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## CMA-ES and Advanced Adaptation Mechanisms

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We are happy to answer questions at any time.

# 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



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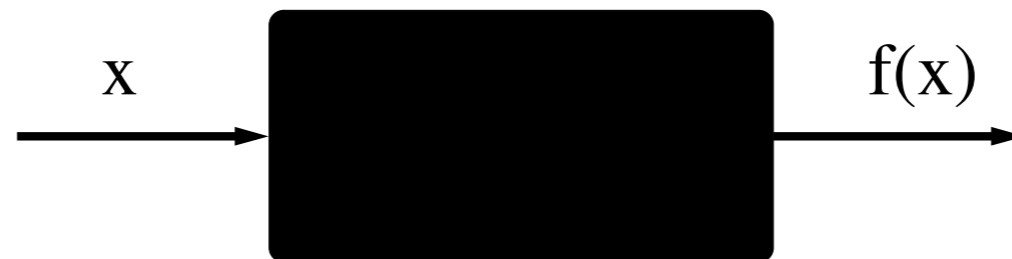
# Problem Statement

## Continuous Domain Search/Optimization

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

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

- **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

- Problems

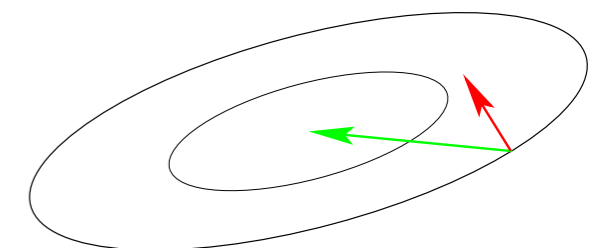
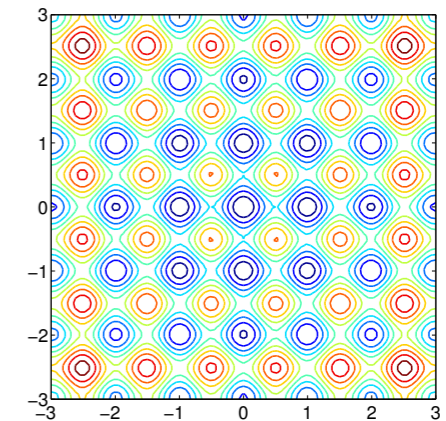
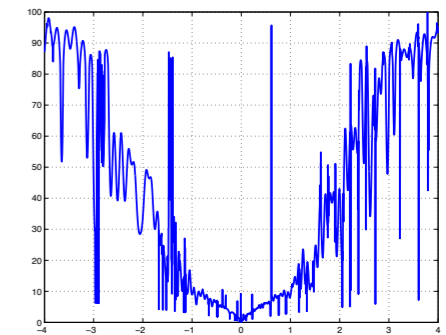
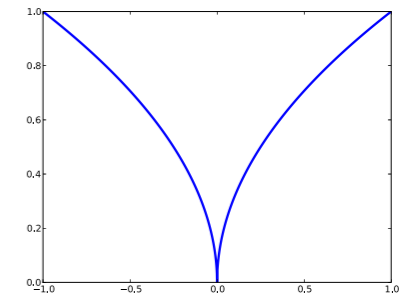
- ▶ exhaustive search is infeasible
- ▶ naive random search takes too long
- ▶ deterministic search is not successful / takes too long

**Approach:** stochastic search, Evolutionary Algorithms

# What Makes a Function Difficult to Solve?

Why stochastic search?

