathcal{N}(0, I)\|} - 1\right)\right)$ 
13  end
14   $m \leftarrow Bm$ 
15   $p_\sigma \leftarrow B^\circ p_\sigma$ 
16  AECMA-Update( $\{Bx_1, \dots, Bx_\mu\}$ ) // update  $B$  and  $B^\circ$ 
17 until stopping criterion is met
```

AE : Adaptive Encoding

CMA : Covariance Matrix Adaptation

CSA-ES : Cumulative *Step-size Adaptation* Evolution Strategy, lines 6–13

Adaptive Encoding

Theorem (Recovery of CMA-ES)

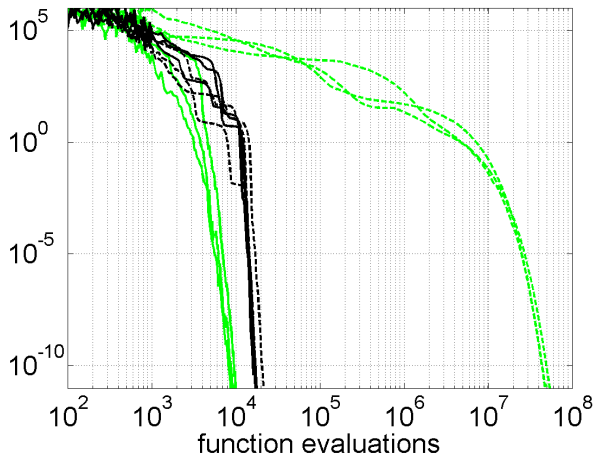
Given AE_{CMA} -Update in Procedure 1, the $AE_{CMA}-(\mu/\mu_W, \lambda)$ -CSA-ES implements the $(\mu/\mu_W, \lambda)$ -CMA-ES.

Adaptive Encoding

- can render *any* continuous domain search algorithm independent of the coordinate system
- anticipated successful applications in particular for population-based stochastic algorithms

Another Case Study

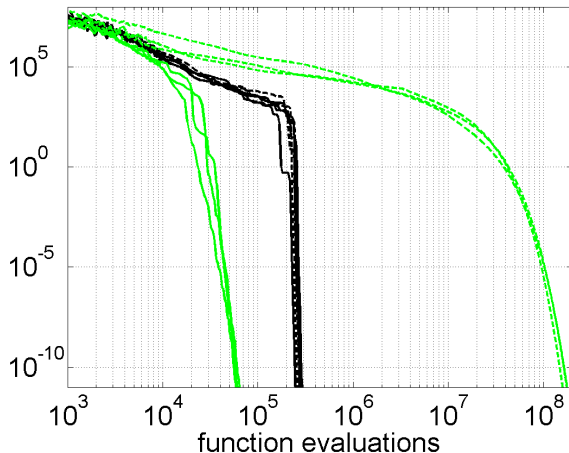
Adaptive Encoding



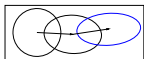
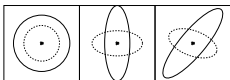
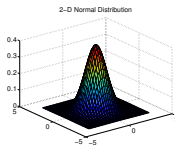
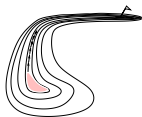
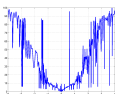
Cauchy-ES (green)
versus Adaptively
Encoded Cauchy-ES
(black)
rotating a separable
function, 10-D

Another Case Study

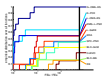
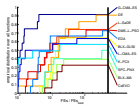
Adaptive Encoding



Cauchy-ES (green)
 versus Adaptively
 Encoded Cauchy-ES
 (black)
 rotating a separable
 function, 30-D



Thank You



```

1 function [F, best_x] = fminsearch(f, x0, options)
2 % Finds the minimum of the function f(x) starting at x0.
3 % See also: fminbnd, fmincon, fminsearch, fminsearch_opts.
4 % Syntax:
5 % [F, best_x] = fminsearch(f, x0)
6 % [F, best_x] = fminsearch(f, x0, options)
7 % Input arguments
8 % f: A function handle that returns the value of the function.
9 % x0: A scalar or vector of real numbers, the starting point.
10 % options: A structure containing the following fields:
11 % 'MaxFunEvals': Maximum number of function evaluations.
12 % 'MaxIter': Maximum number of iterations.
13 % 'TolX': Tolerance for the change in x.
14 % 'TolF': Tolerance for the change in the function value.
15 % 'PlotFcns': A cell array of function handles for plotting the progress.
16 % Output arguments
17 % F: The minimum value of the function.
18 % best_x: The coordinates of the minimum value.
19 % See also: fminbnd, fmincon, fminsearch, fminsearch_opts.
20 % Copyright 1992-2014 by MathWorks, Inc.

```

