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► **To cite this version:**

Nikolaus Hansen. CMA-ES. Parallel Problem Solving from Nature - PPSN XVIII, 18th International Conference, Sep 2024, Hagenberg, Austria. hal-04709819

**HAL Id: hal-04709819**

**<https://inria.hal.science/hal-04709819v1>**

Submitted on 25 Sep 2024

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# CMA-ES

Covariance Matrix Adaptation Evolution Strategy

Nikolaus Hansen  
Inria & Ecole Polytechnique, France

September 2024

I am happy to answer questions at any time!

Need the slides? Available under Talks at my homepage:  
<http://www.cmap.polytechnique.fr/~nikolaus.hansen/talks.html>

# Topics

## 0. Problem statement

## 1. What makes an optimization problem difficult to solve?

## 2. How does the CMA-ES work?

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

## 3. What can users do?

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



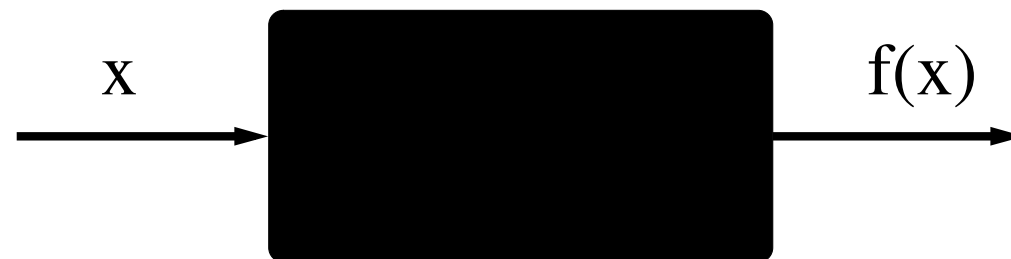
# Problem Statement

## Continuous Domain Search/Optimization

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

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

- **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**  $f(x)$  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

- Difficulties

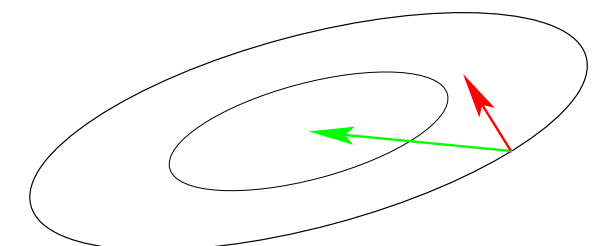
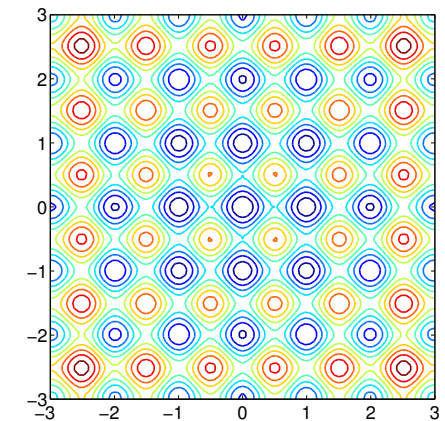
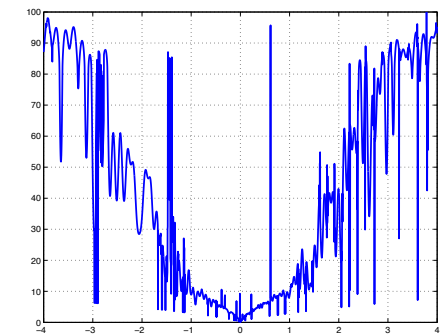
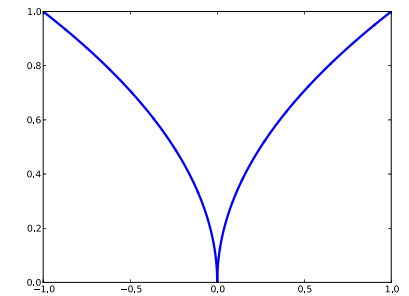
- ▶ exhaustive search is infeasible
- ▶ naive random search takes too long
- ▶ deterministic search is not successful / takes too long

**Approach:** stochastic search, Evolutionary Algorithms

# What Makes a Function Difficult to Solve?

Why stochastic search?

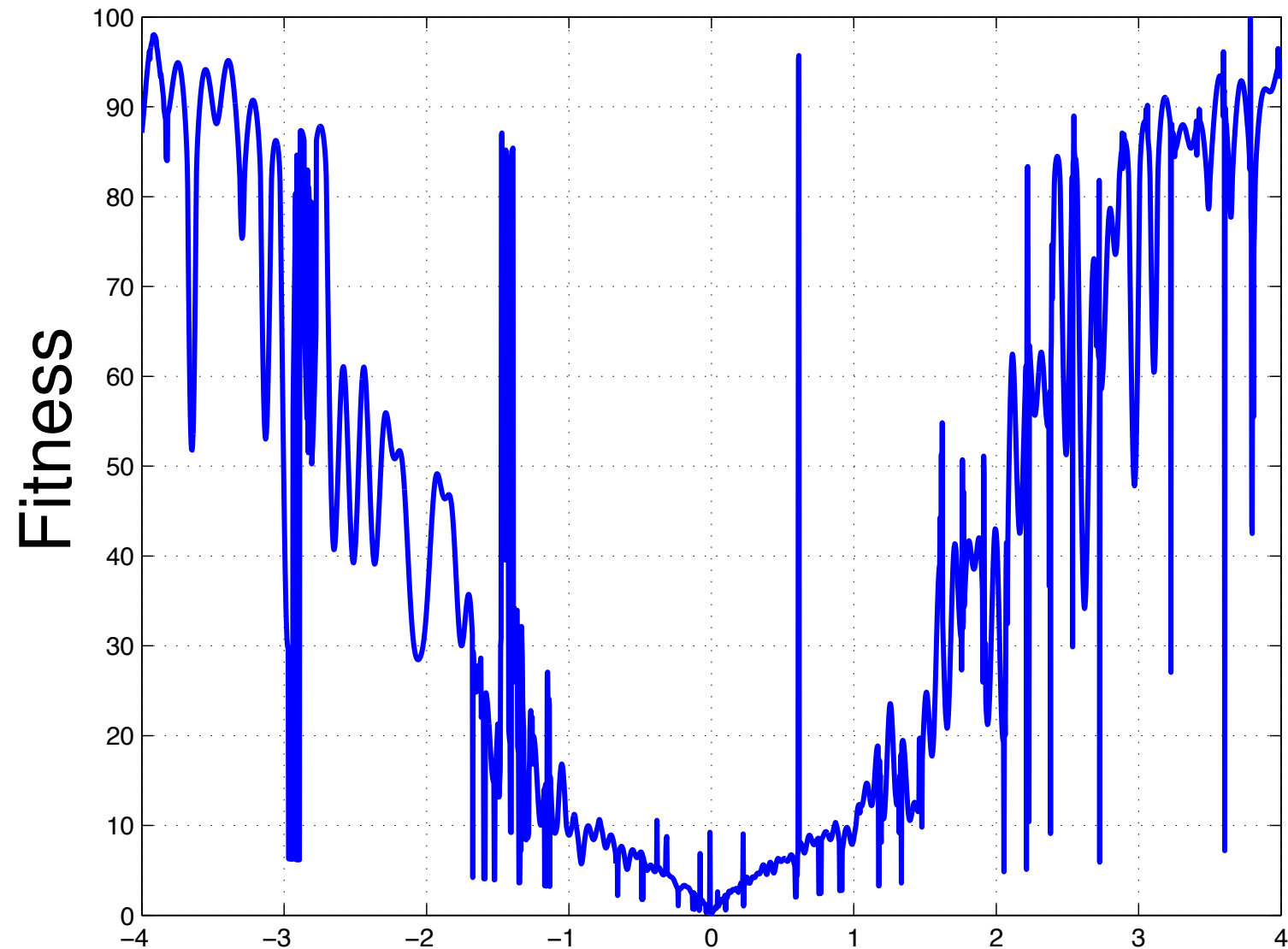
- non-linear, non-quadratic, non-convex  
on linear and quadratic functions much better search policies are available
- ruggedness  
non-smooth, discontinuous, multimodal, and/or noisy function
- dimensionality (size of search space)  
(considerably) larger than three
- non-separability  
dependencies between the objective variables
- ill-conditioning
- non-smooth level sets



gradient direction Newton direction

# Ruggedness

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



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

# Curse of Dimensionality

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

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

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

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

# Separable Problems

## Definition (Separable Problem)

A function  $f$  is separable if

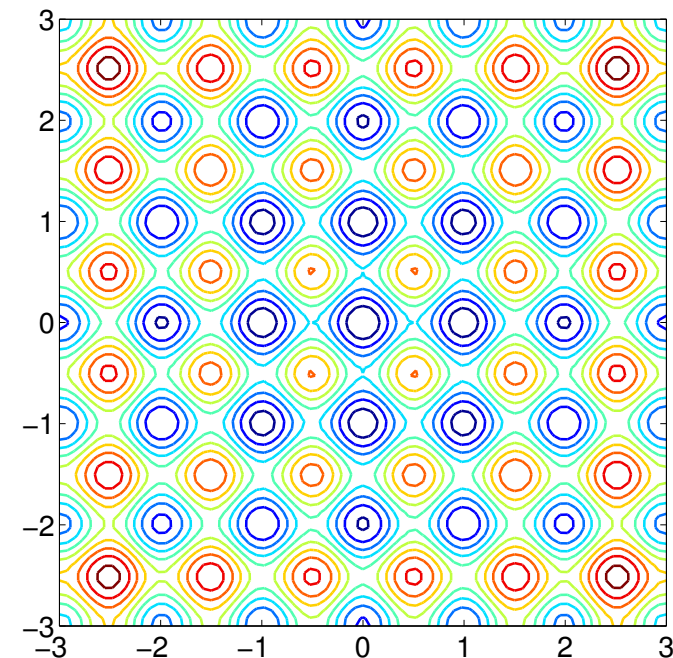
$$\arg \min_{(x_1, \dots, x_n)} f(x_1, \dots, x_n) = \left( \arg \min_{x_1} f(x_1, \dots), \dots, \arg \min_{x_n} f(\dots, x_n) \right)$$

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

Example: Additively decomposable functions

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

Rastrigin function





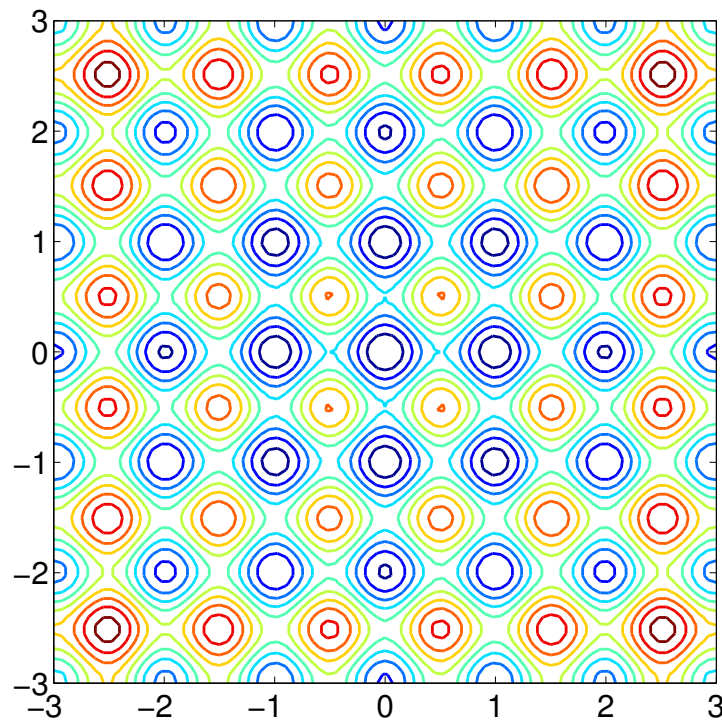
# Non-Separable Problems

Building a non-separable problem from a separable one <sup>(1,2)</sup>

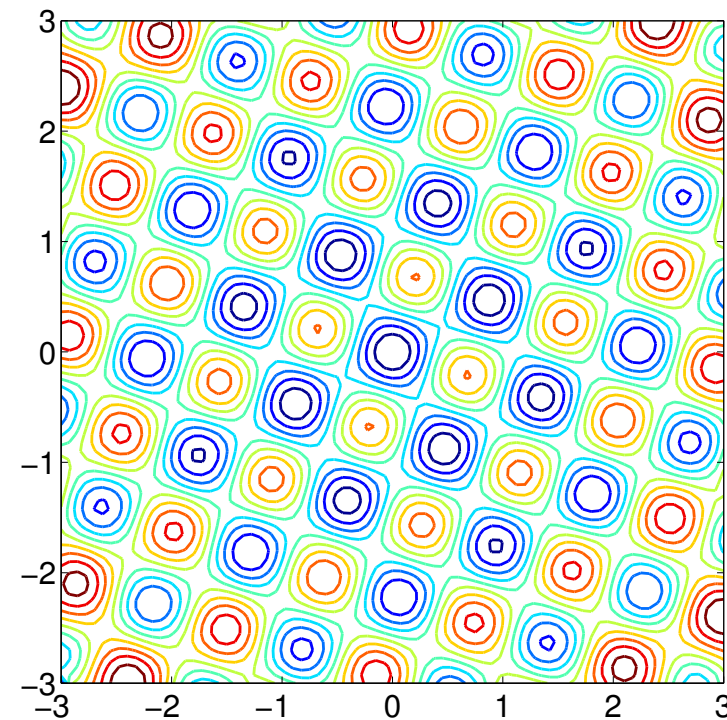
## Rotating the coordinate system

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

**R** rotation matrix



**R**  
→



<sup>1</sup> 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

<sup>2</sup> 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

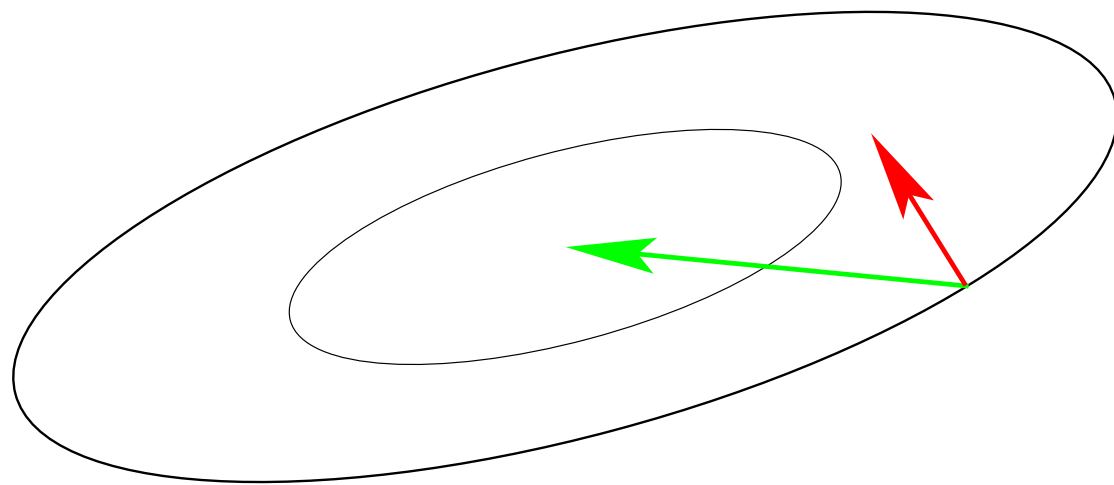
# III-Conditioned Problems

## Curvature of level sets

Consider the convex-quadratic function

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

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



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

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

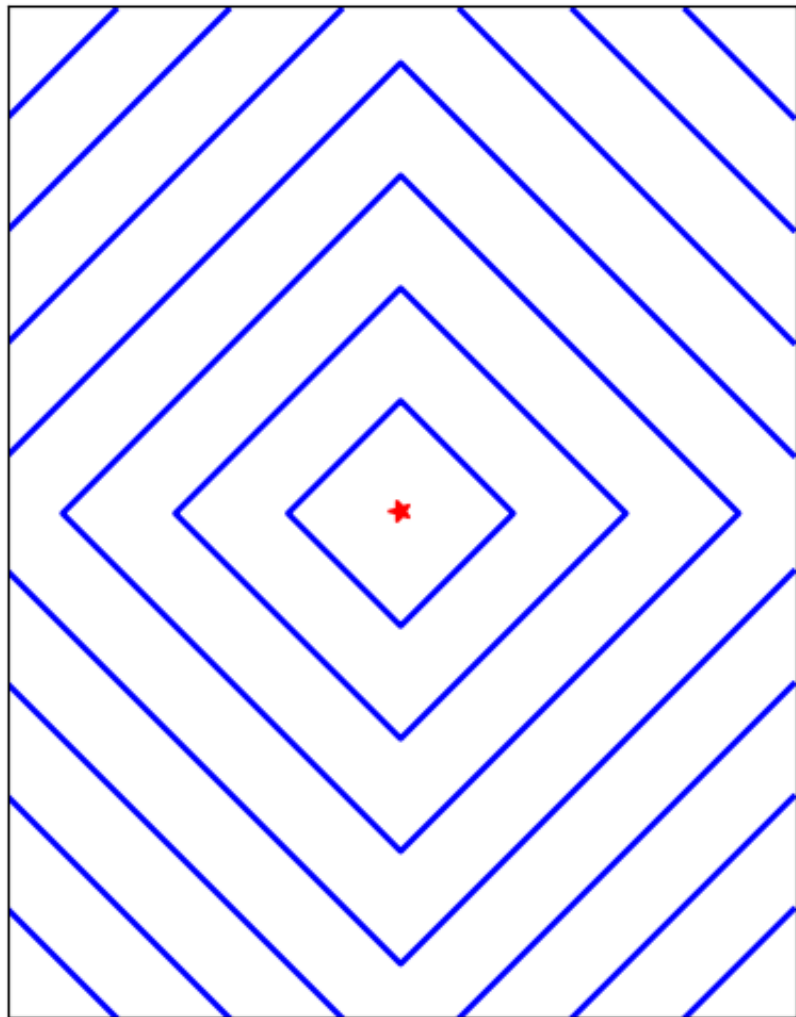
III-conditioning means **squeezed level sets** (high curvature).  
Condition number equals nine here. Condition numbers up to  $10^{10}$   
are not unusual in real world problems.

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

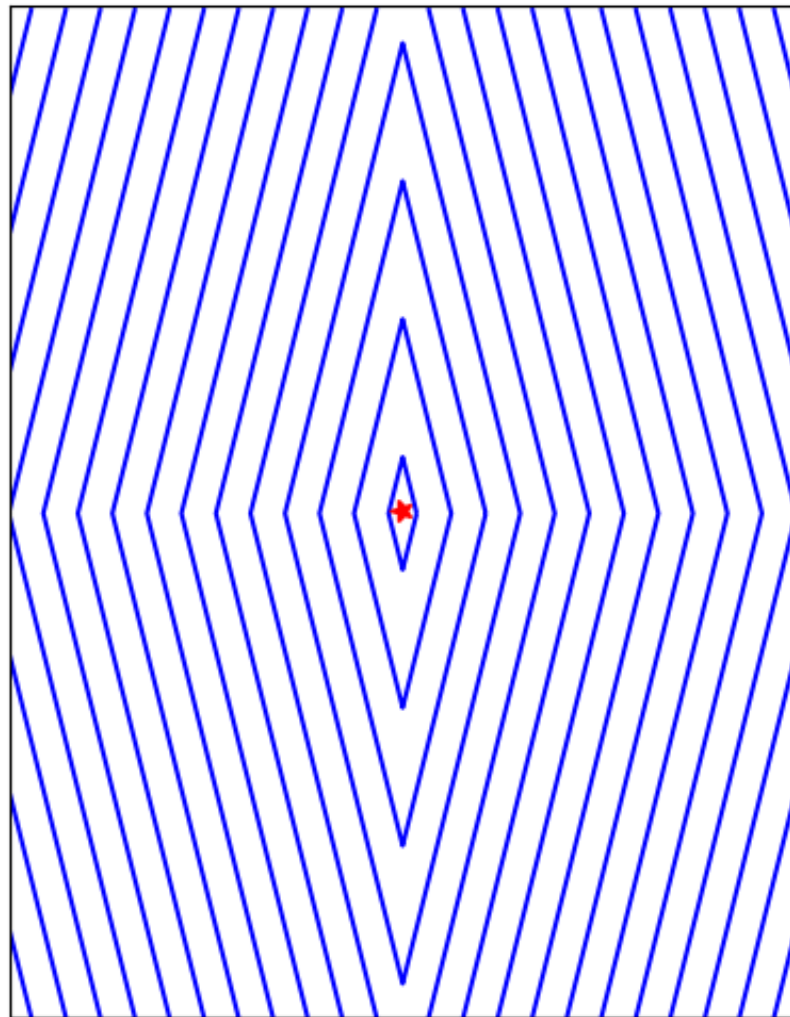


# Non-smooth level sets (sharp ridges)

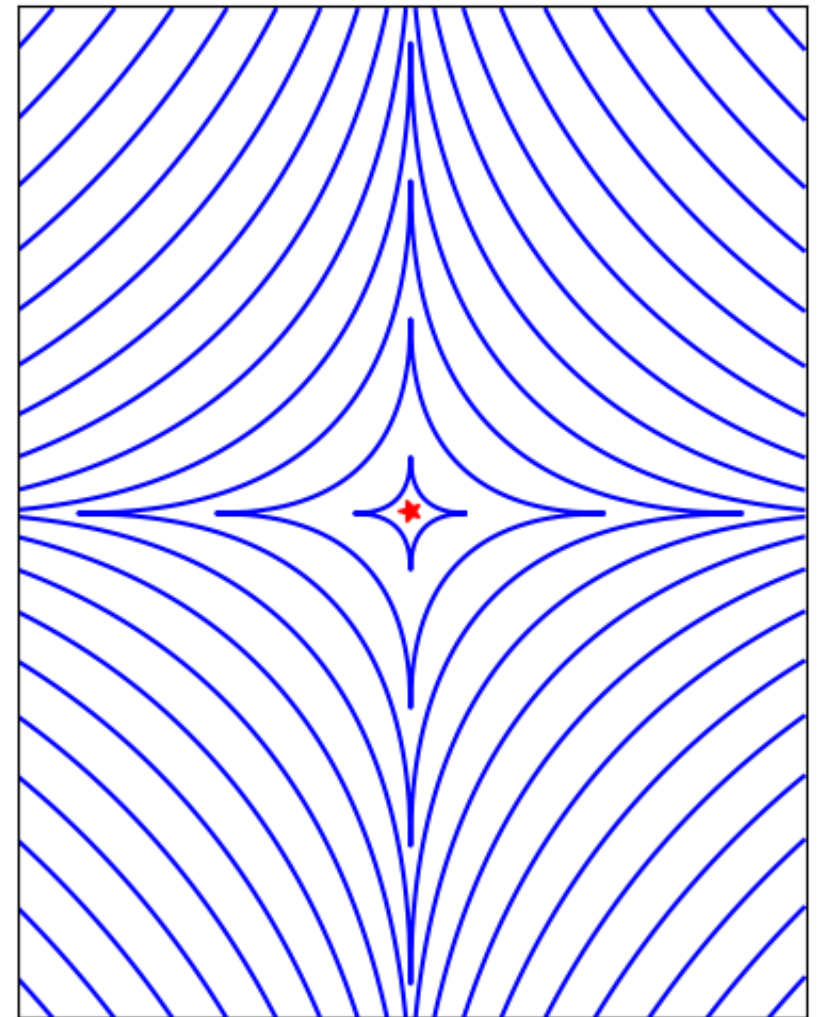
Similar difficulty **but worse** than ill-conditioning



1-norm



scaled 1-norm



1/2-norm

opening angle is the crucial parameter

# What Makes a Function Difficult to Solve?

... and what can be done

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

... metaphors

# Topics

1. What makes the problem difficult to solve?

## 2. How does the CMA-ES work?

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

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

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

# Stochastic Search

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

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

While not terminate

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

Everything depends on the definition of  $P$  and  $F_\theta$

deterministic algorithms are covered as well

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

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

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

# The CMA-ES

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

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

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

**While** not terminate

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

$\mathbf{m} \leftarrow \mathbf{m} + c_m \sigma \mathbf{y}_w$ , where  $\mathbf{y}_w = \sum_{i=1}^\mu w_i \mathbf{y}_{\text{rk}^{-1}(i)}$  update mean

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

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

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

$\mathbf{C} \leftarrow \mathbf{C} + c_\mu \sum_{i=1}^\lambda w_{\text{rk}(i)} (\mathbf{y}_i \mathbf{y}_i^\top - \mathbf{C}) + c_1 (\mathbf{p}_c \mathbf{p}_c^\top - \mathbf{C})$  update  $\mathbf{C}$

*Not covered:* termination, restarts, useful output, search boundaries and encoding, corrections for: positive definiteness guaranty,  $\mathbf{p}_c$  variance loss,  $c_\sigma$  and  $d_\sigma$  for large  $\lambda$

# Stochastic Search

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

While not terminate

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

# Evolution Strategies

New search points are sampled normally distributed

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

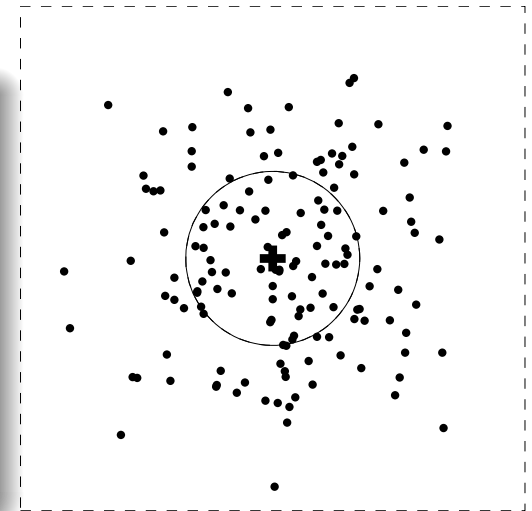
as perturbations of  $\mathbf{m}$ , where  $\mathbf{x}_i, \mathbf{m} \in \mathbb{R}^n$ ,  $\sigma \in \mathbb{R}_+$ ,  $\mathbf{C} \in \mathbb{R}^{n \times n}$

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  $\sigma$ .