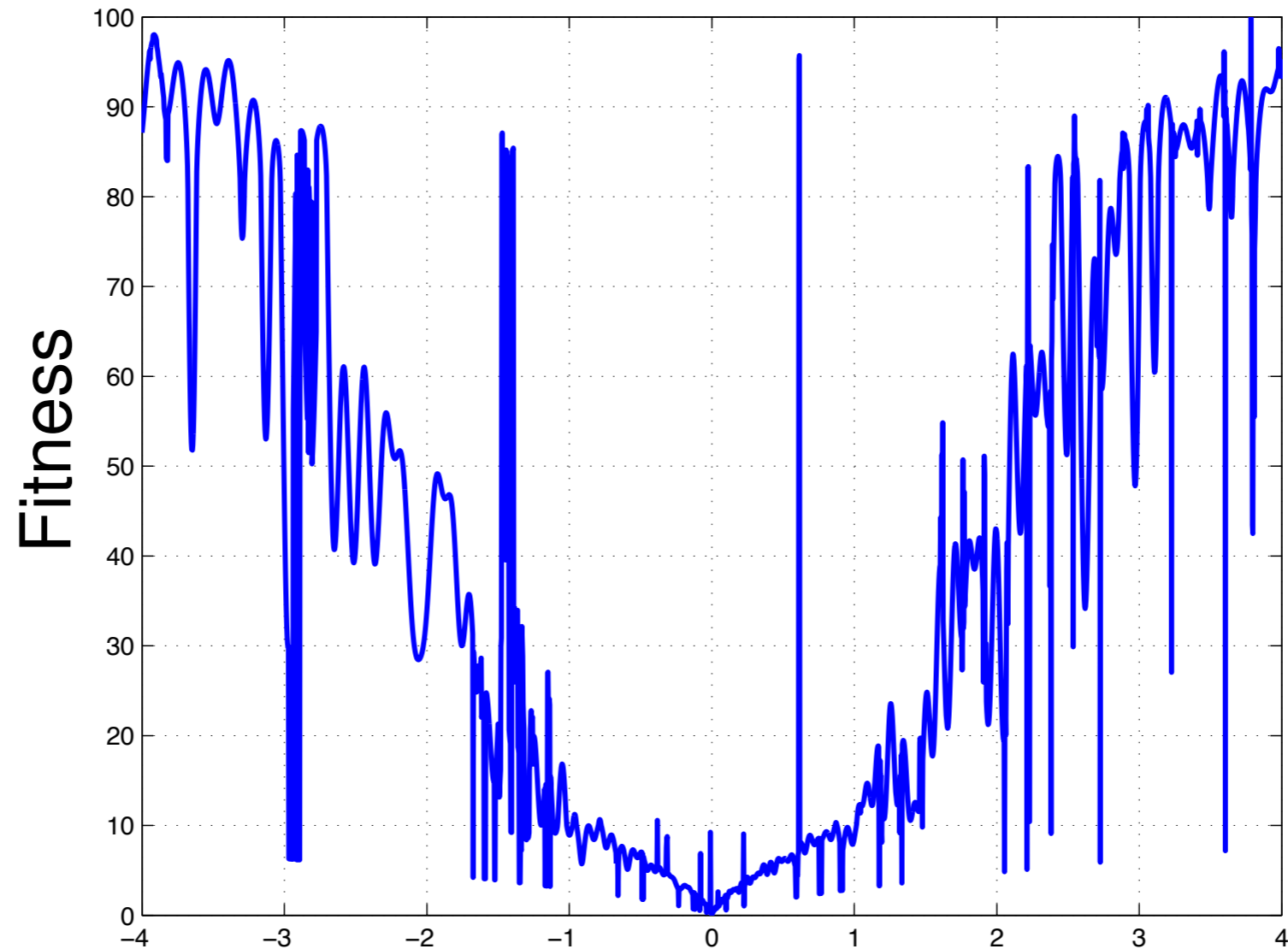
- non-linear, non-quadratic, non-convex  
on linear and quadratic functions much better search policies are available
- ruggedness  
non-smooth, discontinuous, multimodal, and/or noisy function
- dimensionality (size of search space)  
(considerably) larger than three
- non-separability  
dependencies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

# Separable Problems

## Definition (Separable Problem)

A function  $f$  is separable if

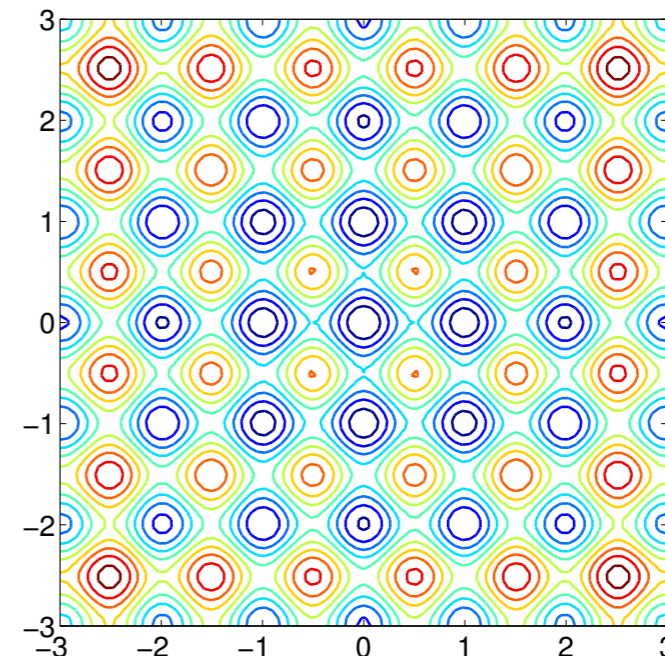
$$\arg \min_{(x_1, \dots, x_n)} f(x_1, \dots, x_n) = \left( \arg \min_{x_1} f(x_1, \dots), \dots, \arg \min_{x_n} f(\dots, x_n) \right)$$