# Why Normal Distributions?

1 widely observed in nature, for example as phenotypic traits

2 only stable distribution with finite variance

stable means that the sum of normal variates is again normal:

$$\mathcal{N}(\mathbf{x}, \mathbf{A}) + \mathcal{N}(\mathbf{y}, \mathbf{B}) \sim \mathcal{N}(\mathbf{x} + \mathbf{y}, \mathbf{A} + \mathbf{B})$$

helpful in **design and analysis** of algorithms  
related to the *central limit theorem*

3 most convenient way to generate **isotropic** search points

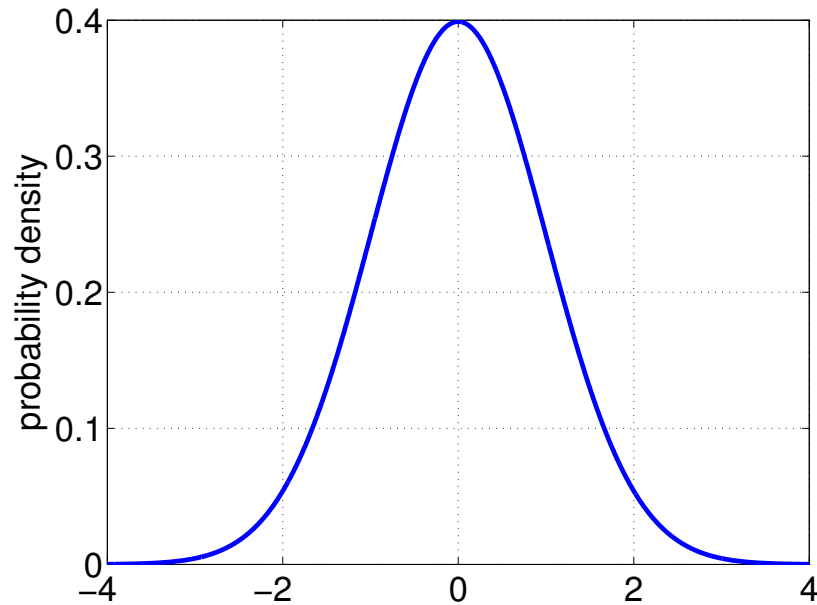
the isotropic distribution does **not favor any direction**, rotational  
invariant

4 maximum entropy distribution with finite variance

the least possible assumptions on  $f$  in the distribution shape

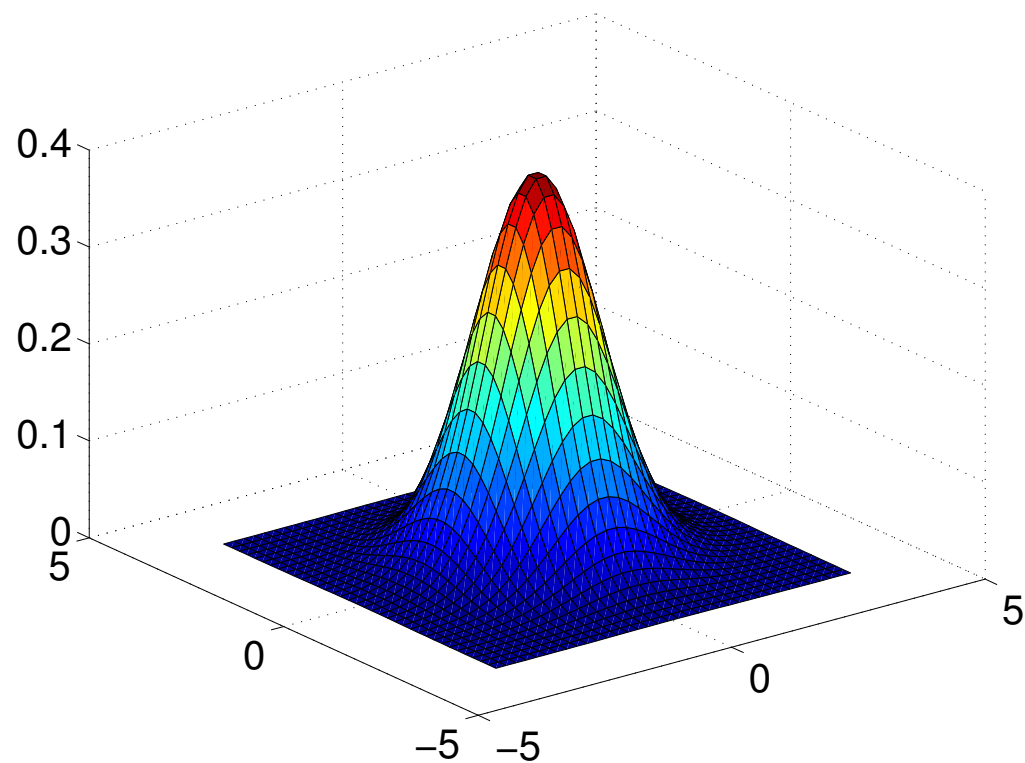
# Normal Distribution

Standard Normal Distribution

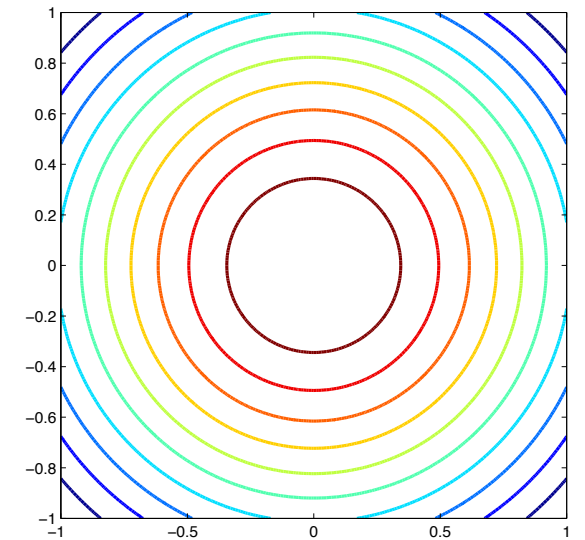


probability density of the 1-D standard normal distribution

2-D Normal Distribution



probability density of a 2-D normal distribution



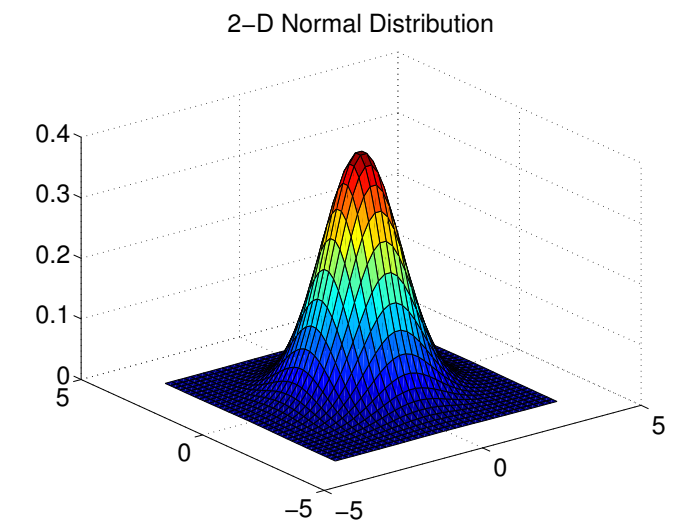


# The Multi-Variate ( $n$ -Dimensional) Normal Distribution

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  $\mathbf{m}$

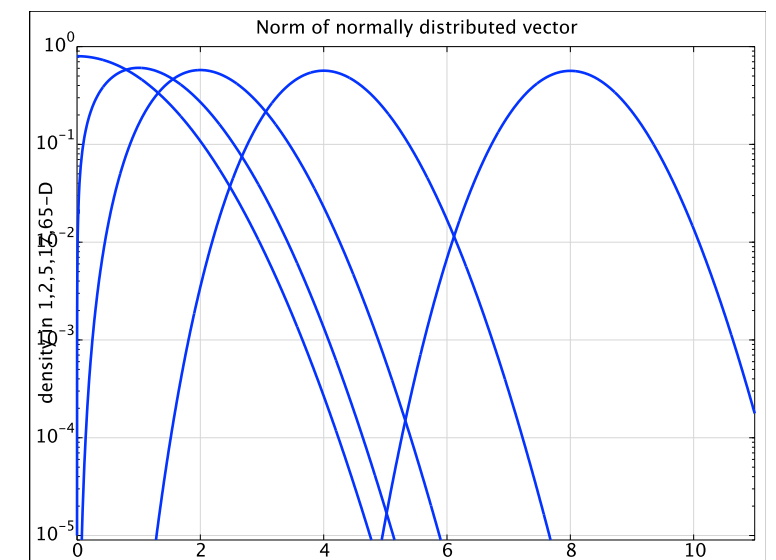
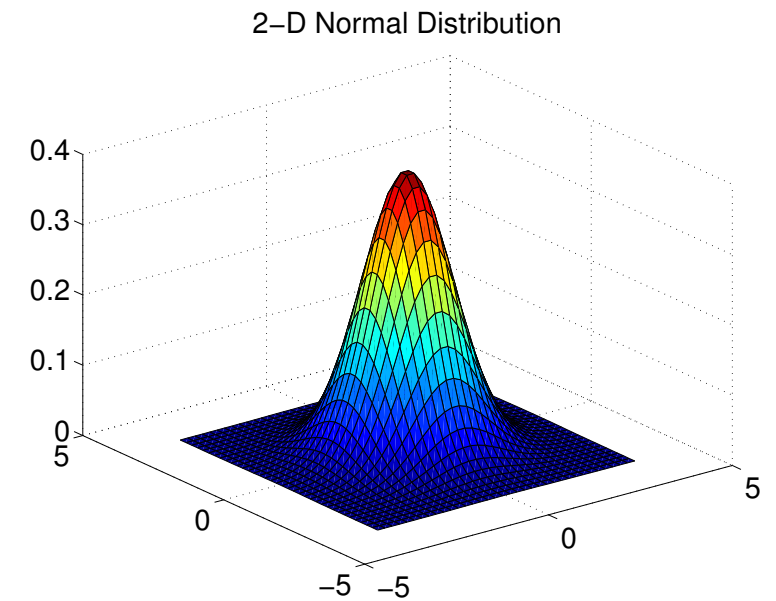
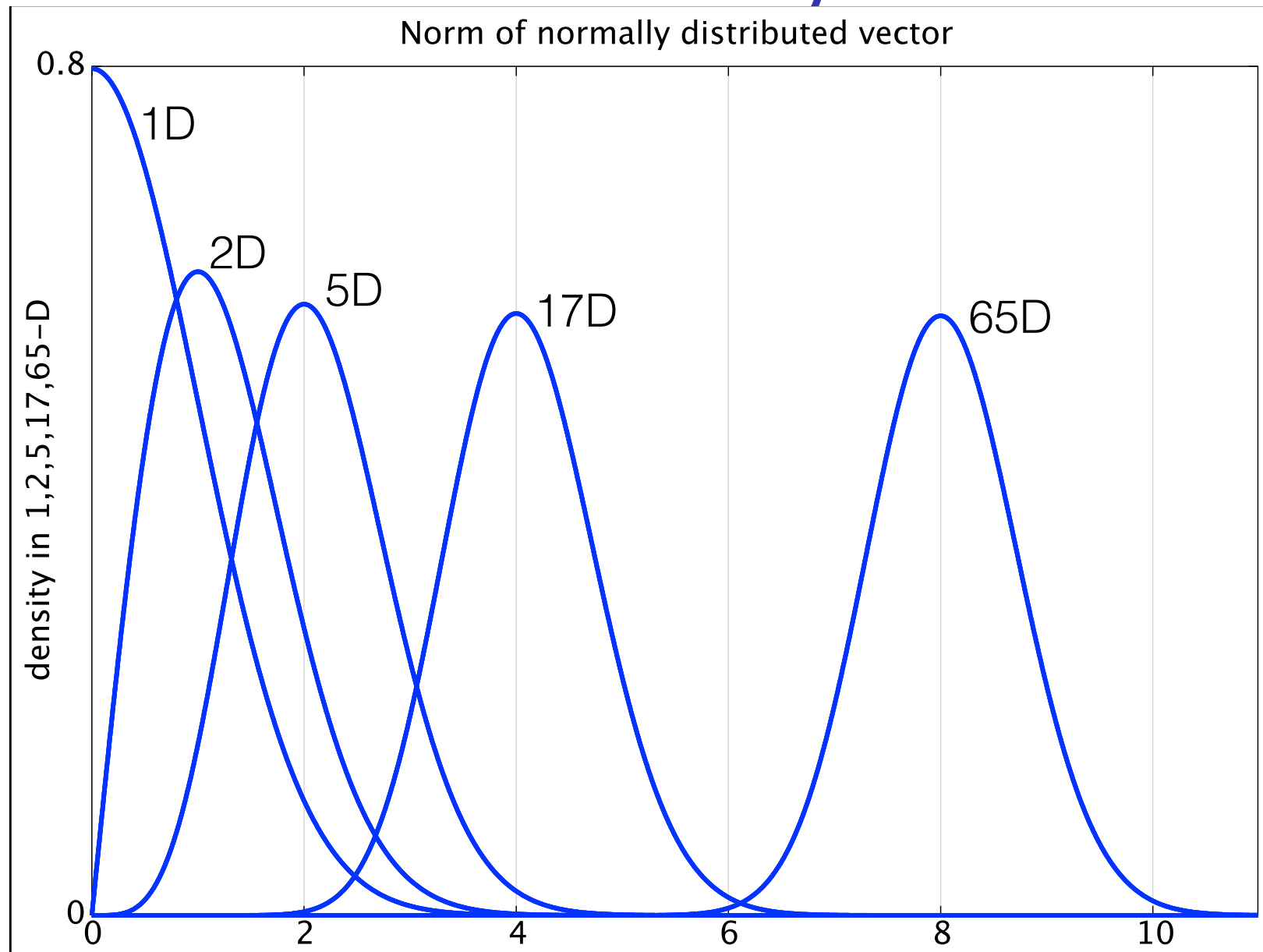
- determines the displacement (translation)
- value with the largest density (modal value)
- the distribution is symmetric about the distribution mean



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

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

# Effect of Dimensionality



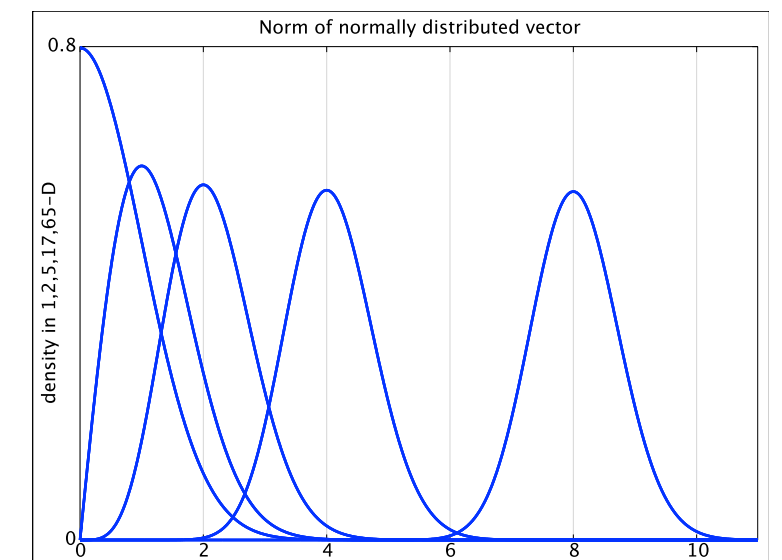
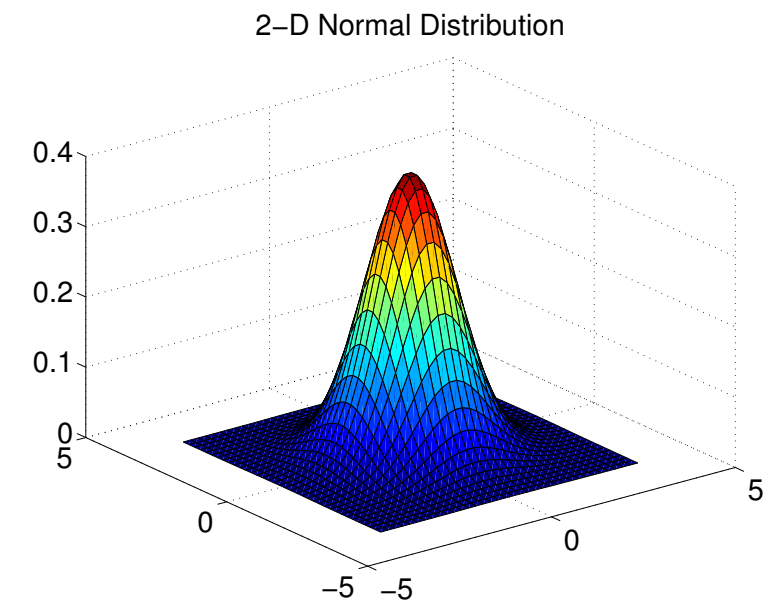
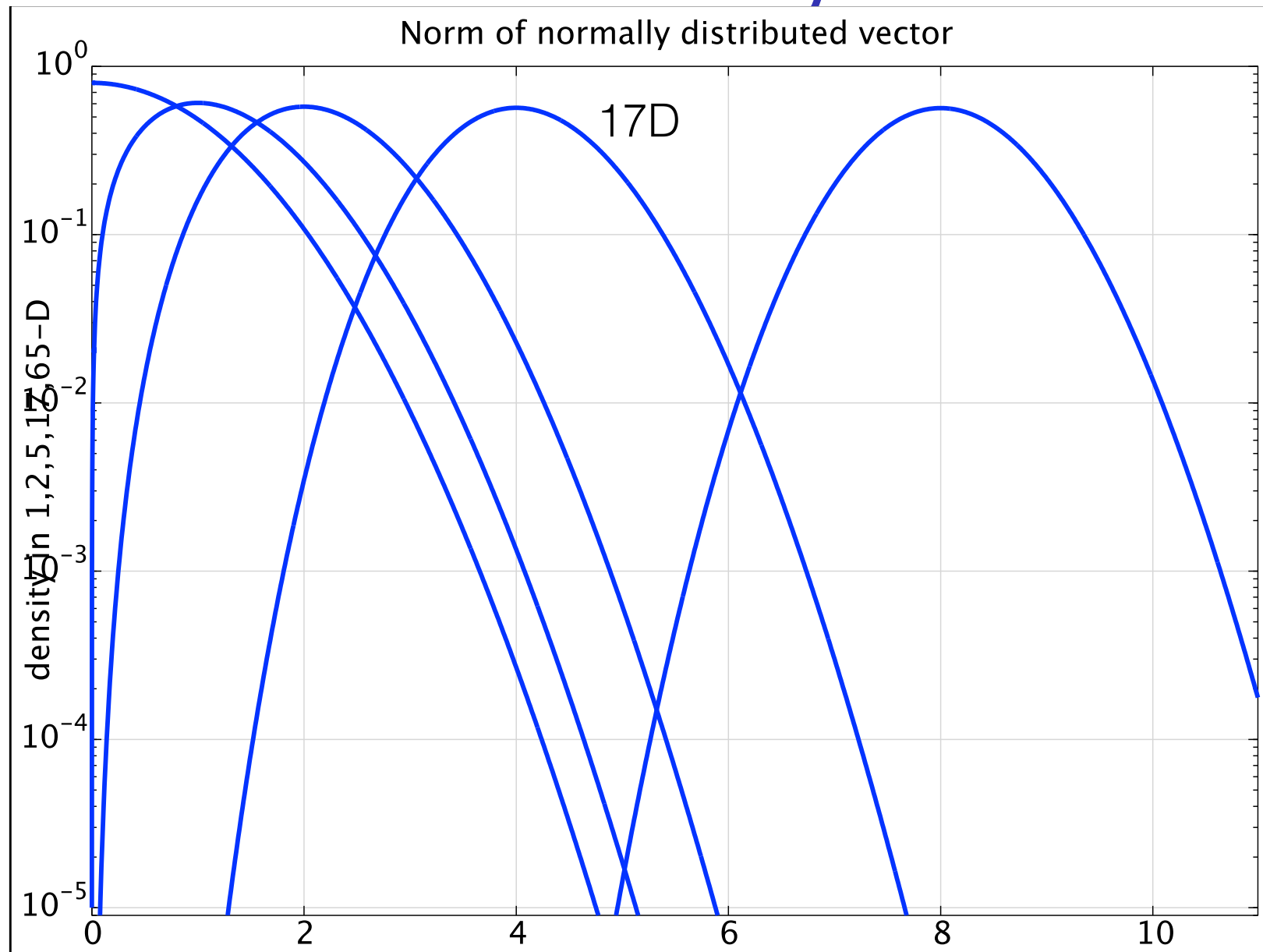
$\|\mathcal{N}(\mathbf{0}, \mathbf{I})\| \longrightarrow \mathcal{N}\left(\sqrt{n-1/2}, 1/2\right)$  with modal value  $\sqrt{n-1}$

yet: maximum entropy distribution

also consider a difference between two vectors:

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

# Effect of Dimensionality



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

yet: maximum entropy distribution

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# Stochastic Search

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

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

While not terminate

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

Everything depends on the definition of  $P$  and  $F_\theta$

deterministic algorithms are covered as well

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

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

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

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

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

where

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

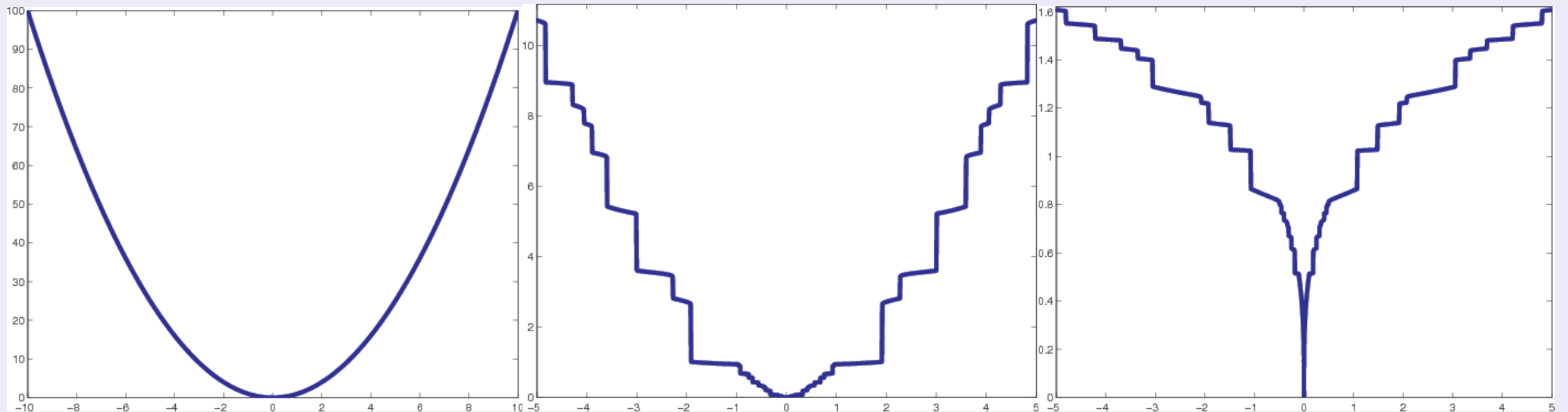
The best  $\mu$  points are selected from the new solutions (non-elitistic) and weighted intermediate recombination is applied.

# Invariance Under Monotonically Increasing Functions

## Rank-based algorithms

Update of all parameters uses only the ranks

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



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

$g$  is strictly monotonically increasing  
 $g$  preserves ranks

3

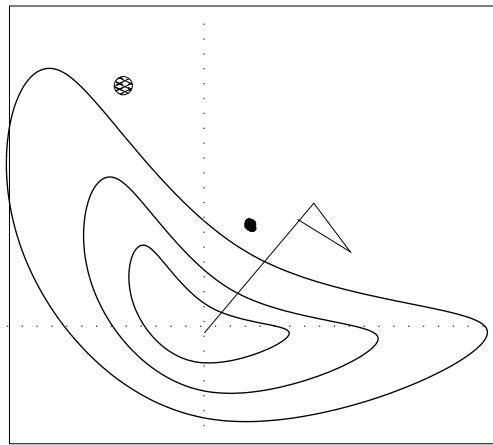
<sup>3</sup> Whitley 1989. The GENITOR algorithm and selection pressure: Why rank-based allocation of reproductive trials is best,

ICGA

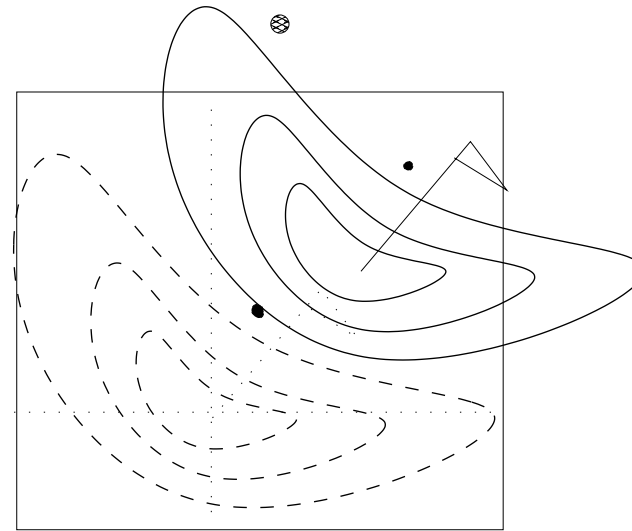
# Basic Invariance in Search Space

- translation invariance

is true for most optimization algorithms



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



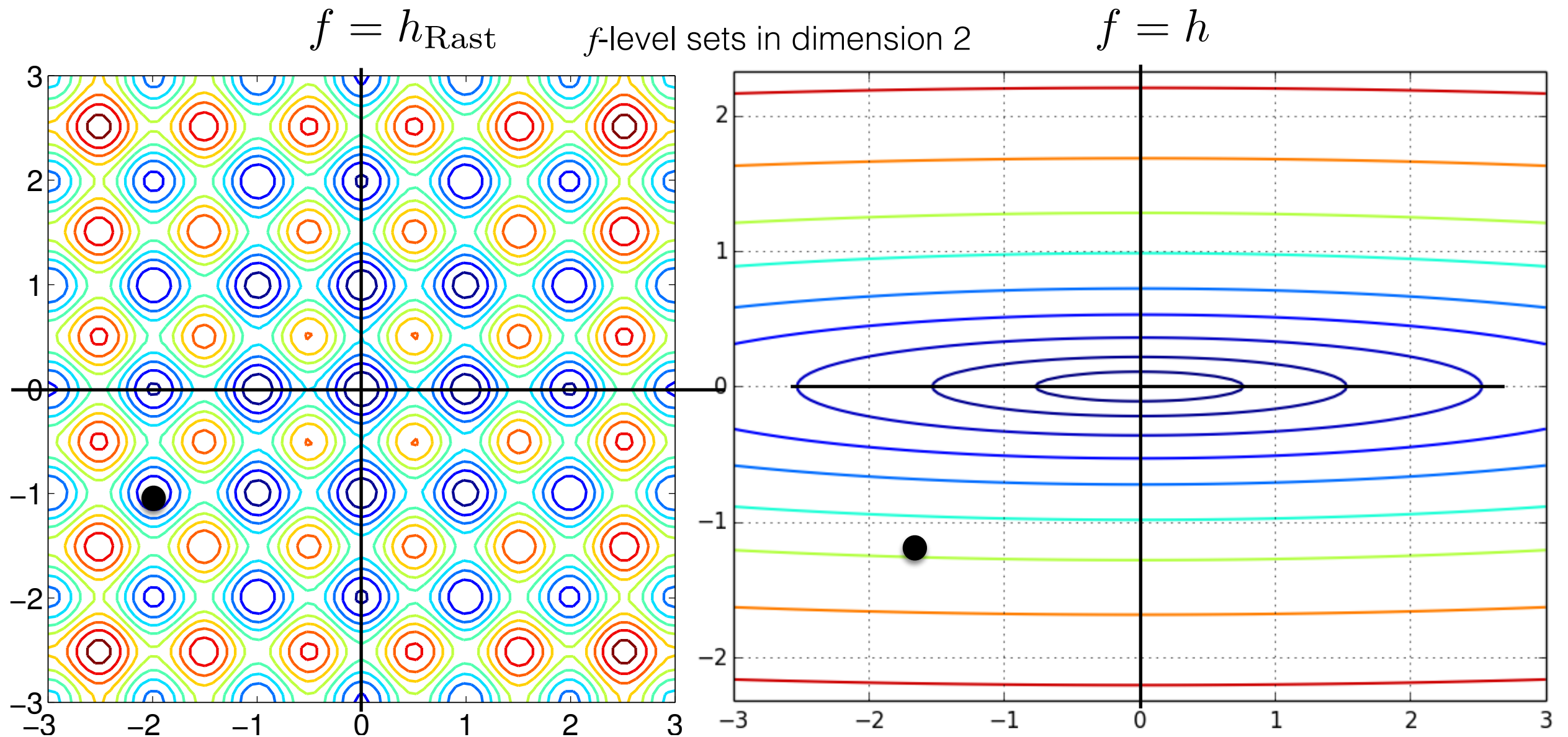
Identical behavior on  $f$  and  $f_a$

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

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



# Invariance Under Rigid Search Space Transformation



for example, invariance under search space rotation  
 (separable  $\Leftrightarrow$  non-separable)

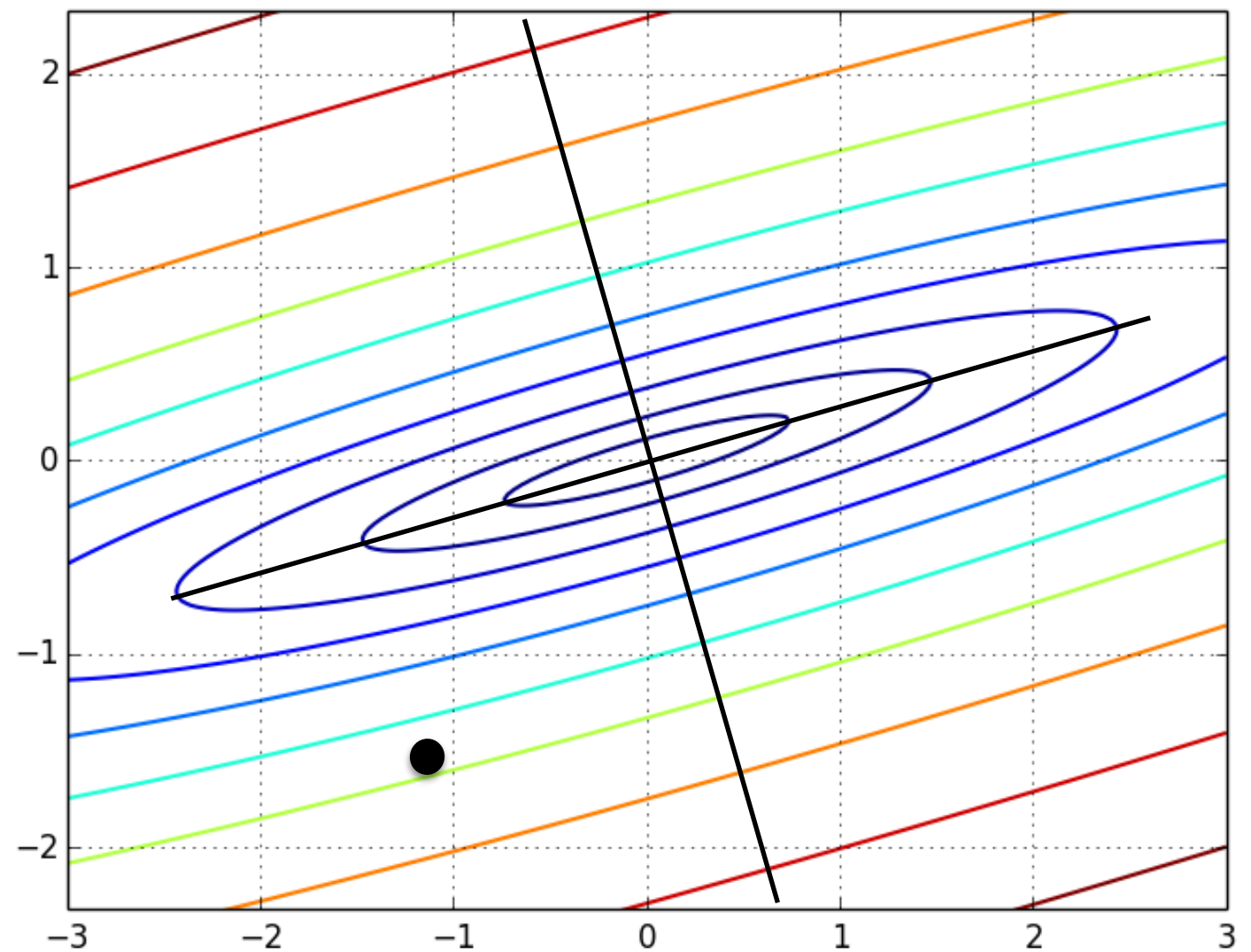
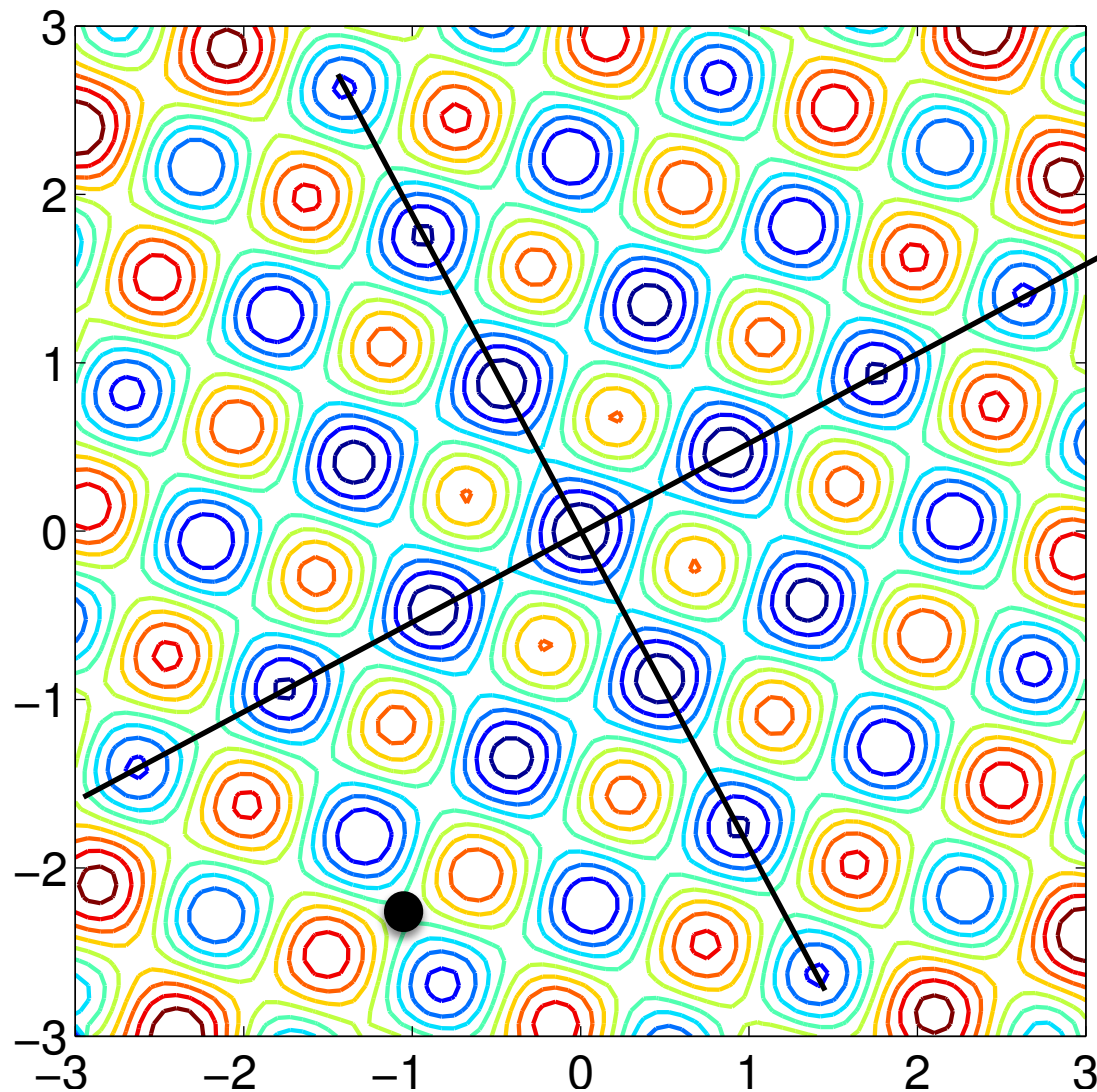


# Invariance Under Rigid Search Space Transformation

$$f = h_{\text{Rast}} \circ R$$

$f$ -level sets in dimension 2

$$f = h \circ R$$



for example, invariance under search space rotation  
(separable  $\Leftrightarrow$  **non-separable**)

# 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

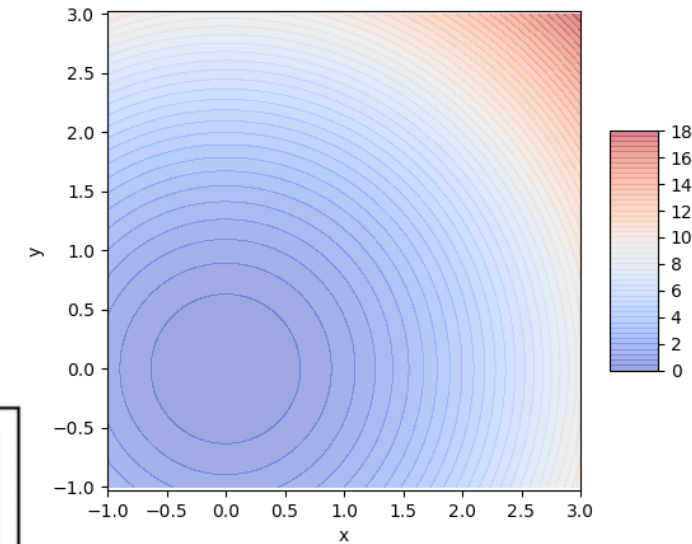
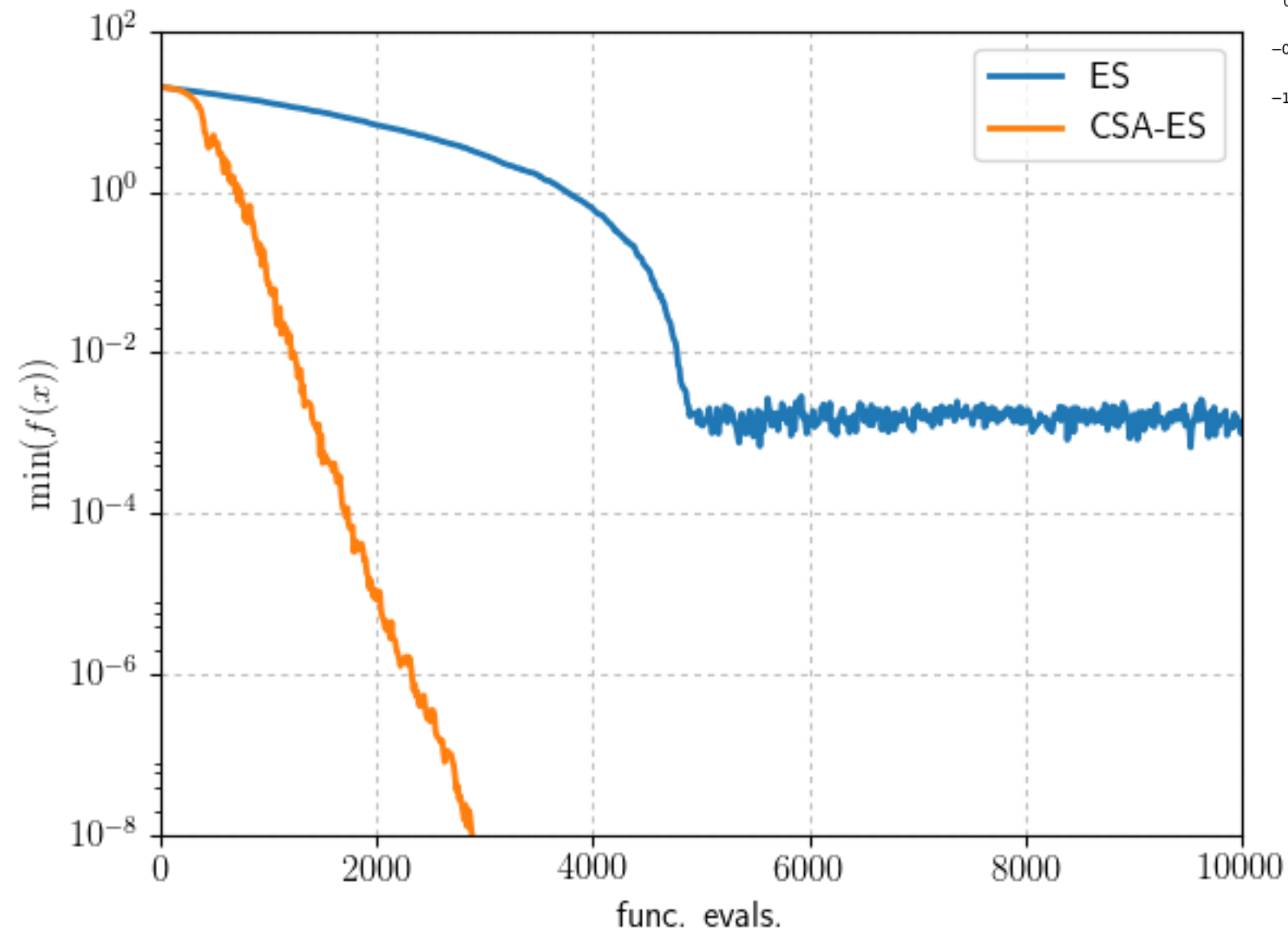
- Empirical performance results
  - ▶ from benchmark functions
  - ▶ from solved real world problems

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

- **Invariance** is a strong **non-empirical** statement about generalization
  - generalizing (identical) performance from a single function to a whole class of functions

consequently, invariance is important for the evaluation of search algorithms

# Summary



On 20D Sphere Function:  $f(\mathbf{x}) = \sum_{i=1}^n x_i^2 = \|\mathbf{x}\|^2$

- ES without adaptation can't approach the optimum  $\Rightarrow$  adaptation required

# Topics

0. Problem statement

1. What makes an optimization problem difficult to solve?

2. How does the CMA-ES work?

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

3. What can users do?

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

# Methods for Step-Size Control

- **1/5-th success rule<sup>ab</sup>**, often applied with “+”-selection
  - increase step-size if more than 20% of the new solutions are successful, decrease otherwise
- **$\sigma$ -self-adaptation<sup>c</sup>**, applied with “,”-selection
  - mutation is applied to the step-size and the better, according to the objective function value, is selected
  - simplified “global” self-adaptation
- **path length control<sup>d</sup>** (Cumulative Step-size Adaptation, CSA)<sup>e</sup>
  - self-adaptation derandomized and non-localized

*f*

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<sup>a</sup>Rechenberg 1973, *Evolutionsstrategie, Optimierung technischer Systeme nach Prinzipien der biologischen Evolution*, Frommann-Holzboog

<sup>b</sup>Schumer and Steiglitz 1968. Adaptive step size random search. *IEEE TAC*

<sup>c</sup>Schwefel 1981, *Numerical Optimization of Computer Models*, Wiley

<sup>d</sup>Hansen & Ostermeier 2001, Completely Derandomized Self-Adaptation in Evolution Strategies, *Evol. Comput.* 9 (2)

<sup>e</sup>Ostermeier *et al* 1994, Step-size adaptation based on non-local use of selection information, *PPSN IV*

<sup>f</sup>Hansen *et al* 2014, How to assess step-size adaptation mechanisms in a derandomised search, *PPSN IX*

# Evolution Strategies

Recalling

New search points are sampled normally distributed

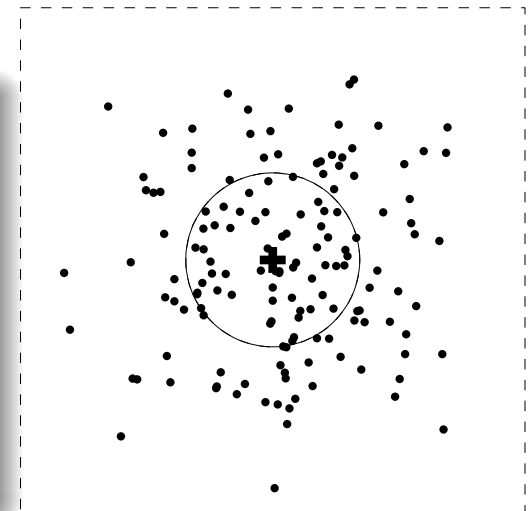
$$\mathbf{x}_i \sim \mathbf{m} + \sigma \mathcal{N}_i(\mathbf{0}, \mathbf{C}) \quad \text{for } i = 1, \dots, \lambda$$

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

where

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

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



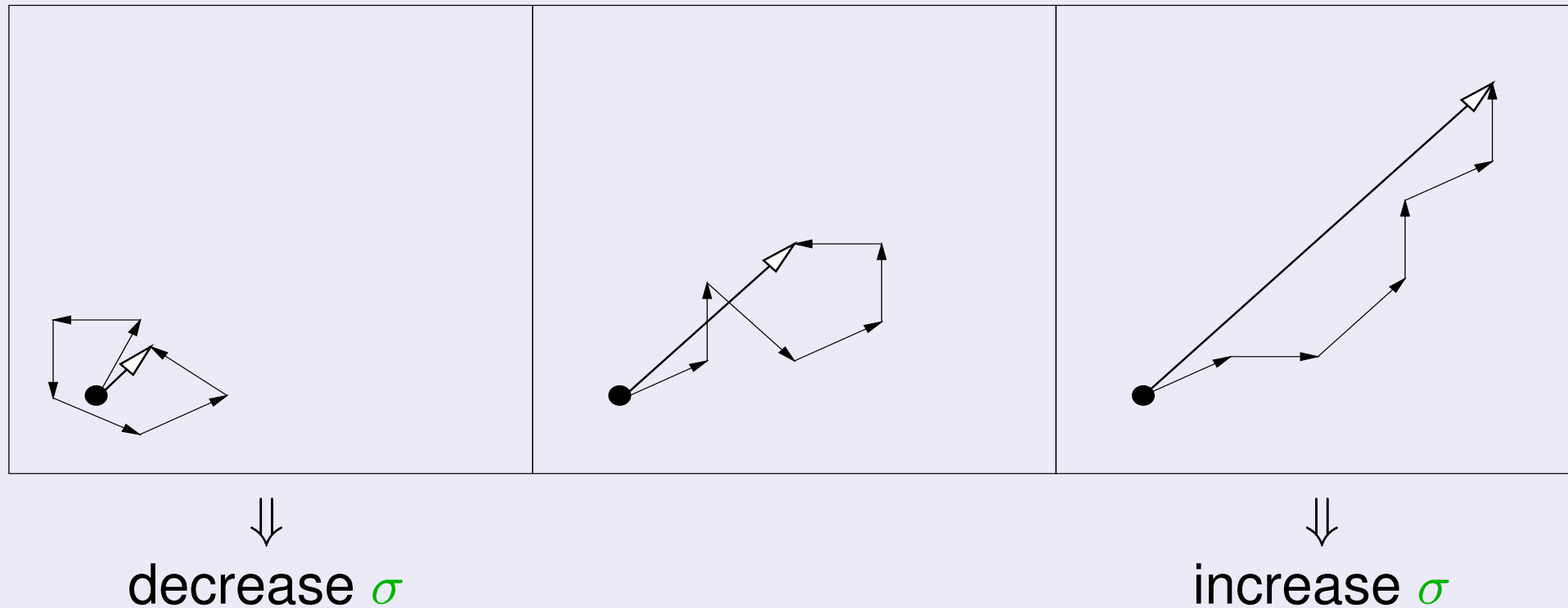
# Path Length Control (CSA)

## The Concept of Cumulative Step-Size Adaptation

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

Measure the length of the *evolution path*

the pathway of the mean vector  $\mathbf{m}$  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  $c_\sigma \approx \mu_w / (n + \mu_w)$ ,  $d_\sigma \approx 1$ .