$\Rightarrow$  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





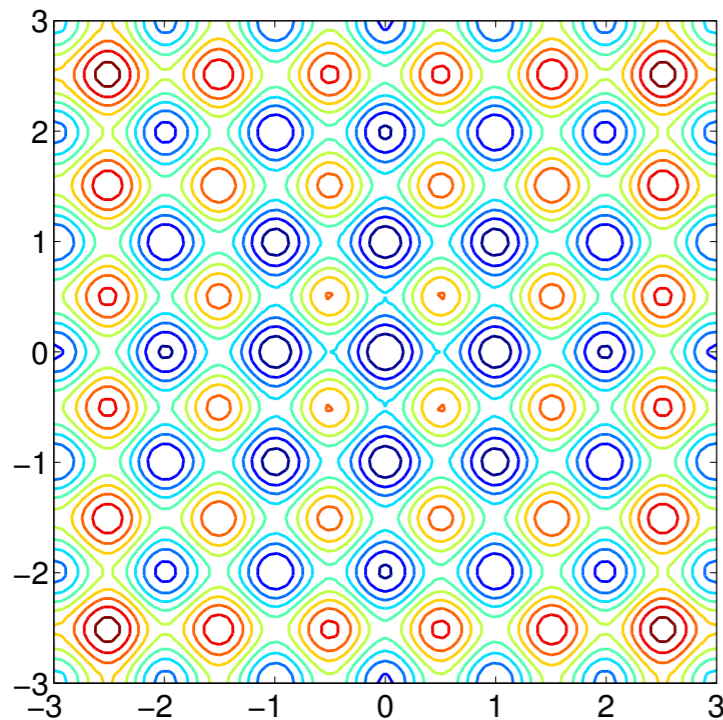
# Non-Separable Problems

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

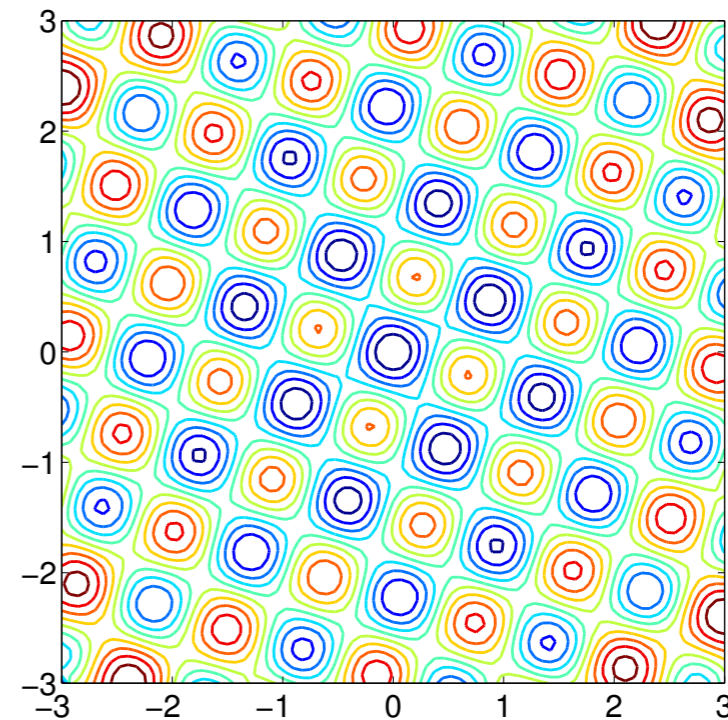
## Rotating the coordinate system

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