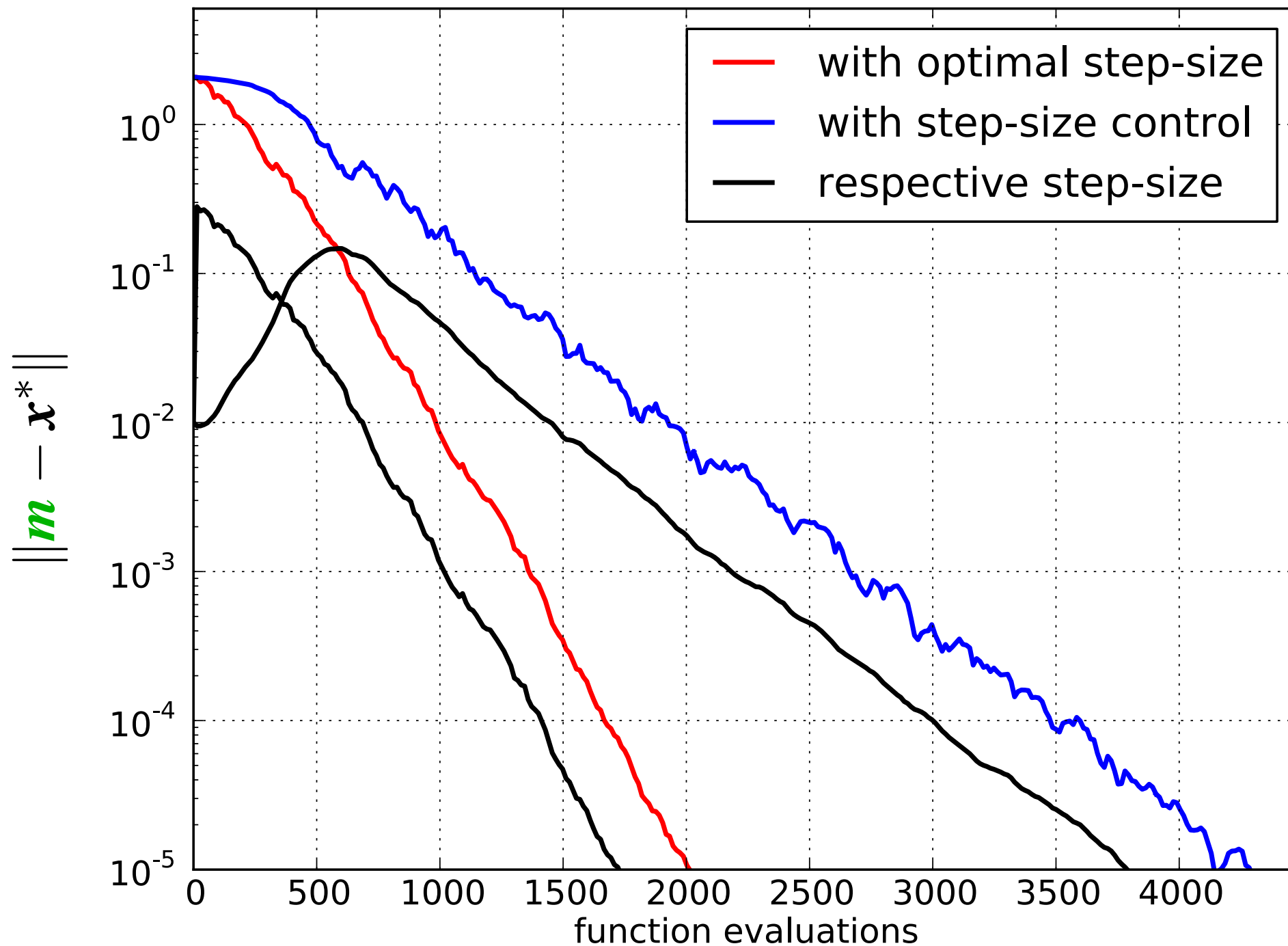
$$\mathbf{m} \leftarrow \mathbf{m} + \sigma \mathbf{y}_w \quad \text{where } \mathbf{y}_w = \sum_{i=1}^{\mu} w_i \mathbf{y}_{i:\lambda} \quad \text{update mean}$$

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

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



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



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

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

# Two-Point Step-Size Adaptation (TPA)

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

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

$$\|\mathbf{x}\|_{\mathbf{C}} := \mathbf{x}^T \mathbf{C}^{-1} \mathbf{x}$$

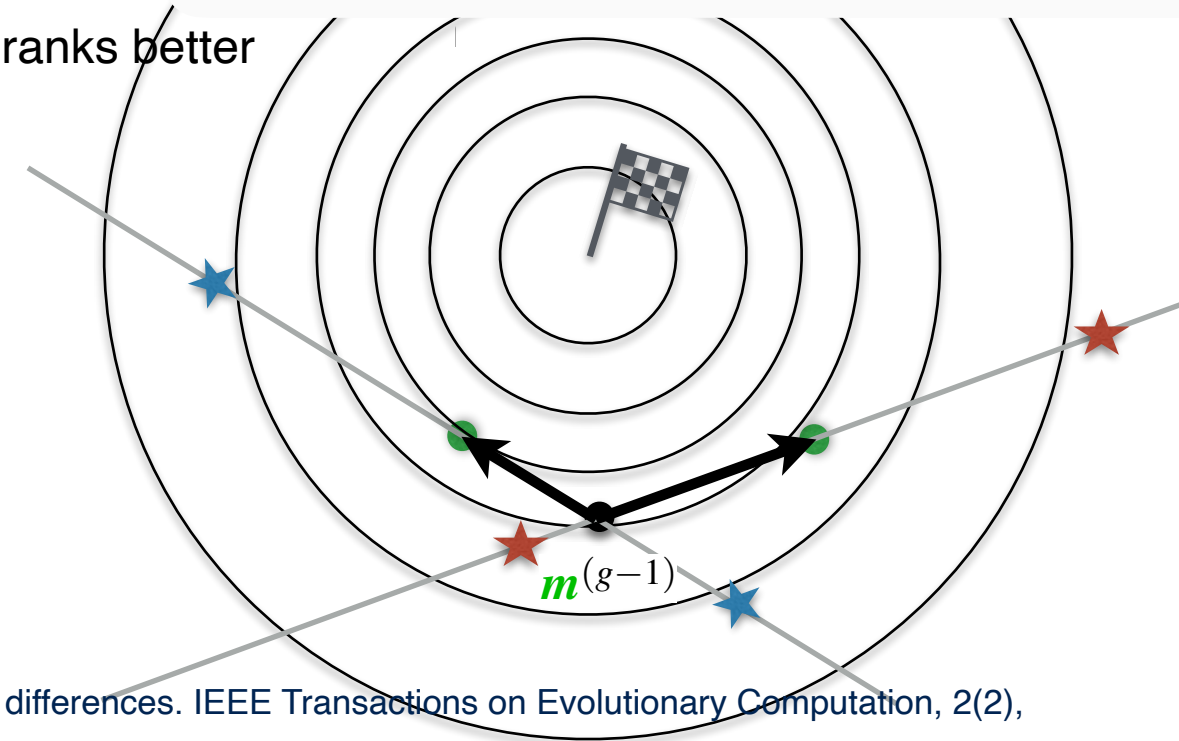
- Compare the ranking of  $\mathbf{x}_1$  and  $\mathbf{x}_2$  among  $\lambda$  current population.

$$s^{(g+1)} = (1 - c_s) s^{(g)} + c_s \underbrace{\frac{\text{rank}(\mathbf{x}_2) - \text{rank}(\mathbf{x}_1)}{\lambda - 1}}_{> 0 \text{ if forward direction ranks better}}$$

- Update the step-size

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

where  $c_s \approx 0.3$  and  $d_\sigma \approx 1 + 2 \ln(n)$



[Salomon, 1998] Salomon, R. (1998). Evolutionary algorithms and gradient search: similarities and differences. *IEEE Transactions on Evolutionary Computation*, 2(2), pages 45–55.

[Hansen, 2008] Hansen, N. (2008). CMA-ES with two-point step-size adaptation. [research report] rr-6527, 2008. Inria-00276854v5.

[Hansen et al, 2014] Hansen, N., Atamna, A., and Auger, A. (2014). How to assess step-size adaptation mechanisms in randomised search. In *Parallel Problem Solving from Nature—PPSN XIII*, pages 60–69. Springer.

[Akimoto and Hansen, 2020] Akimoto, Y. and Hansen, N. (2020). Diagonal acceleration for covariance matrix adaptation evolution strategies. *Evolutionary computation*, 28(3), pages 405–435.

# Step-Size Control: Summary

## Why Step-Size Control?

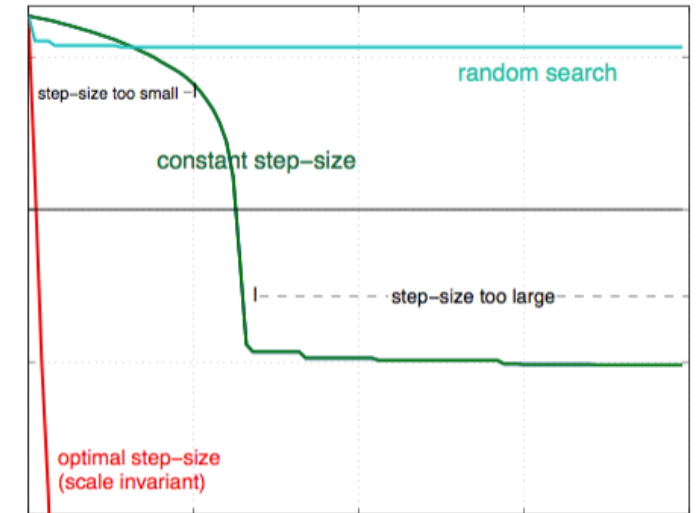
- to achieve linear convergence at near-optimal rate

## Cumulative Step-Size Adaptation

- efficient and robust for  $\lambda \leq N$
- inefficient on functions with (many) ineffective axes

## Alternative Step-Size Adaptation Mechanisms

- Two-Point Step-Size Adaptation
- Median Success Rule<sup>[b]</sup>, Population Success Rule<sup>[c]</sup>



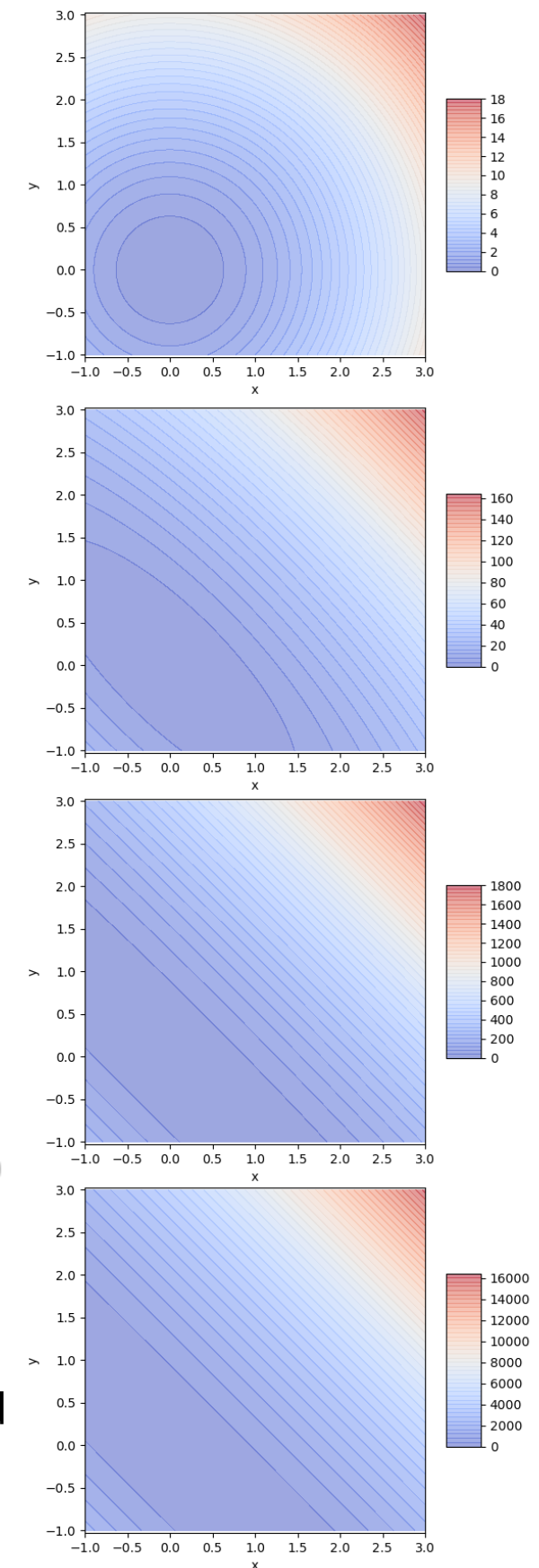
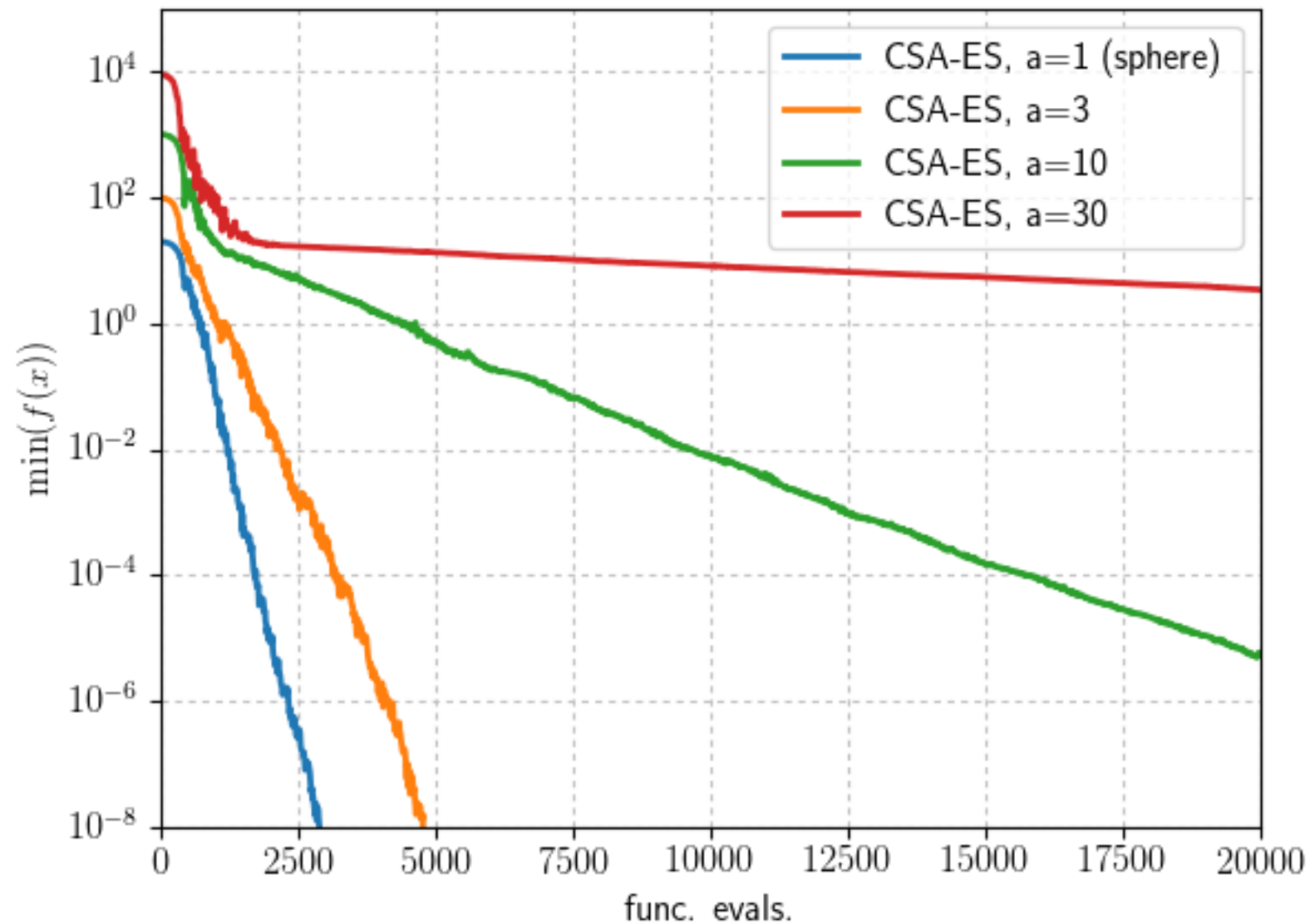
*the effective adaptation of the overall population diversity seems yet to pose open questions, in particular with recombination or without entire control over the realized distribution.<sup>a</sup>*

<sup>a</sup>Hansen et al. How to Assess Step-Size Adaptation Mechanisms in Randomised Search. PPSN 2014

[b] Ait Elhara, O., Auger, A., and Hansen, N. (2013). A median success rule for non-elitist evolution strategies: Study of feasibility. In Proc. of the GECCO, pages 415–422.

[c] Loshchilov, I. (2014). A computationally efficient limited memory CMA-ES for large scale optimization. In Proc. of the GECCO, pages 397–404.

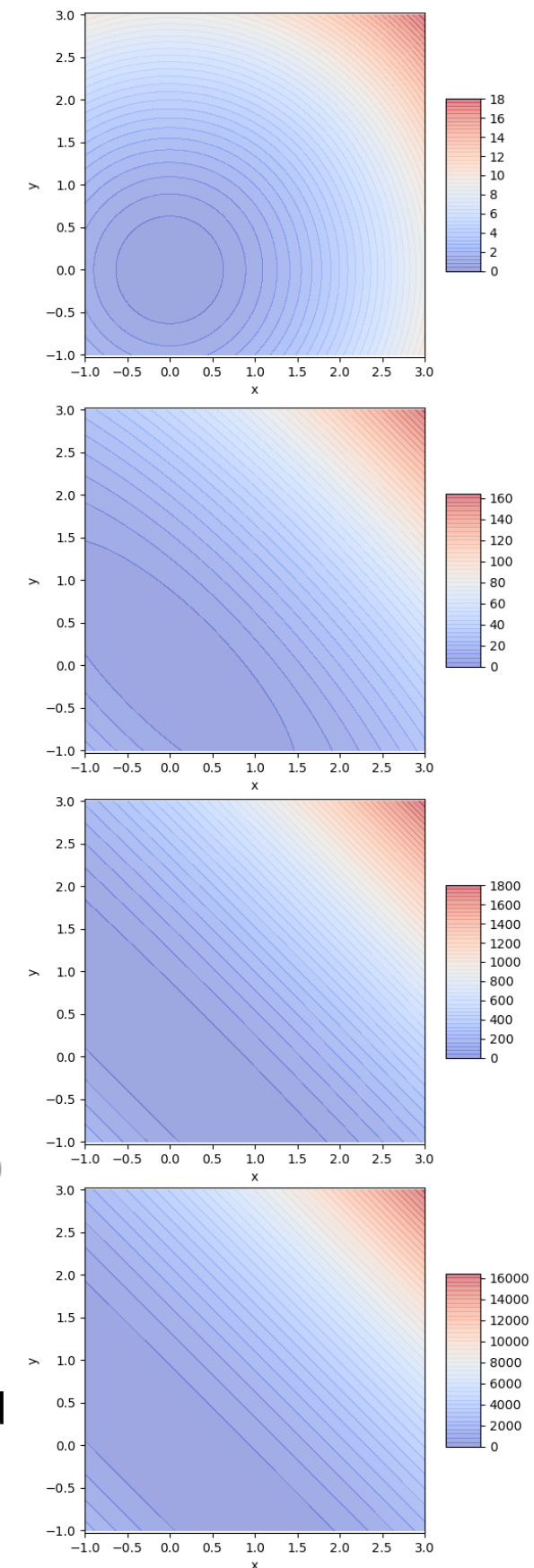
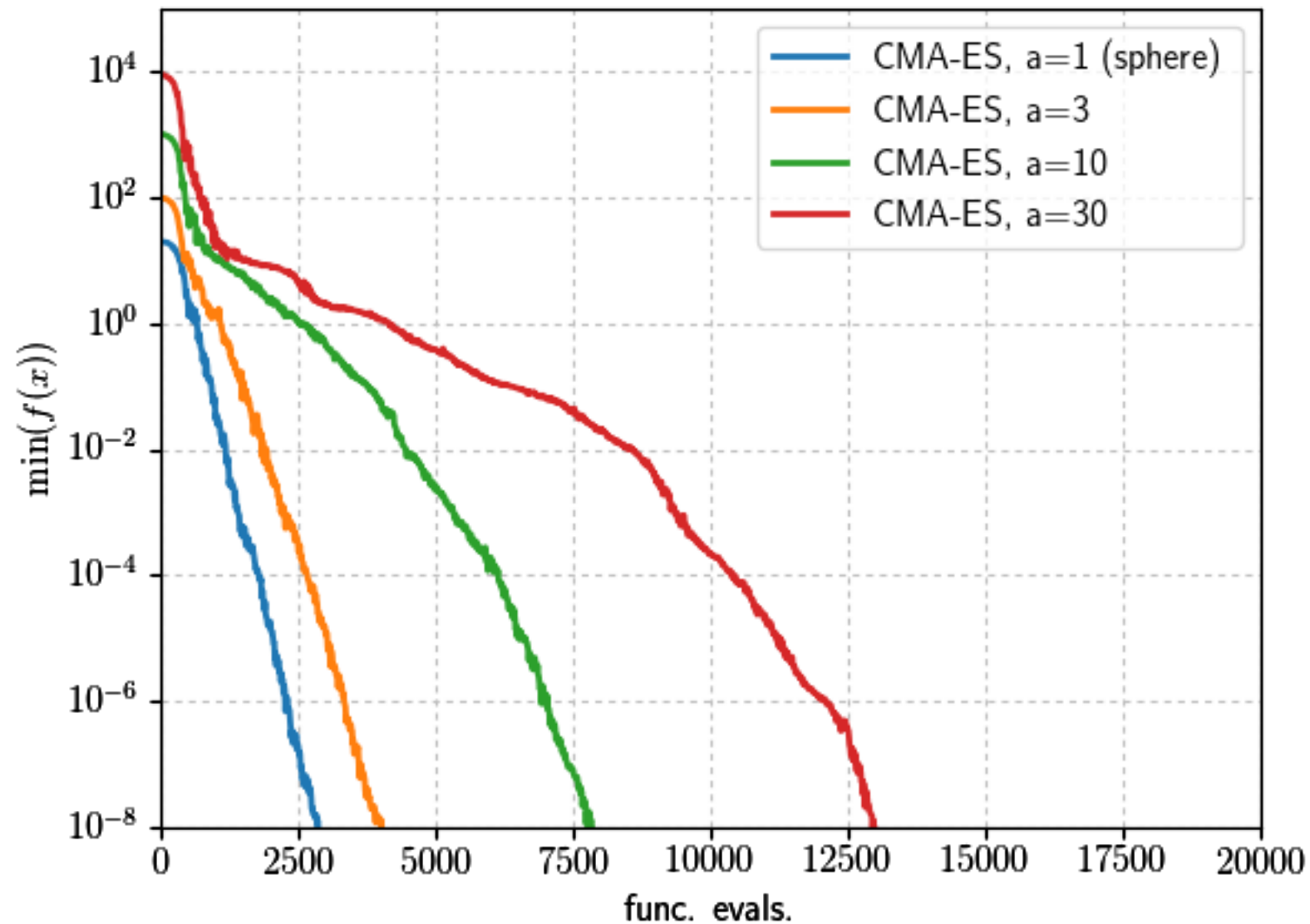
# Step-Size Control Is Not Enough



On 20D TwoAxes Function:  $f(\mathbf{x}) = \sum_{i=1}^{\lfloor n/2 \rfloor} x_i^2 + a \sum_{i=\lfloor n/2 \rfloor + 1}^n x_i^2$

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

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- Covariance Matrix Adaptation

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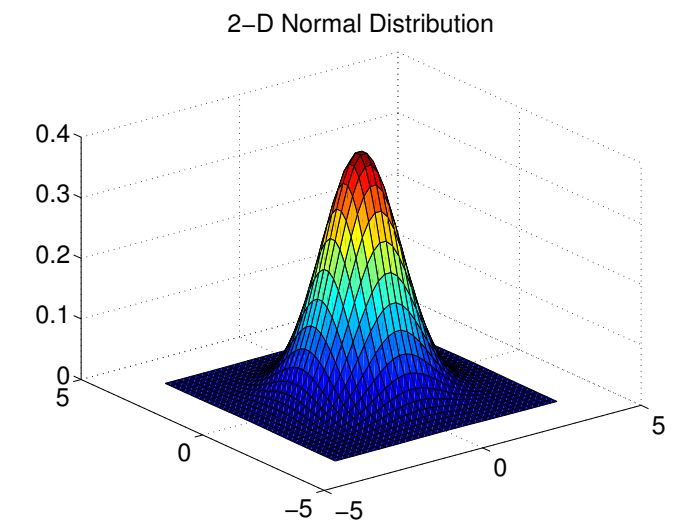
- Normal Distribution, Rank-Based Recombination
- Step-Size Adaptation
- **Covariance Matrix Adaptation**
  - ▶ Rank-One Update and Cumulation
  - ▶ Rank- $\mu$  Update
  - ▶ Active Covariance Update
- Choice of problem formulation and encoding (not covered)
- Choice of initial solution and initial step-size
- Restarts, Increasing Population Size
- Restricted Covariance Matrix

# 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)
- value with the largest density (modal value)
- the distribution is symmetric about the distribution mean



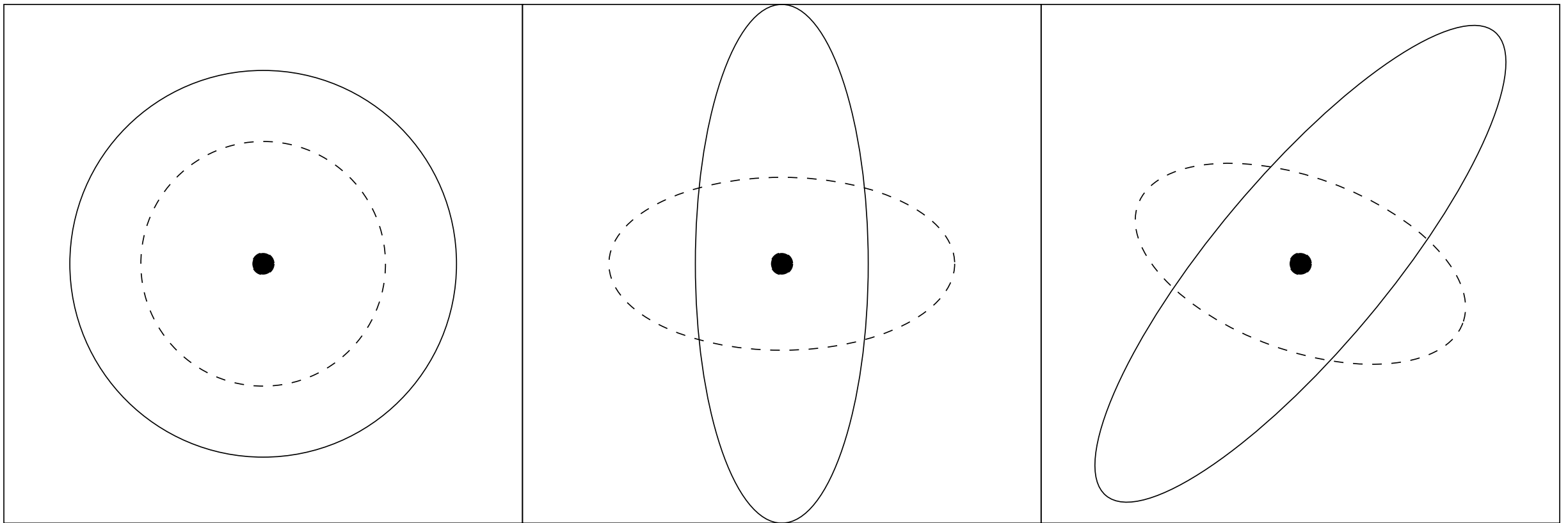
The **covariance matrix**  $\mathbf{C}$

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



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

### 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**  $\sigma$   
 components are  
 independent and identically  
 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  $\mathbf{A}$ .

# Multivariate Normal Distribution and Eigenvalues

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

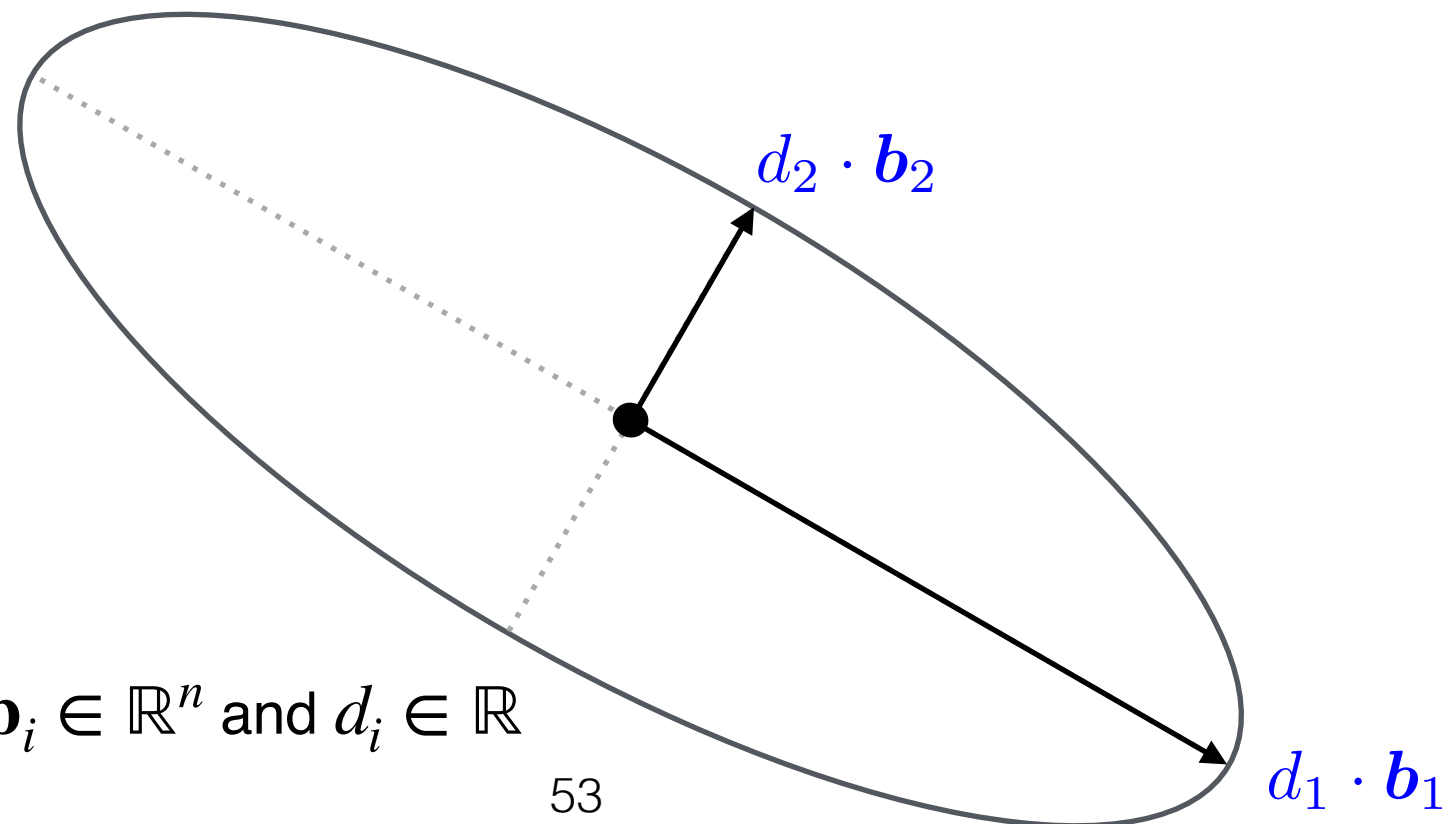
$$\mathbf{C} = d_1^2 \mathbf{b}_1 \mathbf{b}_1^T + \dots + d_N^2 \mathbf{b}_N \mathbf{b}_N^T \quad (1)$$

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

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

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

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



(1)  $\iff$  (2) holds for any  $\mathbf{b}_i \in \mathbb{R}^n$  and  $d_i \in \mathbb{R}$

# Evolution Strategies

Recalling

New search points are sampled normally distributed

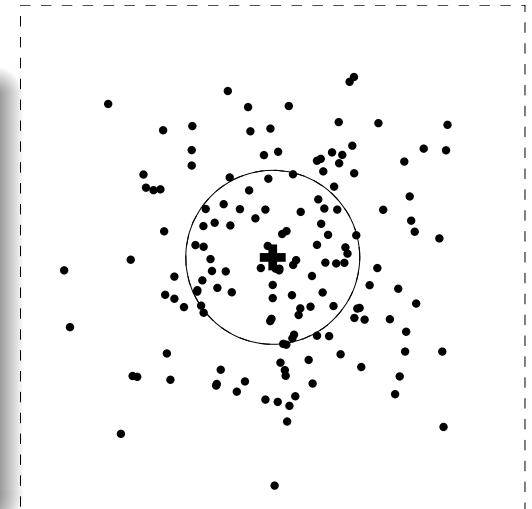
$$\mathbf{x}_i \sim \mathbf{m} + \sigma \mathcal{N}_i(\mathbf{0}, \mathbf{C}) \quad \text{for } i = 1, \dots, \lambda$$

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

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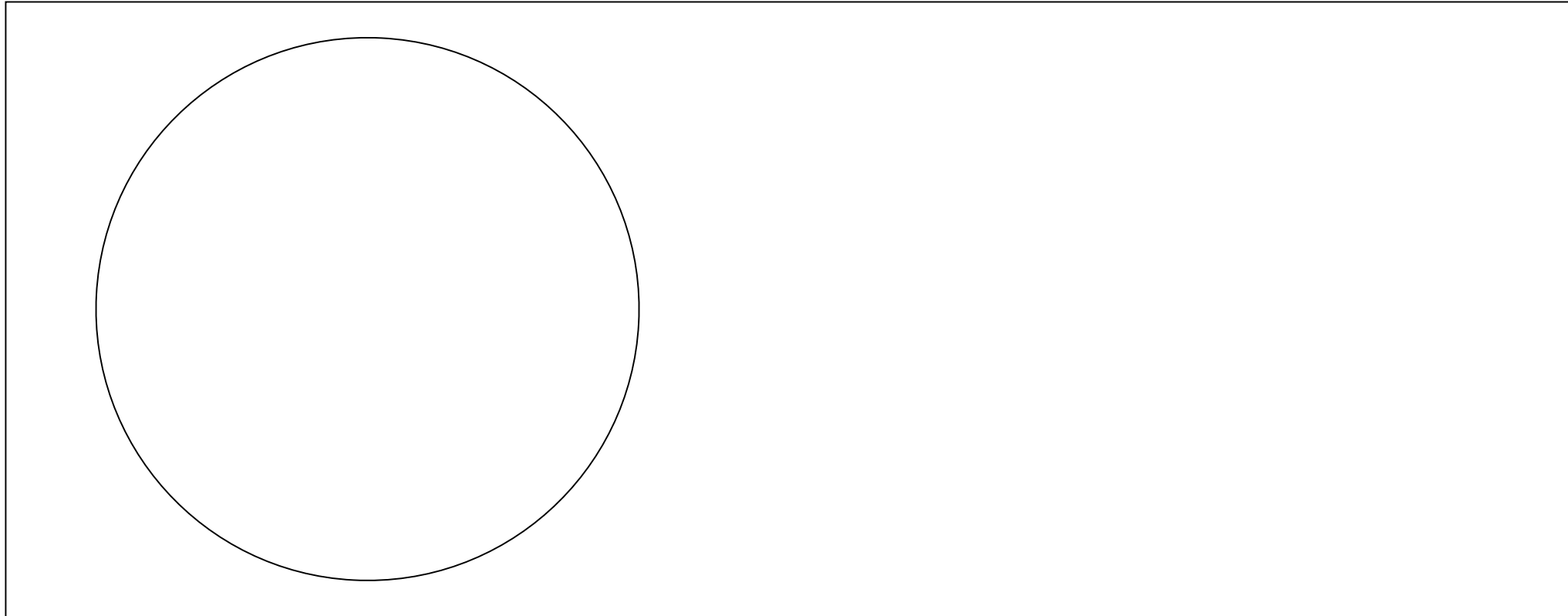
The remaining question is how to update  $\mathbf{C}$ .



# Covariance Matrix Adaptation

## Rank-One Update

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



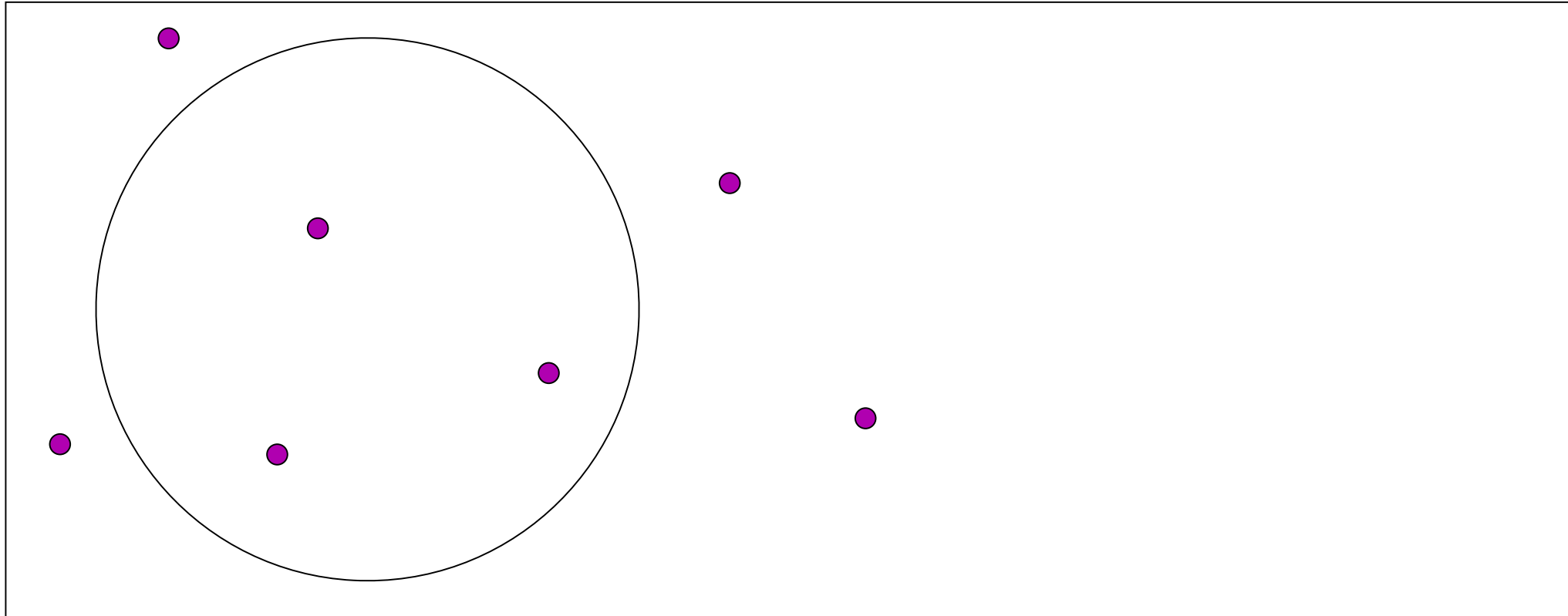
initial distribution,  $\mathbf{C} = \mathbf{I}$

... equations

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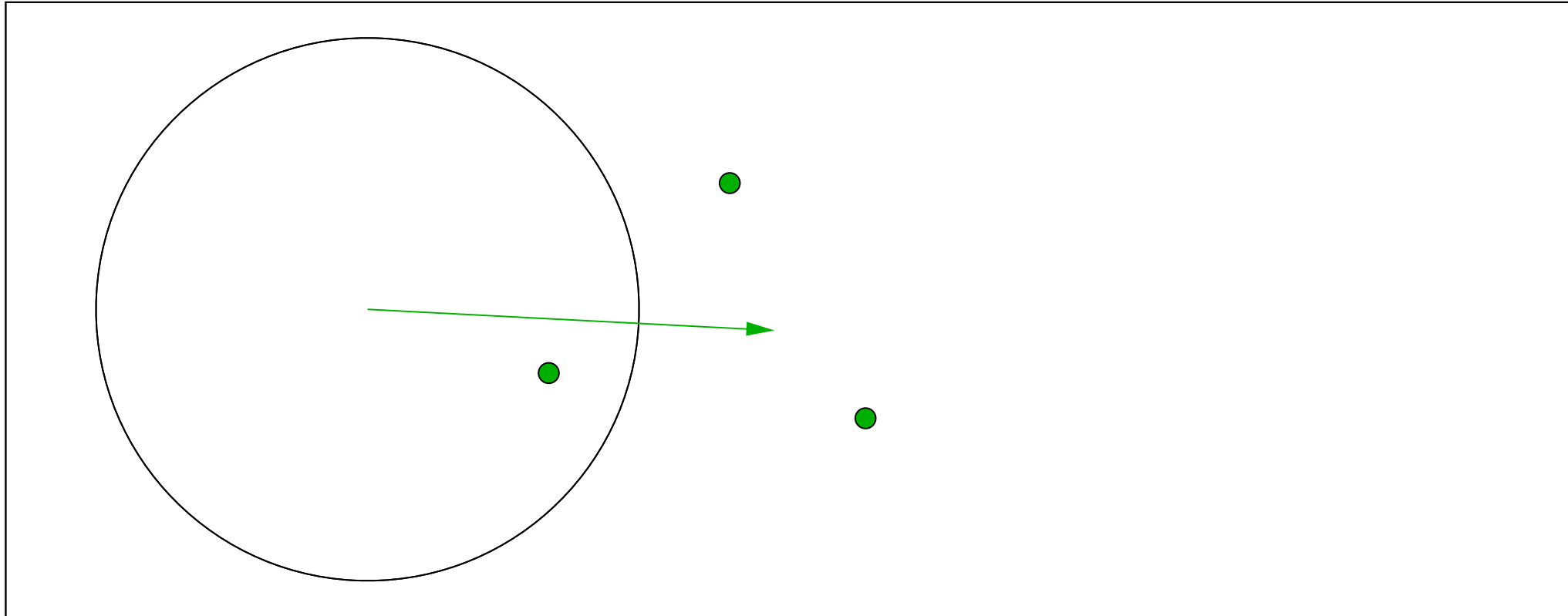
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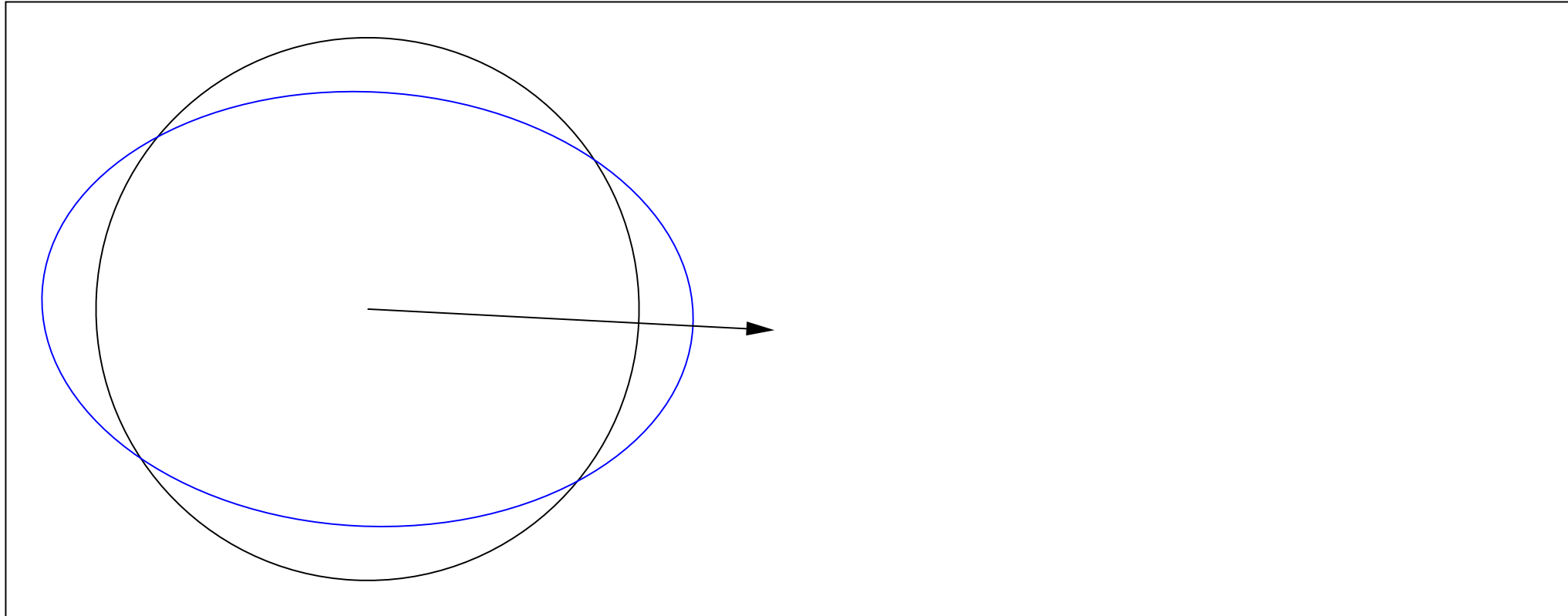
$\mathbf{y}_w$ , movement of the population mean  $\mathbf{m}$  (disregarding  $\sigma$ )

...equations

# Covariance Matrix Adaptation

## Rank-One Update

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



mixture of distribution  $\mathbf{C}$  and step  $\mathbf{y}_w$ ,

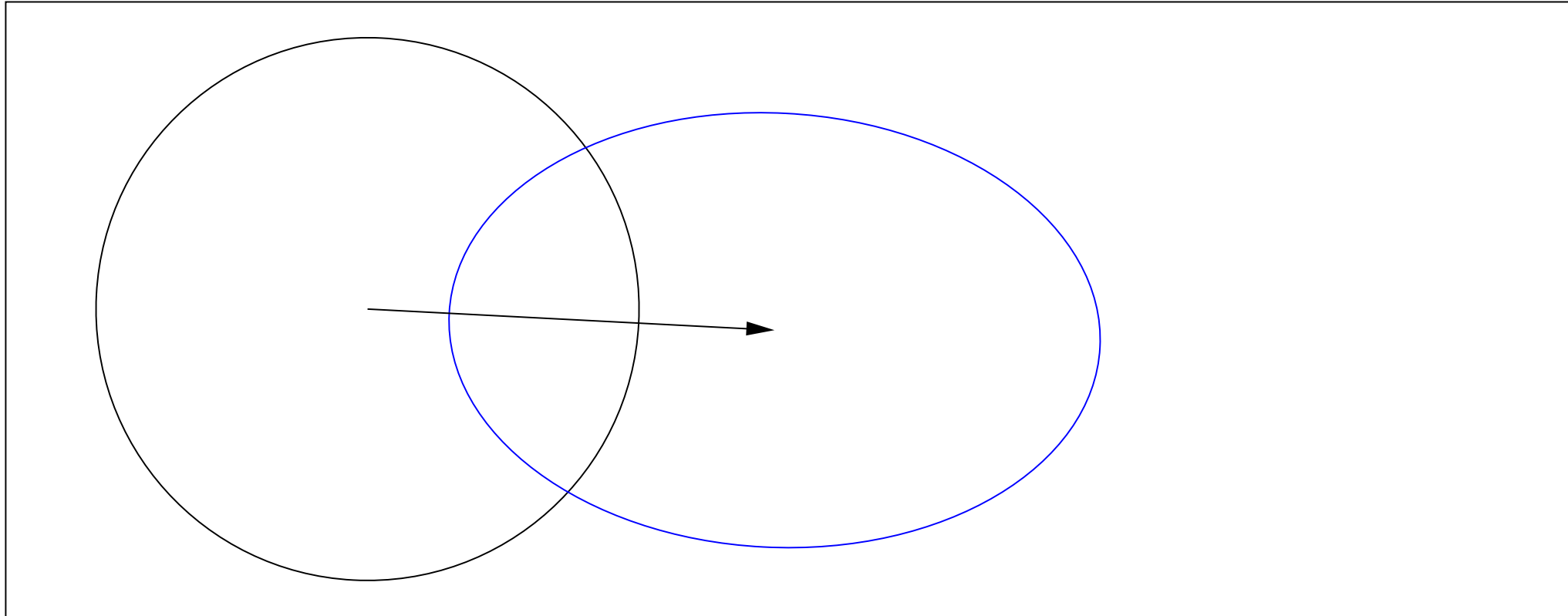
$$\mathbf{C} \leftarrow 0.8 \times \mathbf{C} + 0.2 \times \mathbf{y}_w \mathbf{y}_w^T$$

...equations

# 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 (disregarding  $\sigma$ )

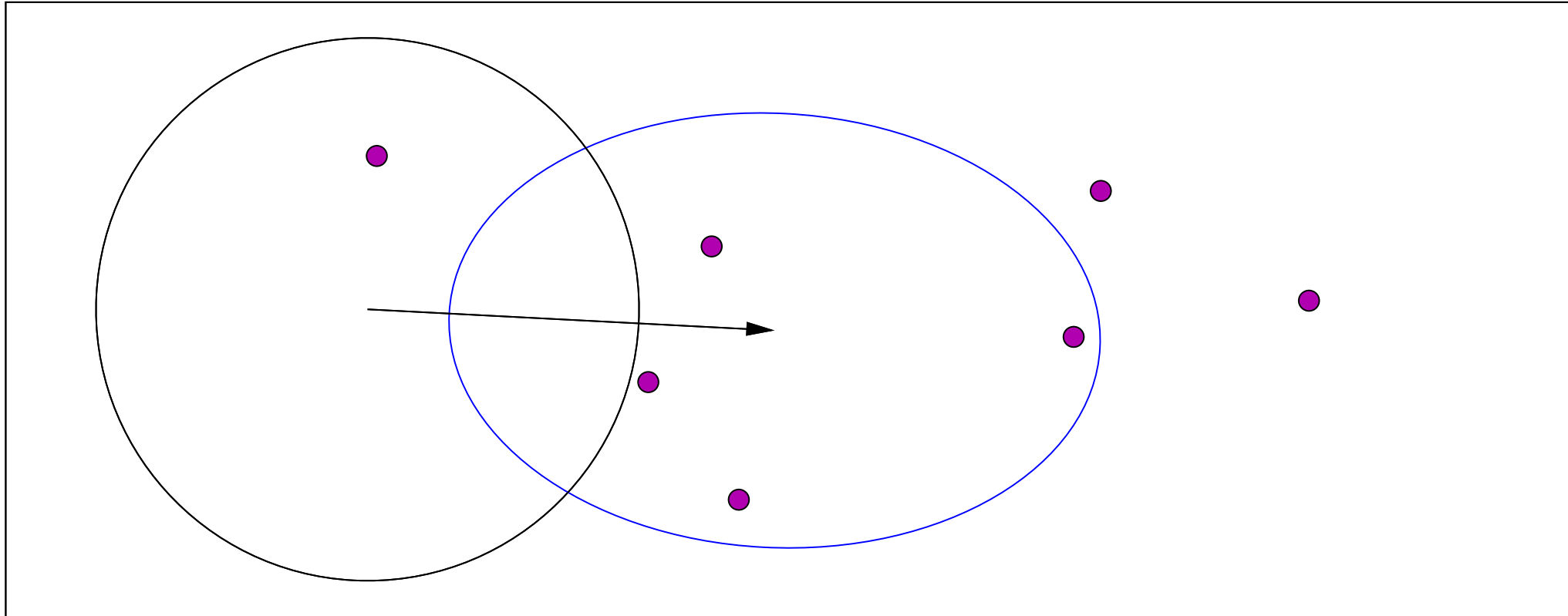
... equations



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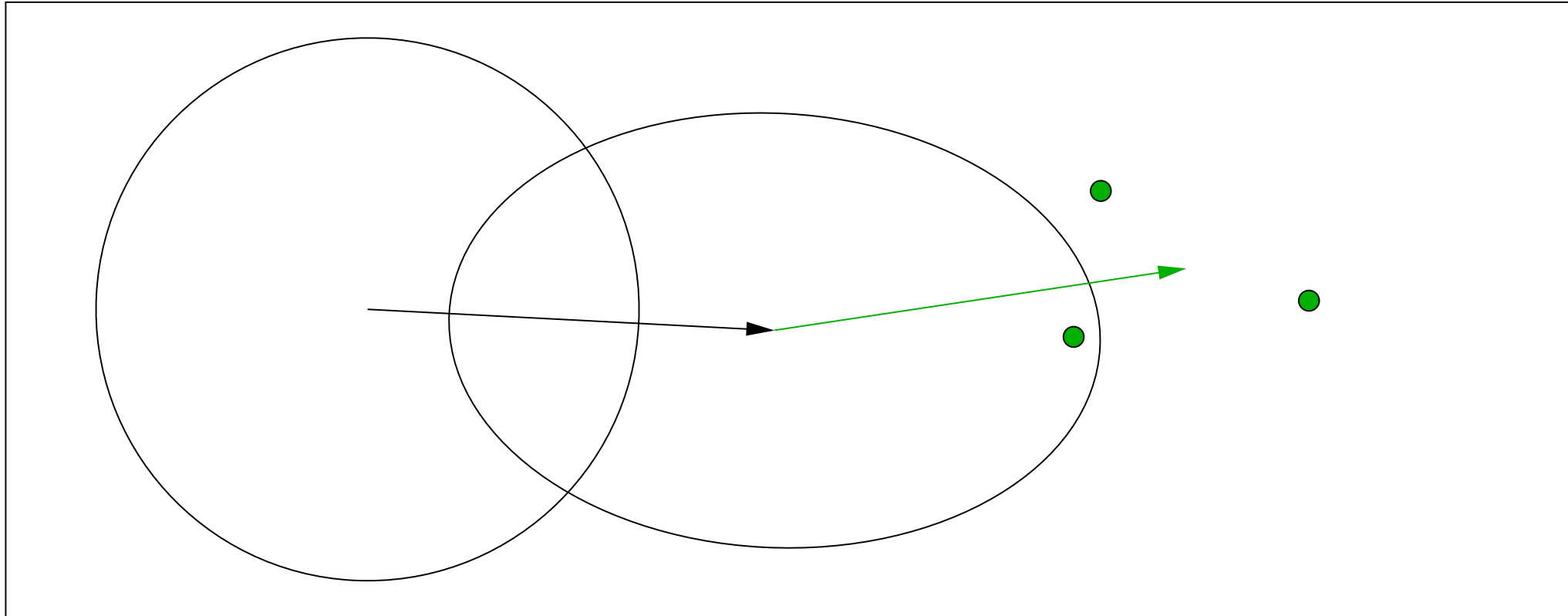
new distribution (disregarding  $\sigma$ )