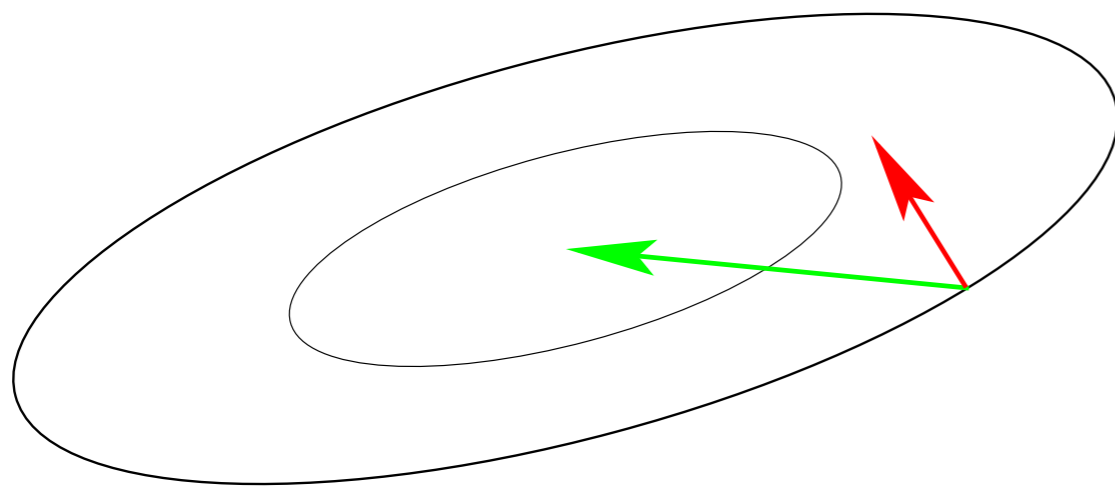
# III-Conditioned Problems

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

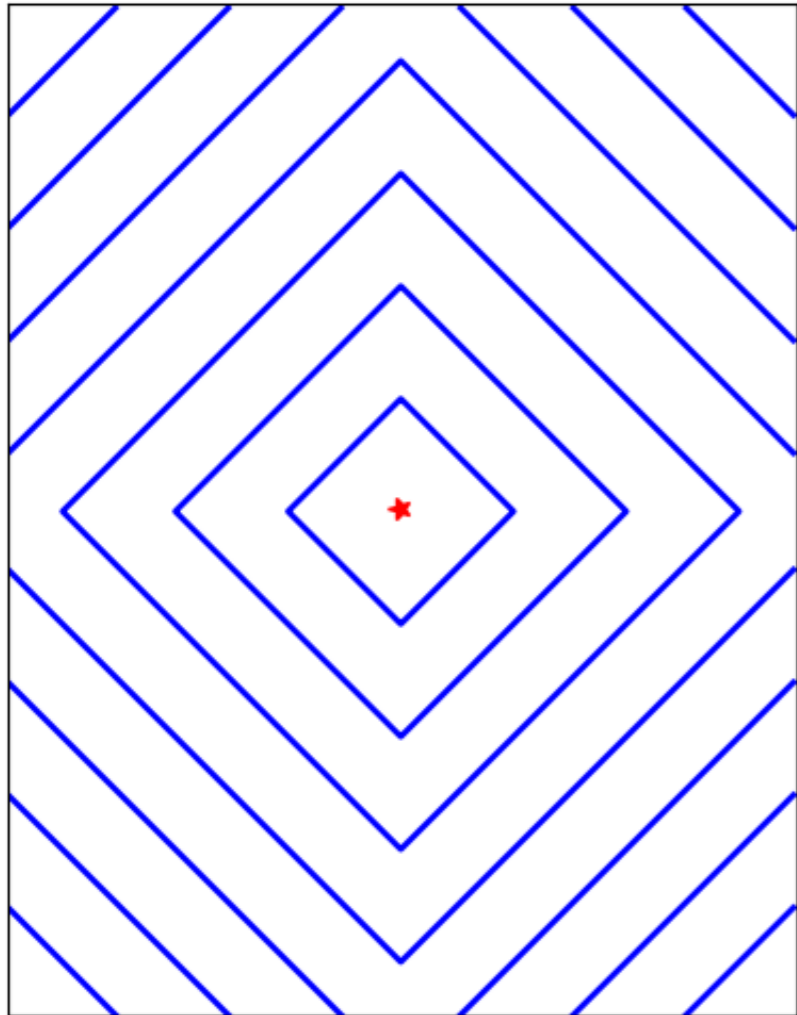
III-conditioning means **squeezed level sets** (high curvature).  
Condition number equals nine here. Condition numbers up to  $10^{10}$   
are not unusual in real world problems.