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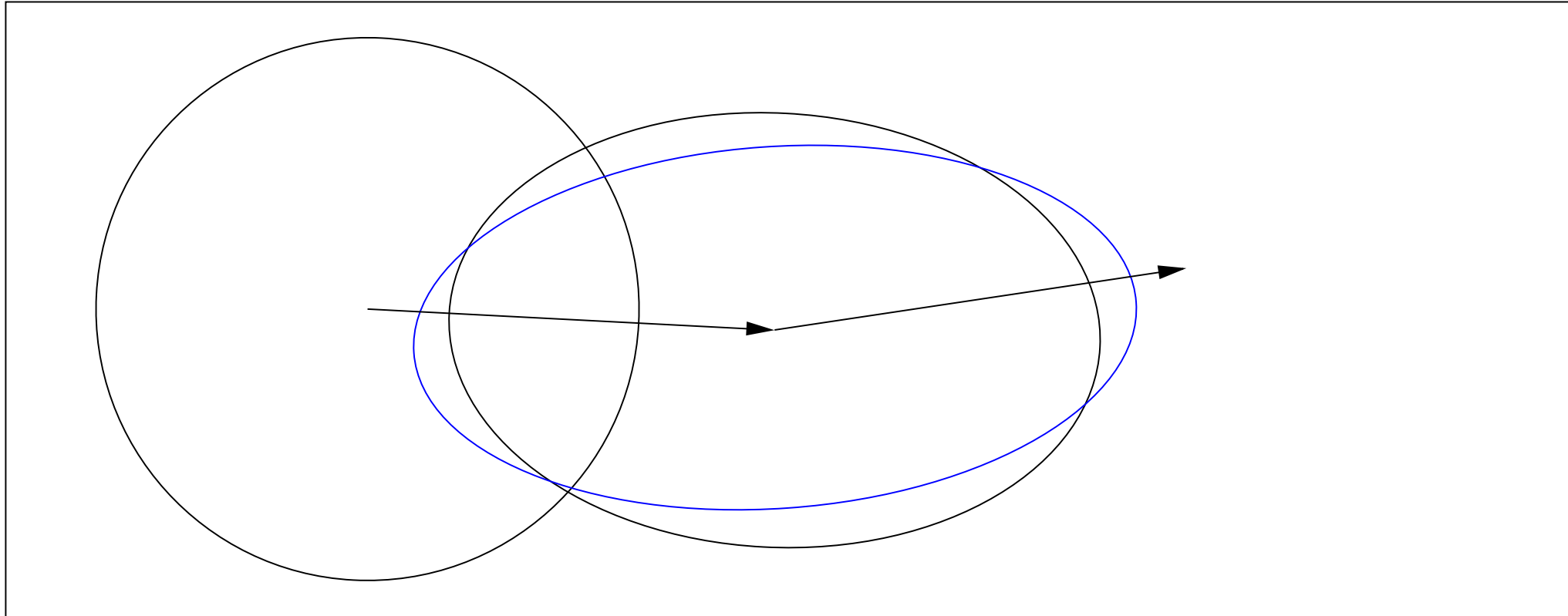
movement of the population mean  $\mathbf{m}$

... equations

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mixture of distribution  $\mathbf{C}$  and step  $\mathbf{y}_w$ ,

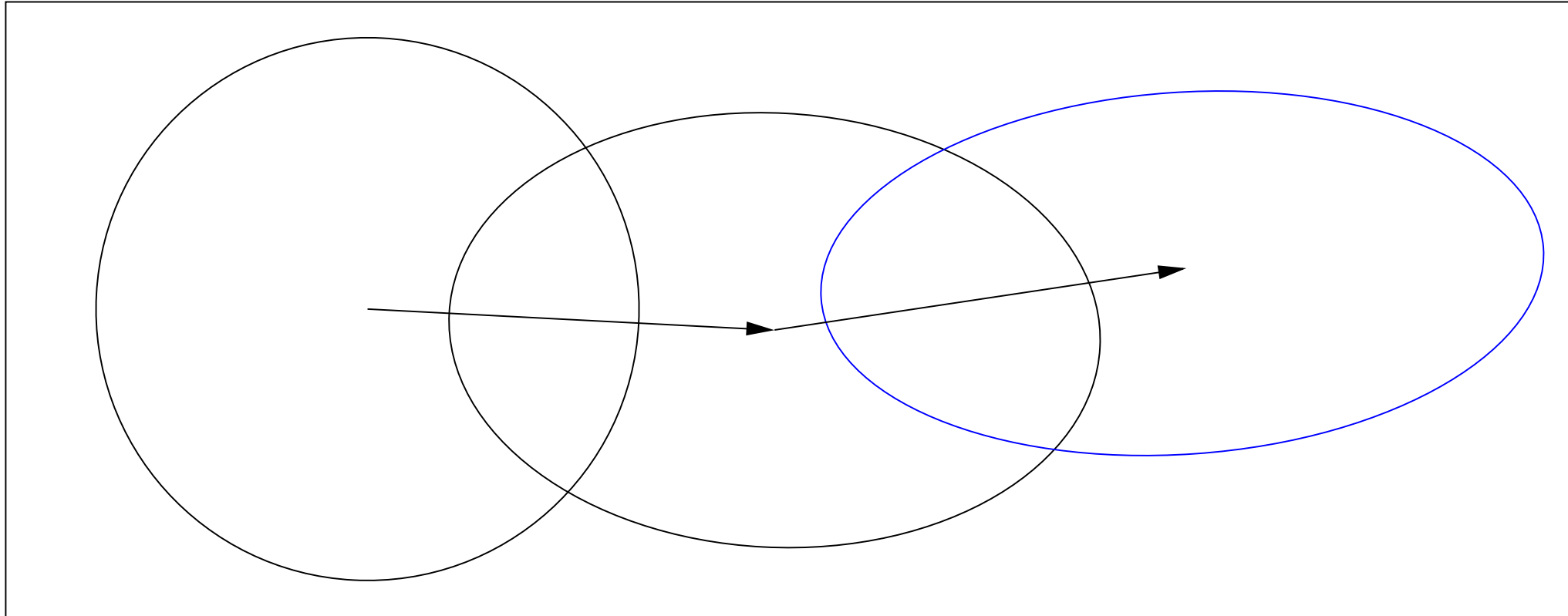
$$\mathbf{C} \leftarrow 0.8 \times \mathbf{C} + 0.2 \times \mathbf{y}_w \mathbf{y}_w^T$$

... equations

# Covariance Matrix Adaptation

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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 likelihood of successful steps**,  $\mathbf{y}_w$ , to appear again

another viewpoint: the adaptation **follows a natural gradient**

approximation of the expected fitness

... equations

# Covariance Matrix Adaptation

## Rank-One Update

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

While not terminate

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

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

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

The rank-one update has been found independently in several domains<sup>6 7 8 9</sup>

<sup>6</sup> Kjellström&Taxén 1981. Stochastic Optimization in System Design, IEEE TCS

<sup>7</sup> Hansen&Ostermeier 1996. Adapting arbitrary normal mutation distributions in evolution strategies: The covariance matrix adaptation, ICEC

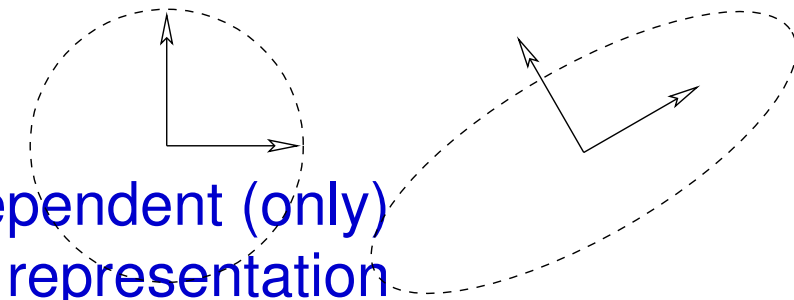
<sup>8</sup> Ljung 1999. System Identification: Theory for the User

<sup>9</sup> Haario et al 2001. An adaptive Metropolis algorithm, JSTOR

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

## 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 principal components / the principal axes of the mutation ellipsoid
- learns a new **rotated problem representation**<sup>[a]</sup>  
components are independent (only)  
in the new representation
- learns a **new** (Mahalanobis) **metric**  
variable metric method
- approximates the **inverse Hessian** on quadratic functions  
transformation into the sphere function
- for  $\mu = 1$ : conducts a **natural gradient ascent** on the distribution  $\mathcal{N}$   
entirely independent of the given coordinate system



[a] invariant under (independently of) search space rotations

# Topics

0. Problem statement

1. What makes an optimization problem difficult to solve?

2. How does the CMA-ES work?

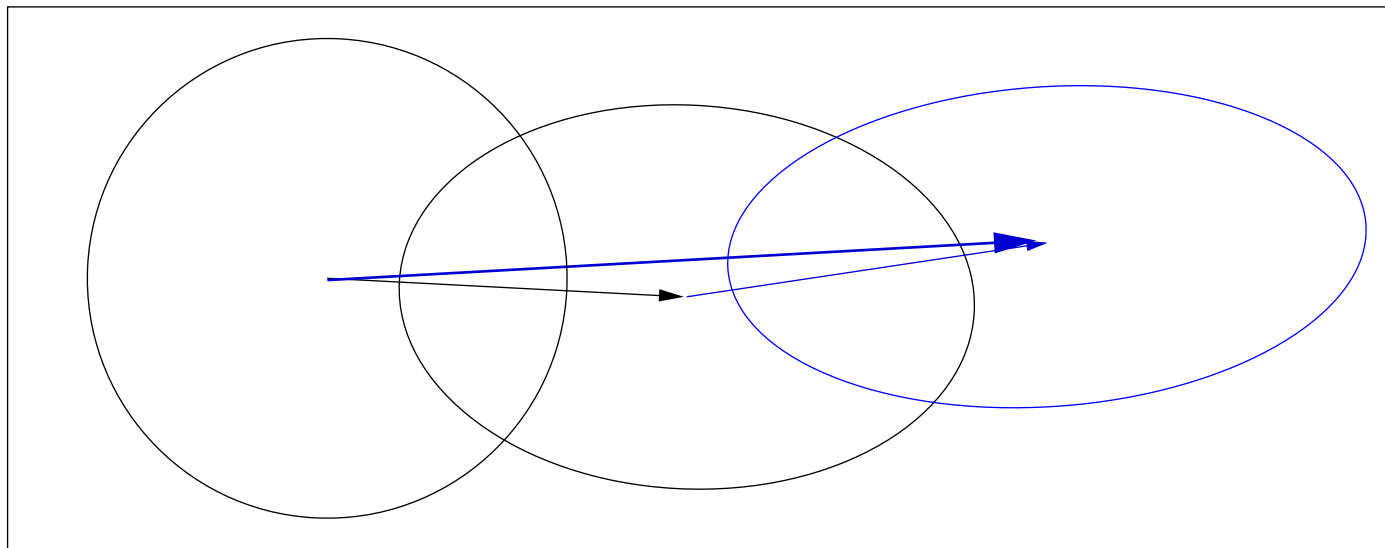
- Normal Distribution, Rank-Based Recombination
- Step-Size Adaptation
- **Covariance Matrix Adaptation**
  - ▶ Rank-One Update and Cumulation
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  - ▶ Active Covariance Update
- Choice of problem formulation and encoding (not covered)
- Choice of initial solution and initial step-size
- Restarts, Increasing Population Size
- Restricted Covariance Matrix

# Cumulation

## The Evolution Path

### Evolution Path

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



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):

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

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
- ...

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

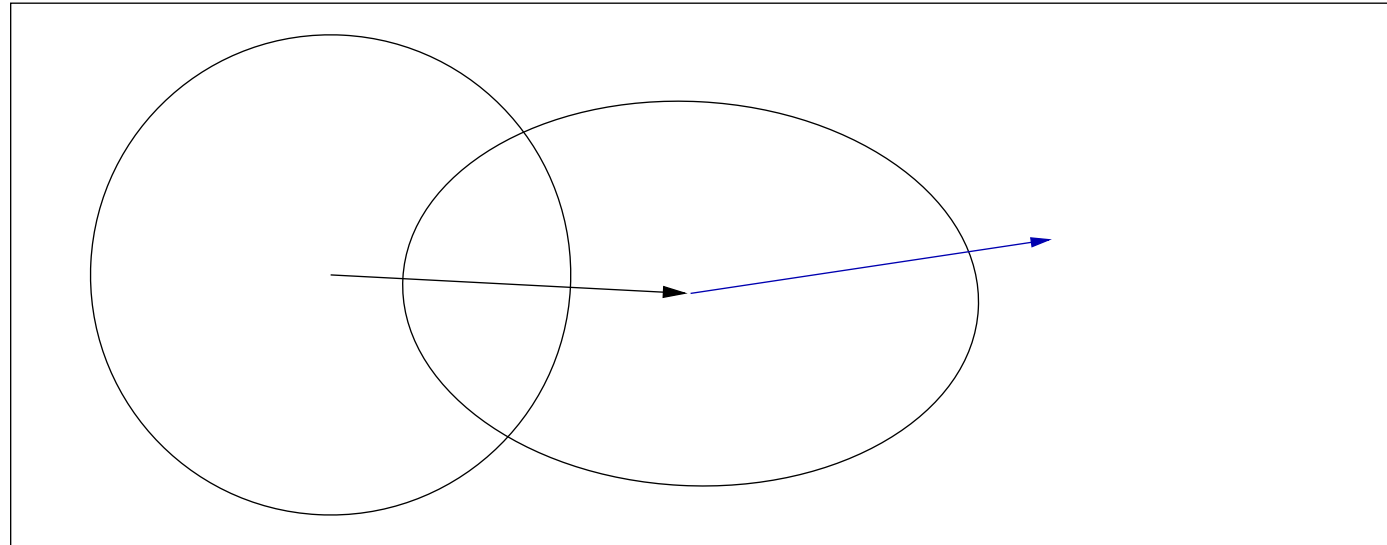
...why?

# Cumulation

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

## 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 lost.



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

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

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

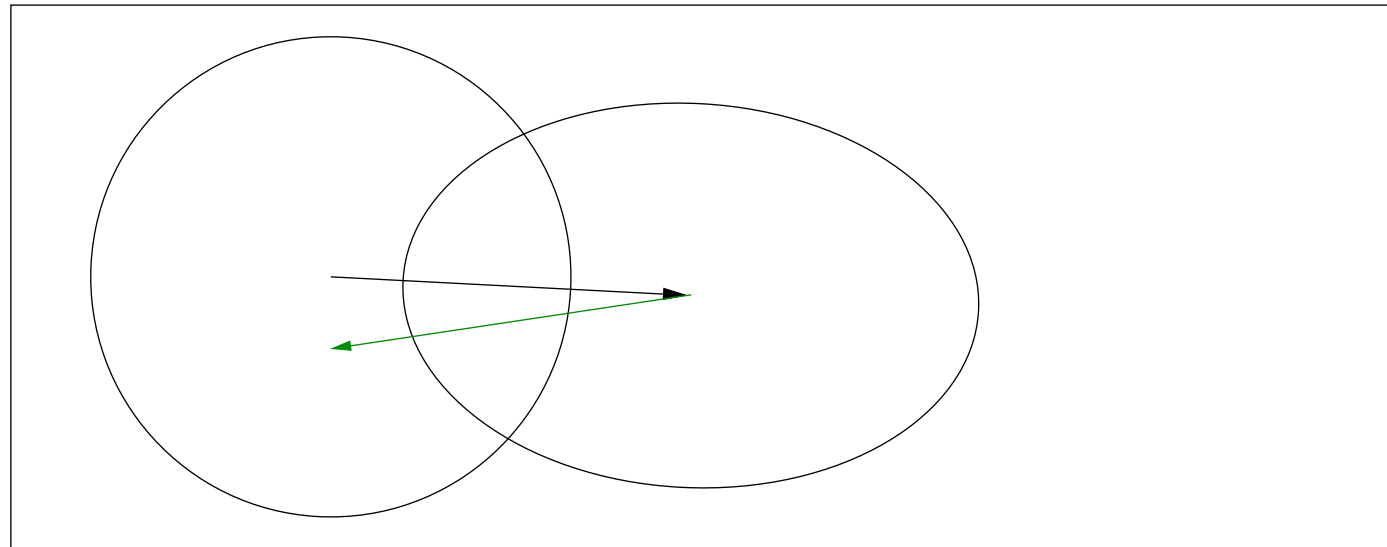
where  $\mu_w = \frac{1}{\sum w_i^2}$ ,  $c_{\text{cov}} \ll c_c \ll 1$  such that  $1/c_c$  is the “backward time horizon”.

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

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

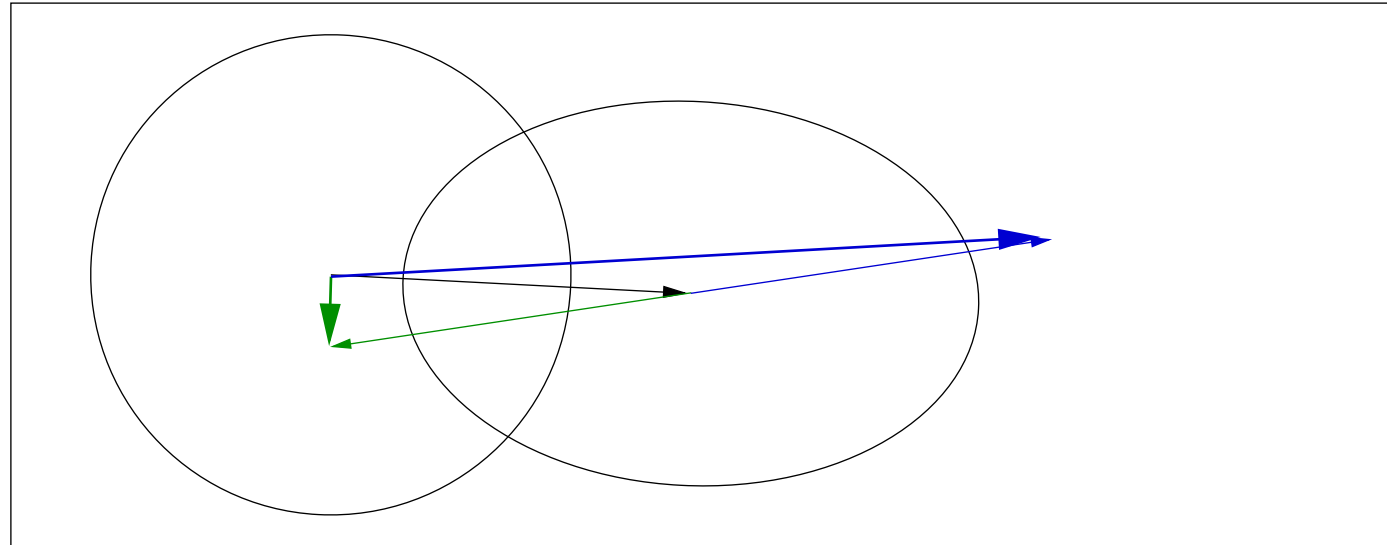
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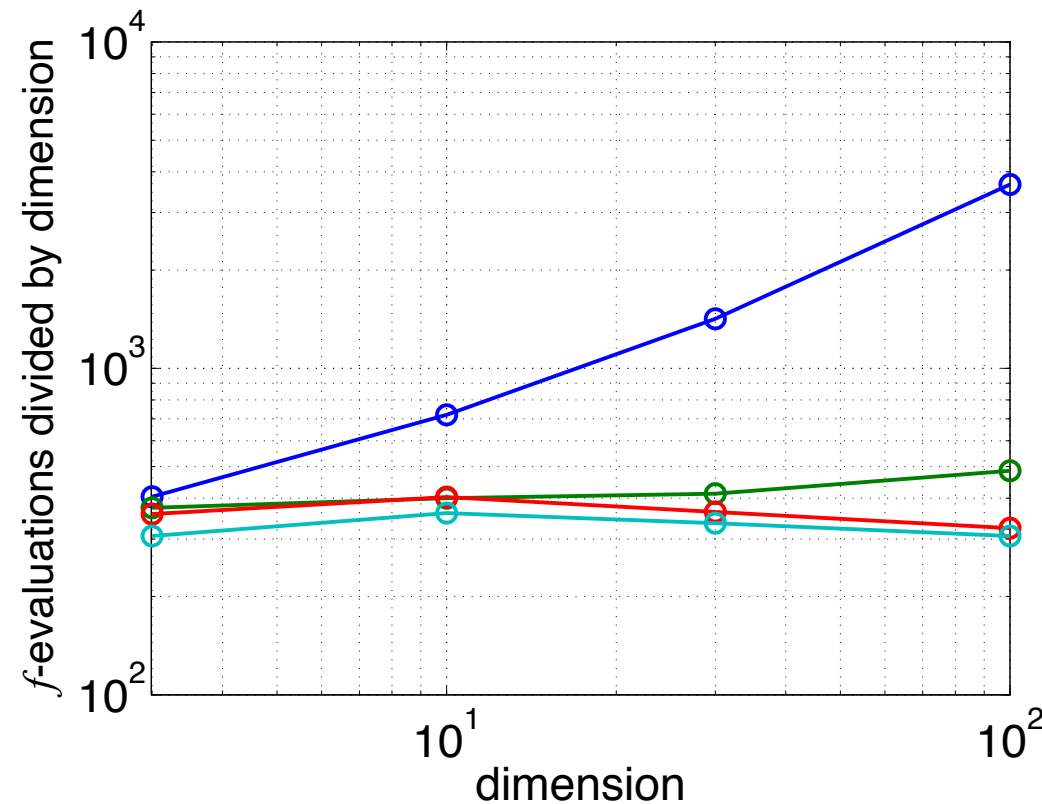
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where  $\mu_w = \frac{1}{\sum w_i^2}$ ,  $c_{\text{cov}} \ll c_c \ll 1$  such that  $1/c_c$  is the “backward time horizon”.

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

<sup>a</sup>Hansen & Auger 2013. Principled design of continuous stochastic search: From theory to practice.

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



$c_c = 1$  (no cumulation)

$c_c = 1/\sqrt{n}$

$c_c = 1/n, 3/(n+3)$

with CSA-ES (without CMA):  $\approx 3 \times 10^7 n$  evaluations

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

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# Rank- $\mu$ 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- $\mu$  update extends the update rule for **large population sizes**  $\lambda$  using  $\mu > 1$  vectors to update  $\mathbf{C}$  at each generation step.

The weighted empirical covariance matrix

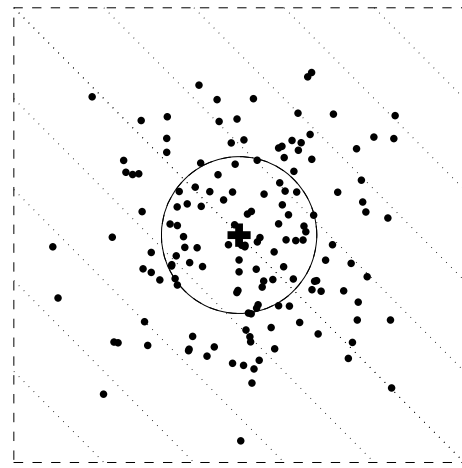
$$\mathbf{C}_\mu = \sum_{i=1}^{\mu} w_i \mathbf{y}_{i:\lambda} \mathbf{y}_{i:\lambda}^T$$

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

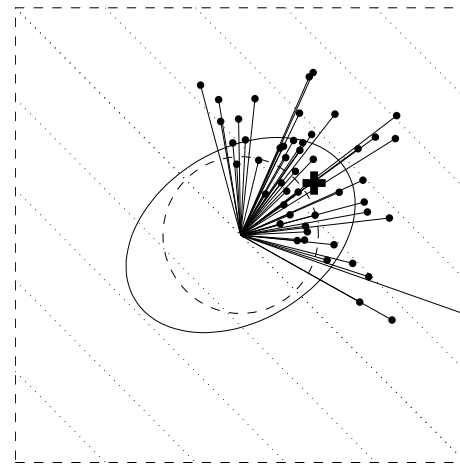
The rank- $\mu$  update then reads

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

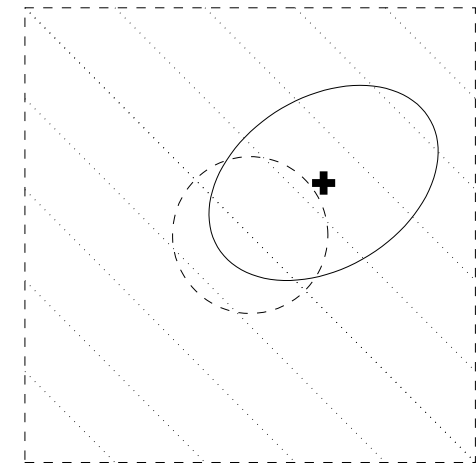
where  $c_{\text{cov}} \approx \mu_w / n^2$  and  $c_{\text{cov}} \leq 1$ .



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



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



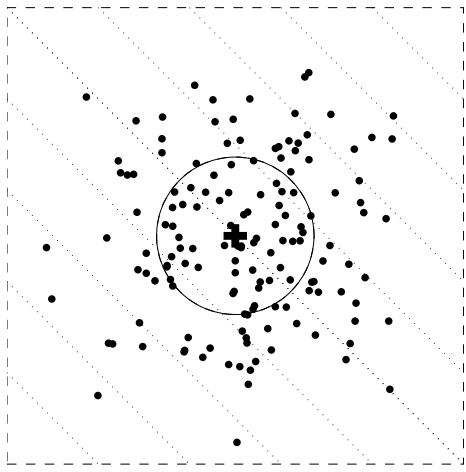
$$m_{\text{new}} \leftarrow m + \frac{1}{\mu} \sum y_{i:\lambda}$$

new distribution

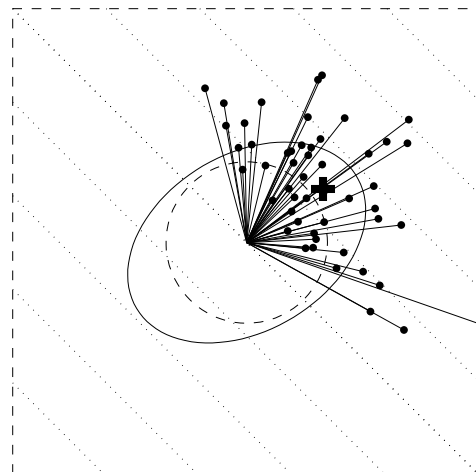
sampling of  $\lambda = 150$   
solutions where  
 $\mathbf{C} = \mathbf{I}$  and  $\sigma = 1$

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

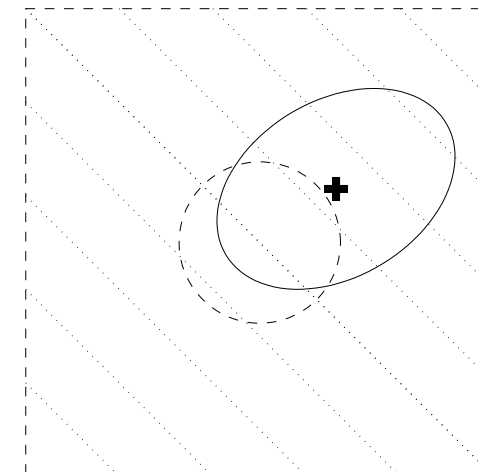


Rank- $\mu$  CMA versus Estimation of Multivariate Normal Algorithm EMNA<sub>global</sub><sup>11</sup>

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

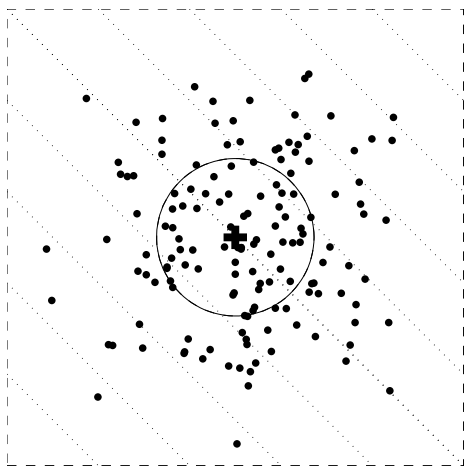


$$\mathbf{C} \leftarrow \frac{1}{\mu} \sum (x_{i:\lambda} - m_{\text{old}})(x_{i:\lambda} - m_{\text{old}})^T$$

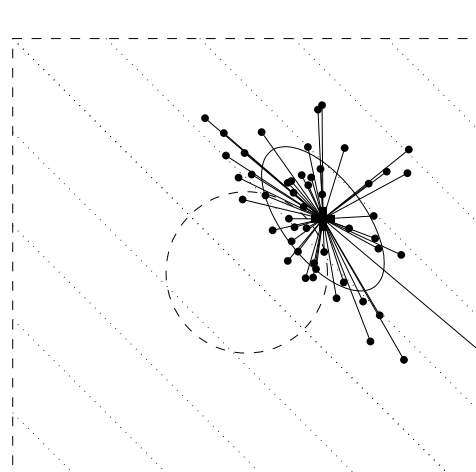


$$m_{\text{new}} = m_{\text{old}} + \frac{1}{\mu} \sum y_{i:\lambda}$$

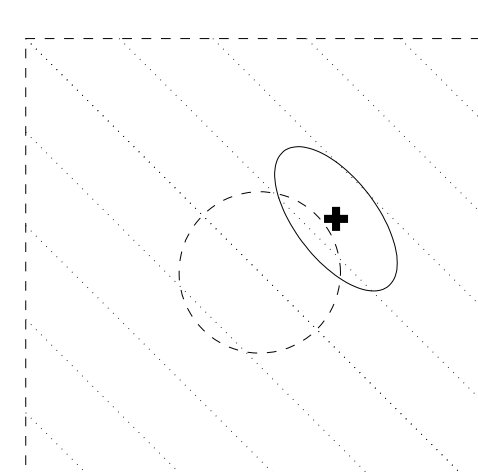
rank- $\mu$  CMA  
conducts a  
PCA of  
steps



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



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



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

EMNA<sub>global</sub>  
conducts a  
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sampling of  $\lambda = 150$   
solutions (dots)

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

new distribution

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

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

## The rank- $\mu$ update

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

Therefore the rank- $\mu$  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- $\mu$  update can be combined

... all equations

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

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# Active Update

utilize negative weights [Jastrebski and Arnold, 2006]

$$\mathbf{C} \leftarrow (1 - c_1 - c_\mu + c_\mu^-) \mathbf{C} + c_1 \mathbf{p}_c \mathbf{p}_c^T + c_\mu \sum_{i=1}^{\lfloor \lambda/2 \rfloor} w_i \mathbf{y}_{i:\lambda} \mathbf{y}_{i:\lambda}^T - \overbrace{c_\mu^- \sum_{i=\lambda-\mu}^{\lambda} |w_i| \mathbf{y}_{i:\lambda} \mathbf{y}_{i:\lambda}^T}^{\text{decreasing the variances in unpromising directions}}$$

- $-|w_i| < 0$  (for  $i \geq \lambda - \mu$ ): negative weight assigned to  $\mathbf{y}_{i:\lambda}$ ,  $\sum_{i=\lambda-\mu}^{\lambda} |w_i| \approx 1$
- $c_\mu^- > 0$ : learning rate for the active update
- increases the variance in the directions of  $\mathbf{p}_c$  and promising steps  $\mathbf{y}_{i:\lambda}$  ( $i \leq \lfloor \lambda/2 \rfloor$ )
- decrease the variance in the directions of unpromising steps  $\mathbf{y}_{i:\lambda}$  ( $i \geq \lambda - \lfloor \lambda/2 \rfloor + 1$ )
- keep the variance in the subspace orthogonal to the above

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

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

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

**While** not terminate

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

$\mathbf{m} \leftarrow \mathbf{m} + c_m \sigma \mathbf{y}_w$ , where  $\mathbf{y}_w = \sum_{i=1}^{\mu} w_i \mathbf{y}_{\text{rk}^{-1}(i)}$  update mean

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

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

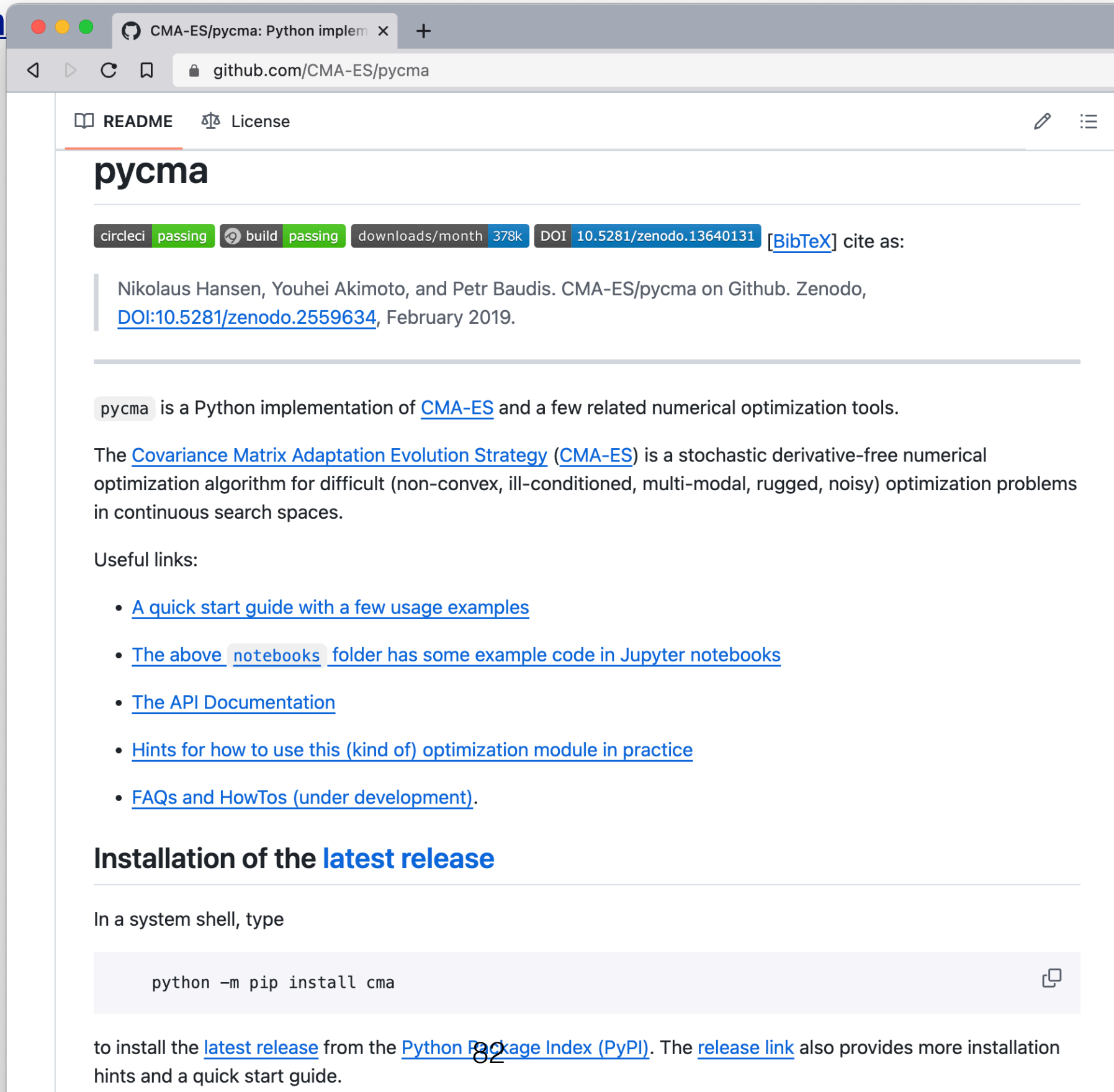
$\sigma \leftarrow \sigma \times \exp \left( \frac{c_\sigma}{d_\sigma} \left( \frac{\|\mathbf{p}_\sigma\|}{\mathbb{E} \|\mathcal{N}(\mathbf{0}, \mathbf{I})\|} - 1 \right) \right)$  update of  $\sigma$

$\mathbf{C} \leftarrow \mathbf{C} + c_\mu \sum_{i=1}^{\lambda} w_{\text{rk}(i)} (\mathbf{y}_i \mathbf{y}_i^\top - \mathbf{C}) + c_1 (\mathbf{p}_c \mathbf{p}_c^\top - \mathbf{C})$  update  $\mathbf{C}$

*Not covered:* termination, restarts, useful output, search boundaries and encoding, corrections for: positive definiteness guaranty,  $\mathbf{p}_c$  variance loss,  $c_\sigma$  and  $d_\sigma$  for large  $\lambda$

# Python CMA-ES Implementation

<https://github.com>



The screenshot shows the GitHub repository page for CMA-ES/pycma. The browser address bar shows the URL `github.com/CMA-ES/pycma`. The repository name `pycma` is prominently displayed. Below the name, there are several status indicators: `circleci` with a green `passing` badge, `build` with a green `passing` badge, `downloads/month` with a blue `378k` badge, and `DOI` with a blue `10.5281/zenodo.13640131` badge. A `[BibTeX]` link is also present. The page content includes a `README` section with the following text:

`pycma` is a Python implementation of [CMA-ES](#) and a few related numerical optimization tools.

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

Useful links:

- [A quick start guide with a few usage examples](#)
- [The above `notebooks` folder has some example code in Jupyter notebooks](#)
- [The API Documentation](#)
- [Hints for how to use this \(kind of\) optimization module in practice](#)
- [FAQs and HowTos \(under development\)](#).

**Installation of the latest release**

In a system shell, type

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

to install the [latest release](#) from the [Python Package Index \(PyPI\)](#). The [release link](#) also provides more installation hints and a quick start guide.



# Python CMA-ES Demo

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

## Optimizing the 11D Rosenbrock Function

```

1 import cma
2
3 x, es = cma.fmin2(cma.ff.rosen, 11 * [0.1], 0.1, {'verb_disp_overwrite': 200})
4 es.plot(); # cma.plot() # works too

```

✓ 1.2s

Python

(5\_w,11)-aCMA-ES (mu\_w=3.4,w\_1=42%) in dimension 11 (seed=329070, Fri Sep 13 13:55:03 2024)

Iterat	#Fevals	function value	axis ratio	sigma	min&max	std	t[m:s]
1	11	1.807461200564364e+01	1.0e+00	9.01e-02	9e-02	9e-02	0:00.0
2	22	1.609456060870233e+01	1.1e+00	8.18e-02	8e-02	8e-02	0:00.0
3	33	1.501834332056772e+01	1.2e+00	7.39e-02	7e-02	7e-02	0:00.0
100	1100	7.225343889168434e+00	5.6e+00	1.84e-02	8e-03	2e-02	0:00.1
200	2200	3.475523910468565e+00	1.1e+01	2.94e-02	8e-03	3e-02	0:00.1
619	6809	2.441368464931154e-14	6.4e+01	2.14e-07	4e-09	1e-07	0:00.3

termination on tolfun=1e-11 (Fri Sep 13 13:55:04 2024)

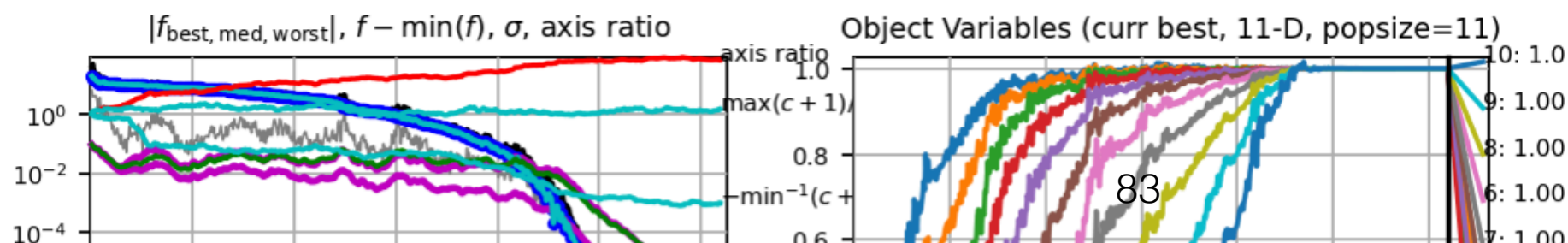
final/bestever f-value = 1.235402e-14 1.235402e-14 after 6810/6810 evaluations

incumbent solution: [1. 1. 1. 1. 1. 1. 1. 1. ...]

std deviations: [3.73610667e-09 3.79778919e-09 3.80249505e-09 3.97976791e-09

4.15284285e-09 5.01249494e-09 8.22295518e-09 1.37738208e-08 ...]

Figure 374





```

35 1.501854552050772e+01 1.2e+00 7.55e-02 7e-02 7e-02 0:00.0
100 1100 7.225343889168434e+00 5.6e+00 1.84e-02 8e-03 2e-02 0:00.1
200 2200 3.475523910468565e+00 1.1e+01 2.94e-02 8e-03 3e-02 0:00.1
619 6809 2.441368464931154e-14 6.4e+01 2.14e-07 4e-09 1e-07 0:00.3

```

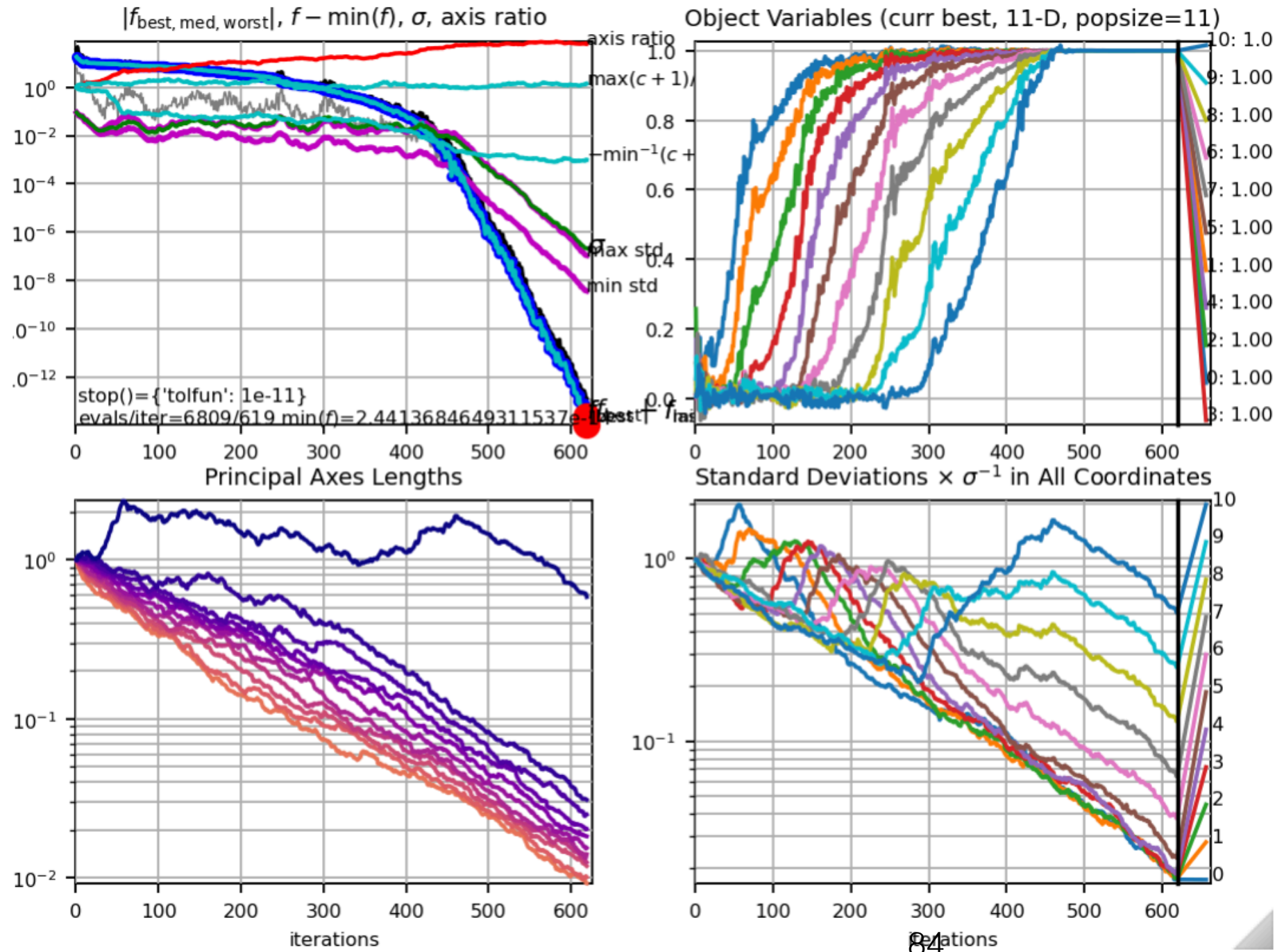
termination on tolfun=1e-11 (Fri Sep 13 13:55:04 2024)

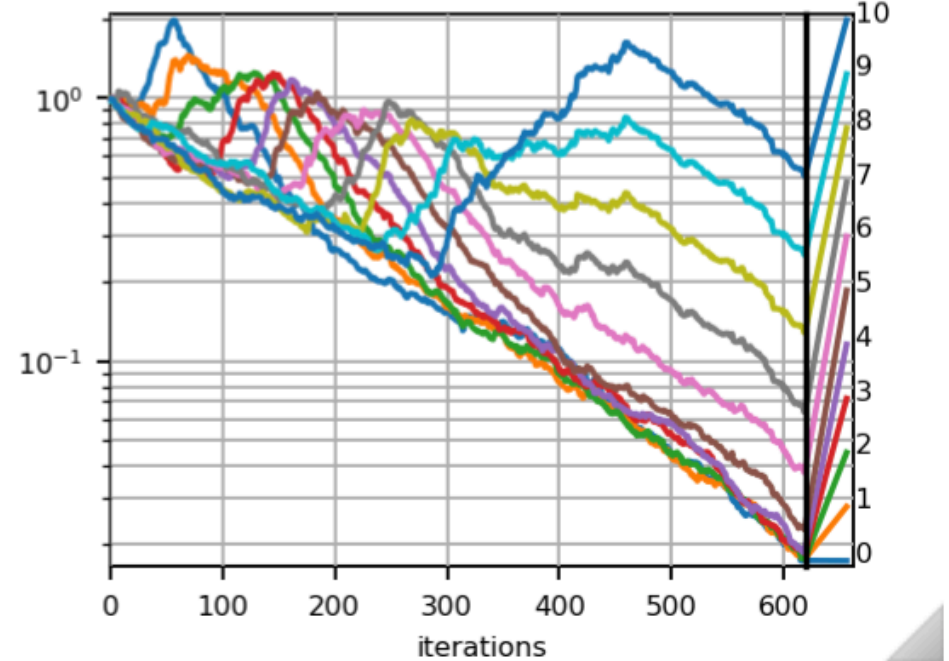
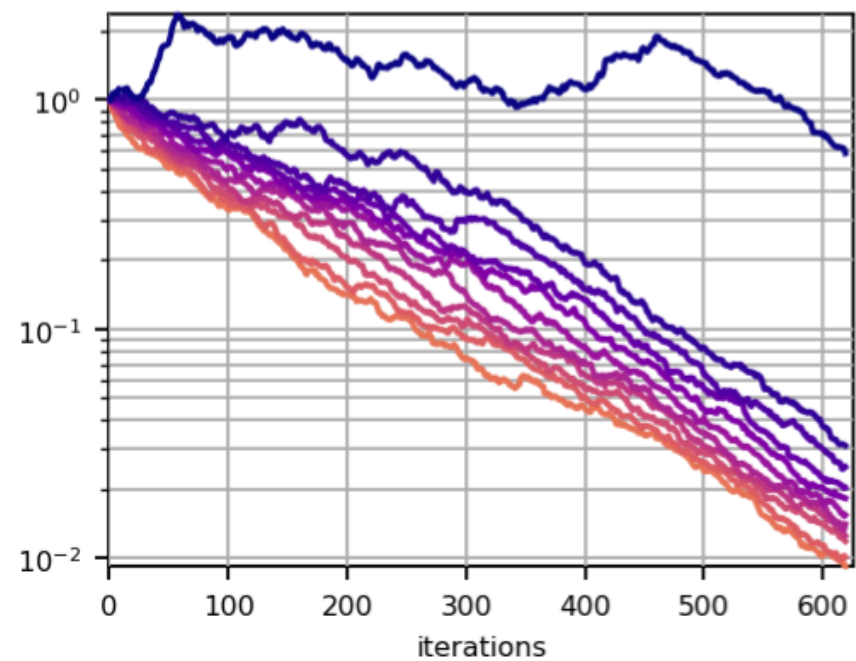
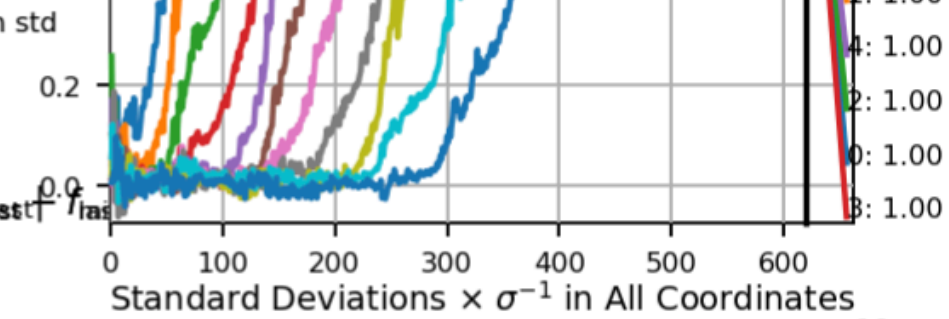
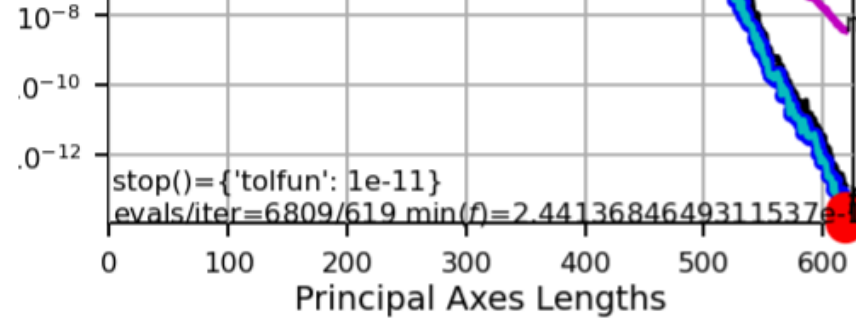
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Figure 374





```
1 cma.CMAOptions('tol')
```

✓ 0.0s

Python

```
{'mindx': '0 #v minimal std in any arbitrary direction, cave interference with tol*',
 'minstd': '0 #v minimal std (scalar or vector) in any coordinate direction, cave interference with tol*',
 'tolconditioncov': '1e14 #v stop if the condition of the covariance matrix is above `tolconditioncov`',
 'tolfacupx': '1e3 #v termination when step-size increases by tolfacupx (diverges). That is, the initial step-size',
 'tolflatfitness': '1 #v iterations tolerated with flat fitness before termination',
 'tolfun': '1e-11 #v termination criterion: tolerance in function value, quite useful',
 'tolfunhist': '1e-12 #v termination criterion: tolerance in function value history',
 'tolfunrel': '0 #v termination criterion: relative tolerance in function value: Delta f current < tolfunrel * (me',
 'tolstagnation': 'int(100 + 100 * N**1.5 / popsize) #v termination if no improvement over tolstagnation iteration',
 'tolupsigma': '1e20 #v sigma/sigma0 > tolupsigma * max(eivenvals(C)**0.5) indicates "creeping behavior" with usua',
 'tolx': '1e-11 #v termination criterion: tolerance in x-changes',
 'tolxstagnation': '[1e-9, 20, 0.1] #v termination thresholds for Delta of [mean, iterations, iterations fraction]
```