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**.

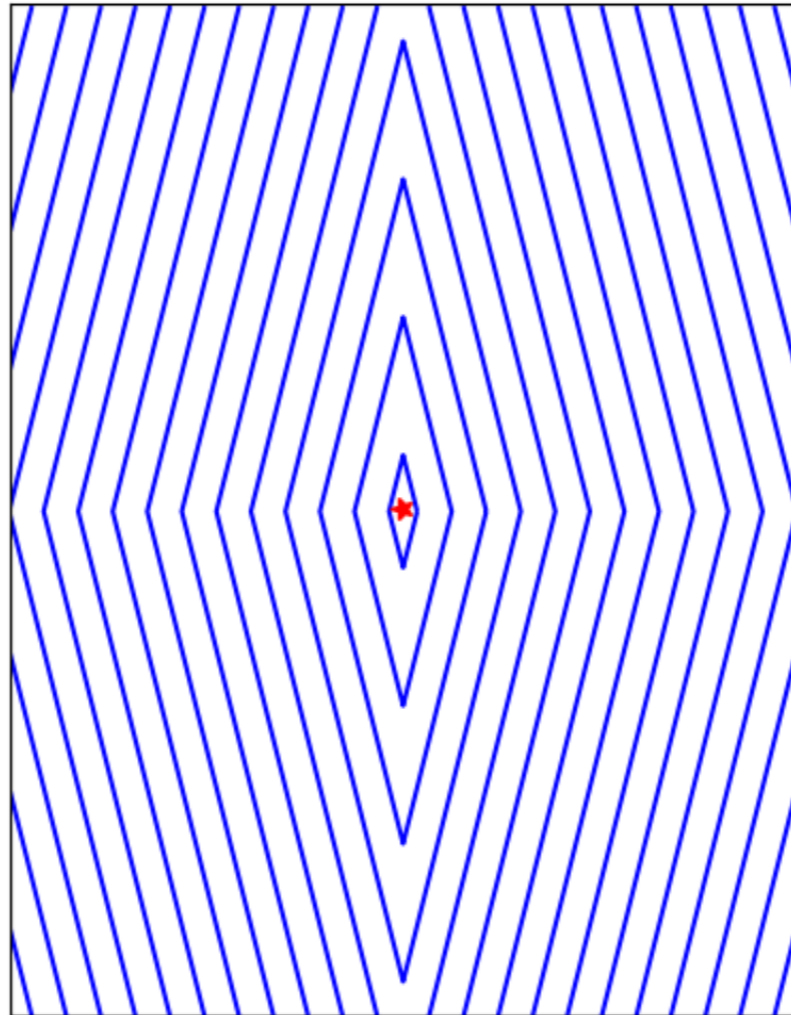


# Non-smooth level sets (sharp ridges)

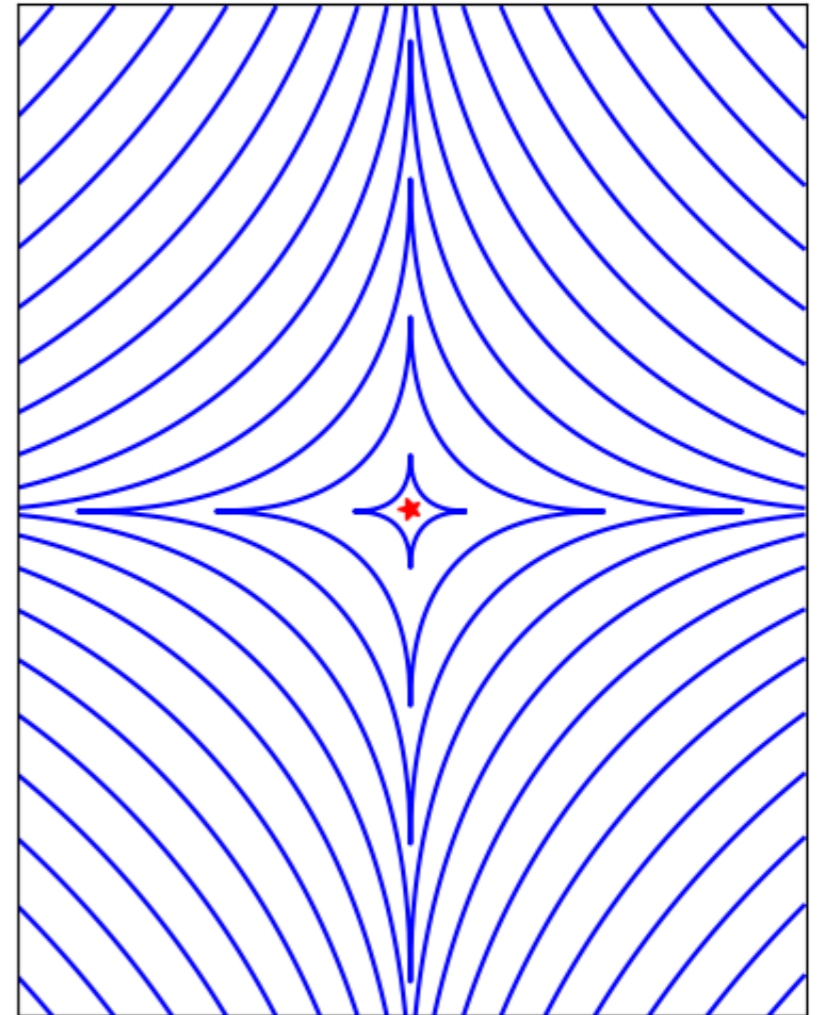
Similar difficulty **but worse** than ill-conditioning



1-norm



scaled 1-norm



1/2-norm

# 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	<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

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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*

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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  $\mathbf{y}_w = \sum_{i=1}^\mu w_{\text{rk}(i)} \mathbf{y}_i$  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  $\lambda$

# Evolution Strategies

New search points are sampled normally distributed

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

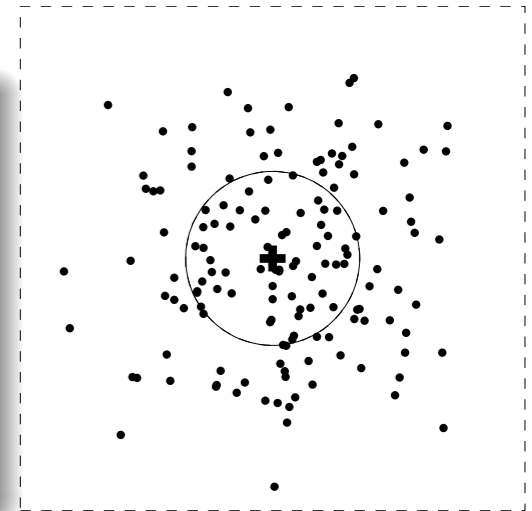
as perturbations of  $\mathbf{m}$ , where  $\mathbf{x}_i, \mathbf{m} \in \mathbb{R}^n$ ,  $\sigma \in \mathbb{R}_+$ ,  $\mathbf{C} \in \mathbb{R}^{n \times n}$