# Topics

0. Problem statement

1. What makes an optimization problem difficult to solve?

2. How does the CMA-ES work?

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

3. What can users do?

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



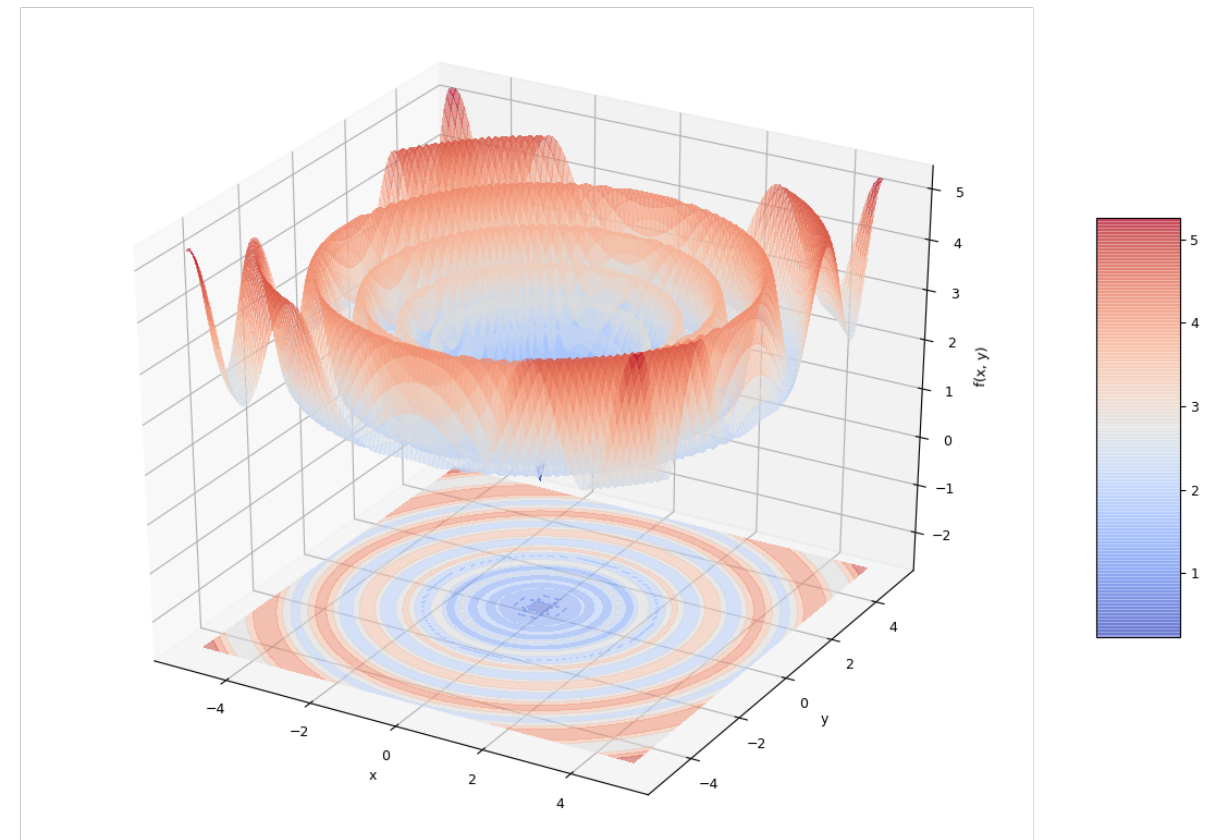
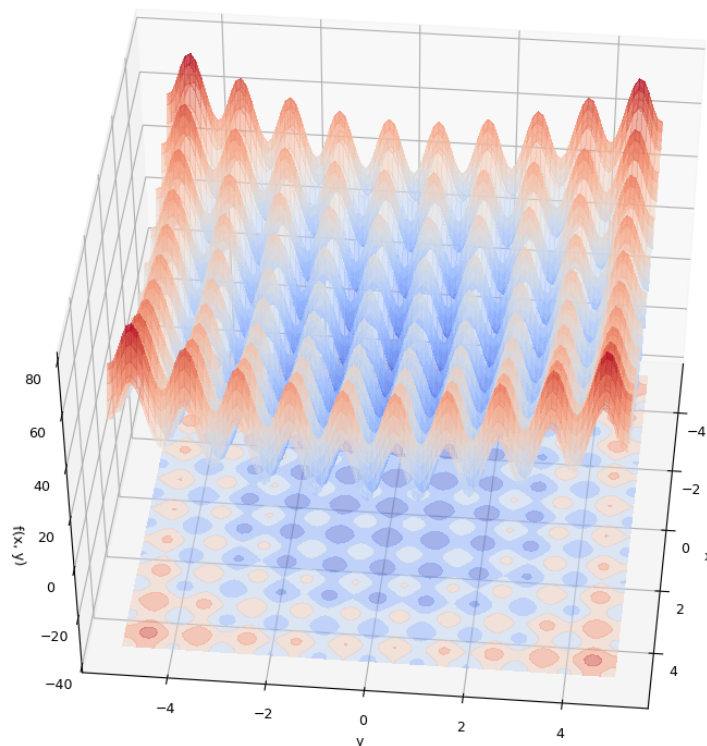
# Multimodality

Approaches for multimodal functions: Try again with

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

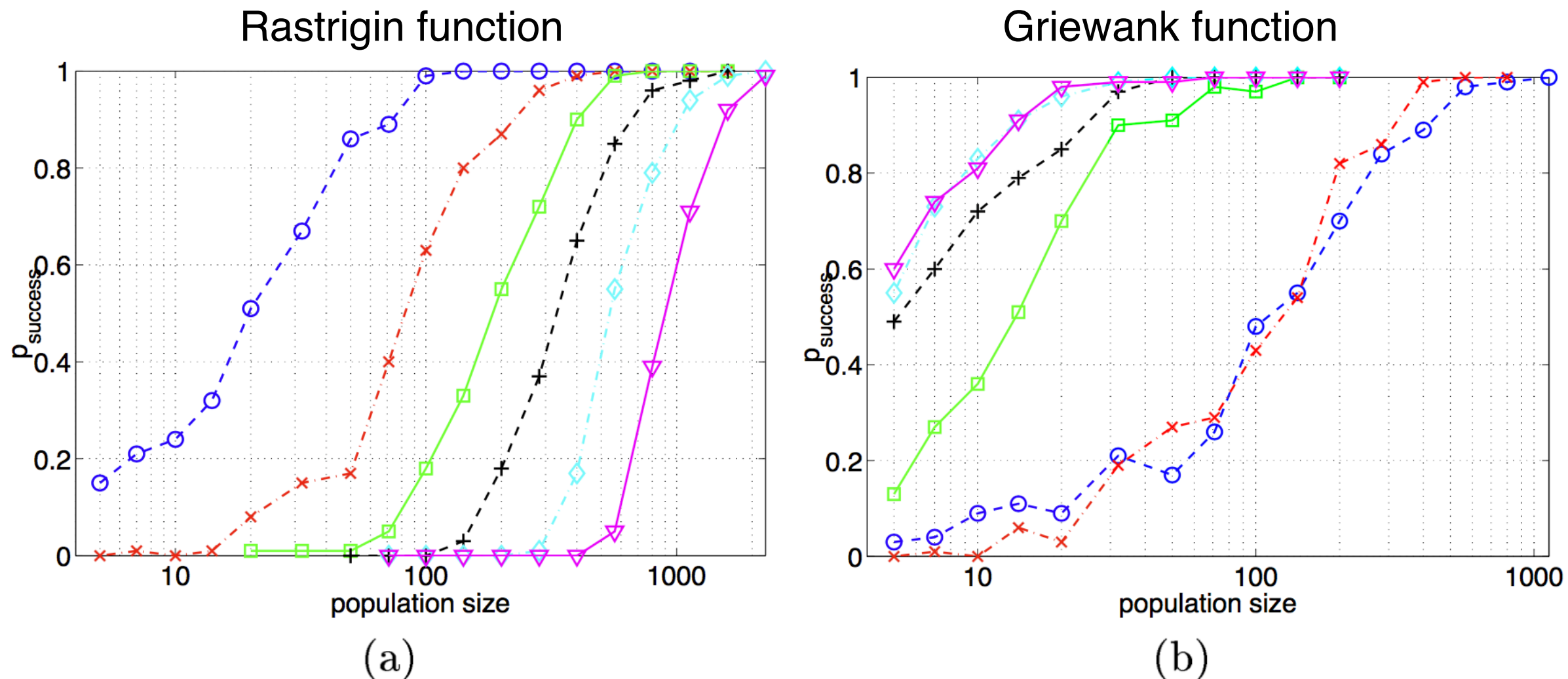
A restart with a **large population size** helps if the objective function has a **well global structure**

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



# Multimodality

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



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

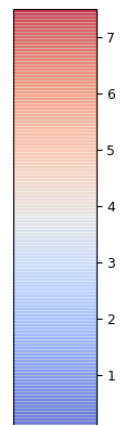
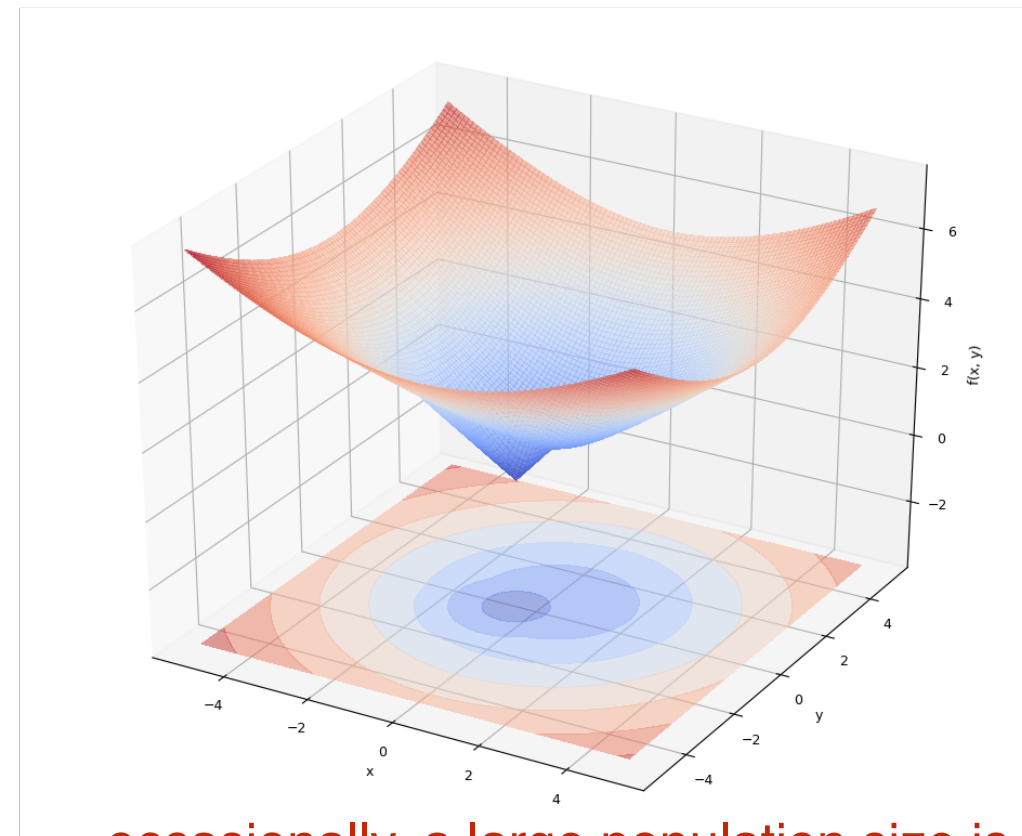
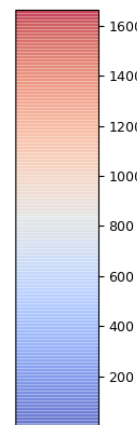
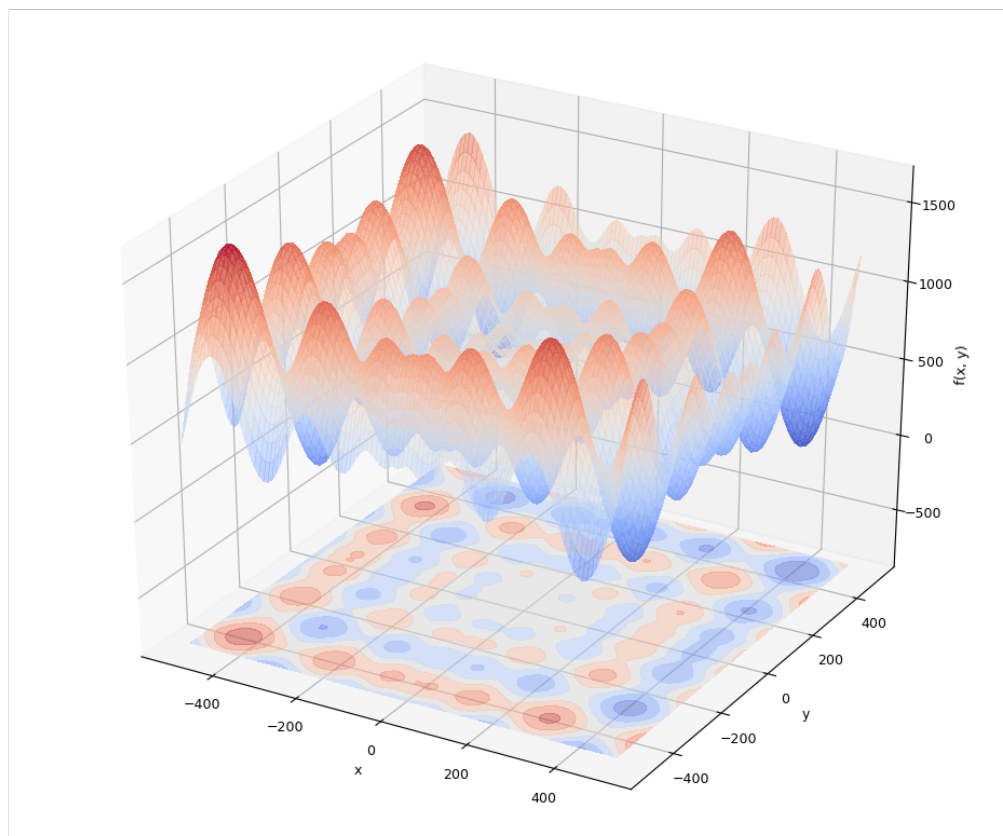
# Multimodality

Approaches for multimodal functions: Try again with

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

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

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



occasionally, a large population size is even counterproductive

# Restart Strategy

It makes the CMA-ES parameter free

**IPOP: Restart with increasing the population size**

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

**BIPOP: IPOP regime + Local search regime**

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

# Summary and Final Remarks



# The Continuous Search Problem

**Difficulties** of a non-linear optimization problem are

- dimensionality and non-separability

demands to exploit problem structure, e.g. neighborhood  
caveat: design of benchmark functions

- ill-conditioning

demands to acquire a second order model

- ruggedness

demands a non-local (stochastic? population based?) approach

# Main Characteristics of (CMA) Evolution Strategies

- 1 Multivariate normal distribution to generate new search points  
follows the maximum entropy principle
- 2 Rank-based selection  
implies invariance, same performance on  $g(f(\mathbf{x}))$  for any increasing  $g$   
more invariance properties are featured
- 3 Step-size control facilitates fast (log-linear) convergence and possibly linear scaling with the dimension  
in CMA-ES based on an **evolution path** (a non-local trajectory)
- 4 *Covariance matrix adaptation (CMA)* **increases the likelihood of previously successful steps** and can improve performance by orders of magnitude

the update follows the natural gradient  
 $\mathbf{C} \propto \mathbf{H}^{-1} \iff$  adapts a variable metric  
 $\iff$  new (rotated) problem representation  
 $\implies f : \mathbf{x} \mapsto g(\mathbf{x}^T \mathbf{H} \mathbf{x})$  reduces to  $\mathbf{x} \mapsto \mathbf{x}^T \mathbf{x}$

# Limitations

## of CMA Evolution Strategies

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

# Thank you

**Source code** for CMA-ES in C, C++, Java, Matlab, Octave, Python, R, Scilab  
and

**Practical hints** for problem formulation, variable encoding, parameter setting  
are available (or linked to) at

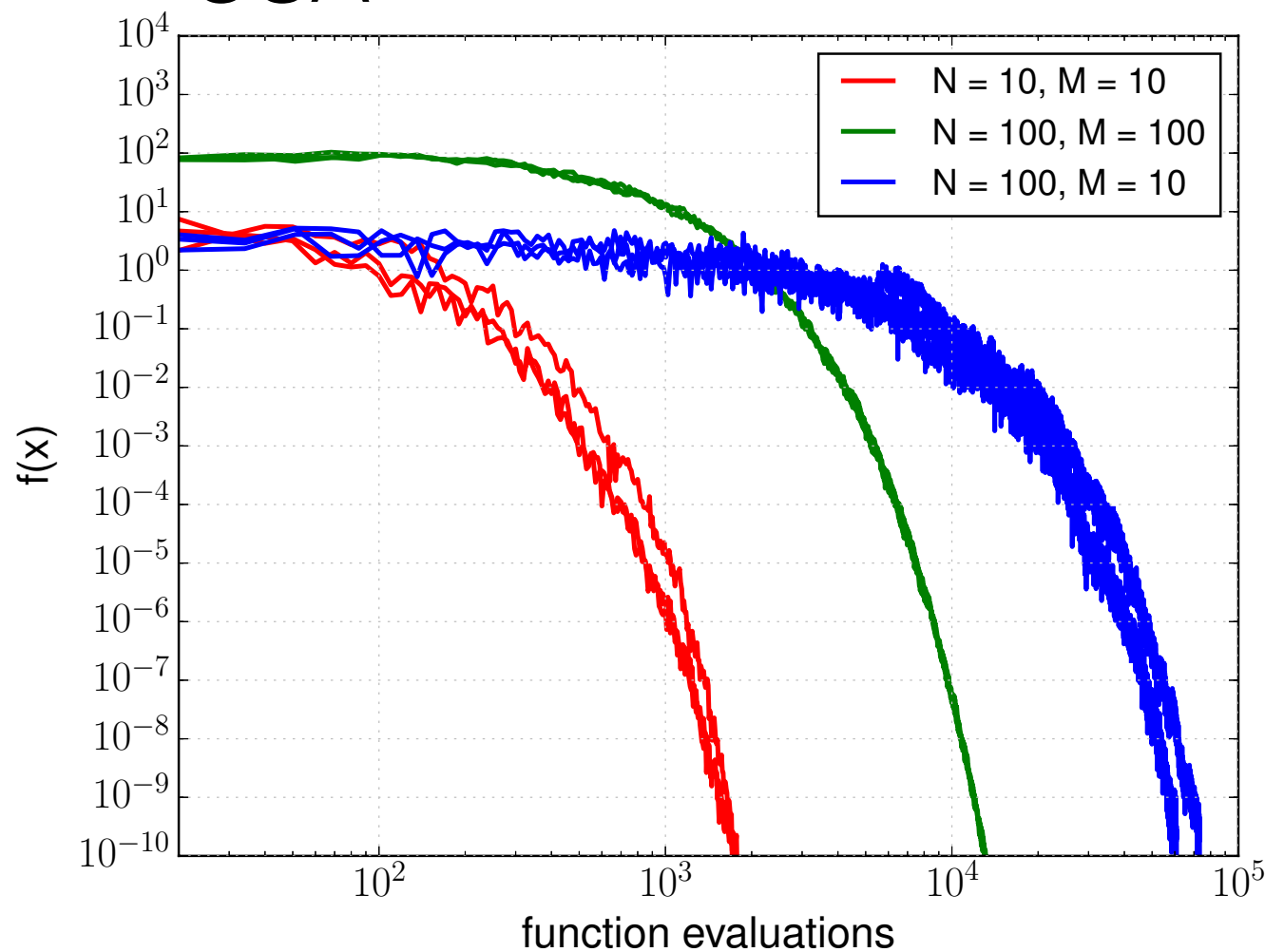
<https://cma-es.github.io/>

# On Sphere with Low Effective Dimension

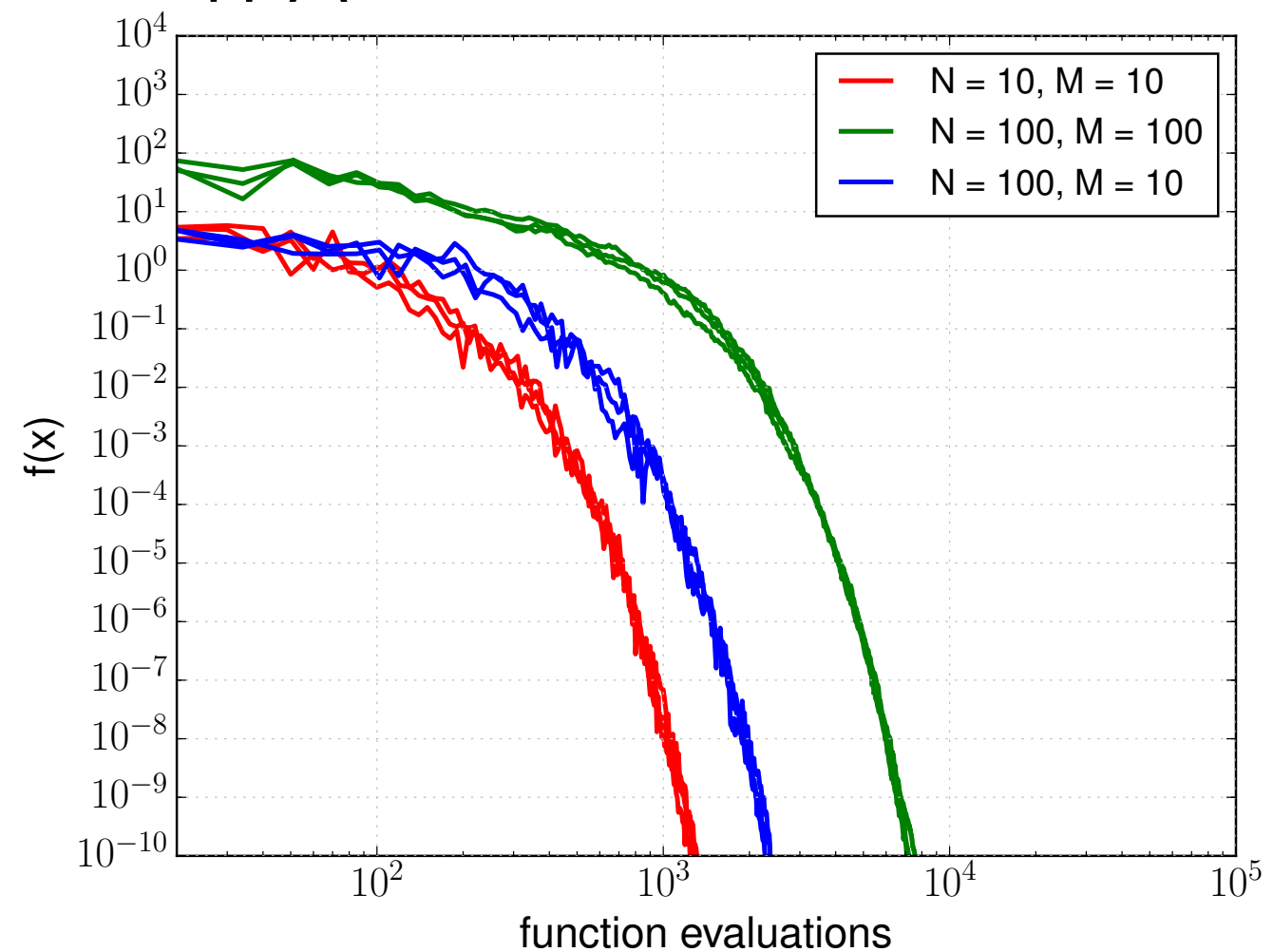
On a function with low effective dimension

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

## CSA



## TPA



# Maximum Likelihood Update

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

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

independently of the given covariance matrix

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

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

$$\log p_{\mathcal{N}}(\mathbf{x} | \mathbf{m}, \mathbf{C}) = -\frac{1}{2} \log \det(2\pi \mathbf{C}) - \frac{1}{2} (\mathbf{x} - \mathbf{m})^{\text{T}} \mathbf{C}^{-1} (\mathbf{x} - \mathbf{m})$$

$p_{\mathcal{N}}$  is the density of the multi-variate normal distribution

# Strategy Internal Parameters

- related to selection and recombination
  - ▶  $\lambda$ , offspring number, new solutions sampled, population size
  - ▶  $\mu$ , parent number, solutions involved in updates of  $m$ ,  $C$ , and  $\sigma$
  - ▶  $w_{i=1,\dots,\mu}$ , recombination weights
- related to  $C$ -update
  - ▶  $c_c$ , decay rate for the evolution path
  - ▶  $c_1$ , learning rate for rank-one update of  $C$
  - ▶  $c_\mu$ , learning rate for rank- $\mu$  update of  $C$
- related to  $\sigma$ -update
  - ▶  $c_\sigma$ , decay rate of the evolution path
  - ▶  $d_\sigma$ , damping for  $\sigma$ -change

Parameters were identified in carefully chosen experimental set ups. **Parameters do not in the first place depend on the objective function** and are not meant to be in the users choice.

Only(?) the population size  $\lambda$  (and the initial  $\sigma$ ) might be reasonably varied in a wide range, *depending on the objective function*

Useful: restarts with increasing population size (IPOP)