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

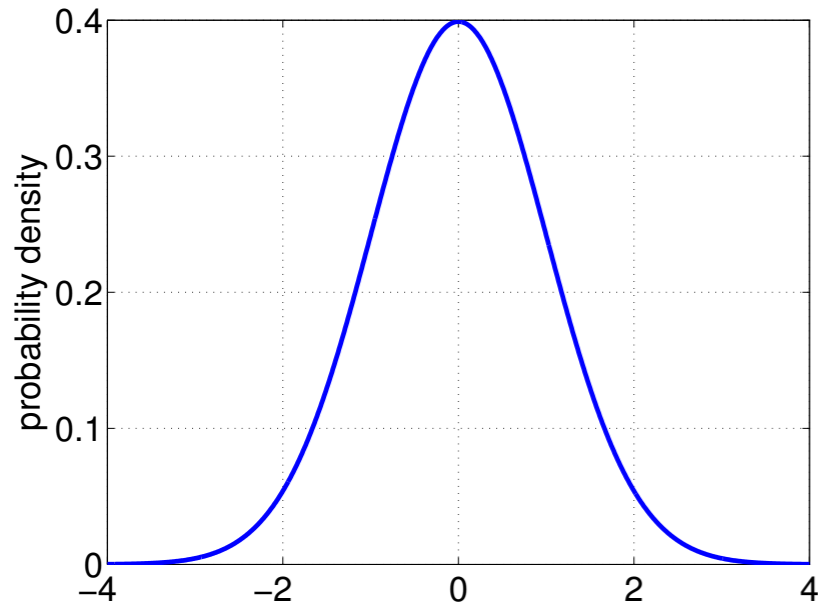
the isotropic distribution does **not favor any direction**, rotational  
invariant

4 maximum entropy distribution with finite variance

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

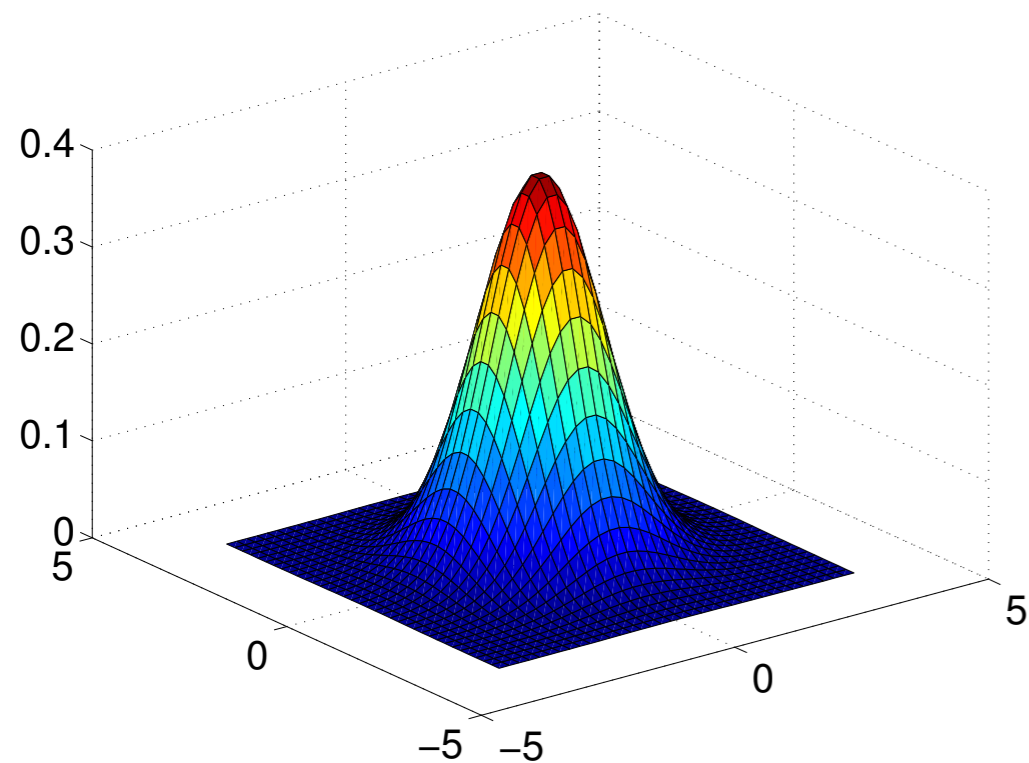
# Normal Distribution

Standard Normal Distribution

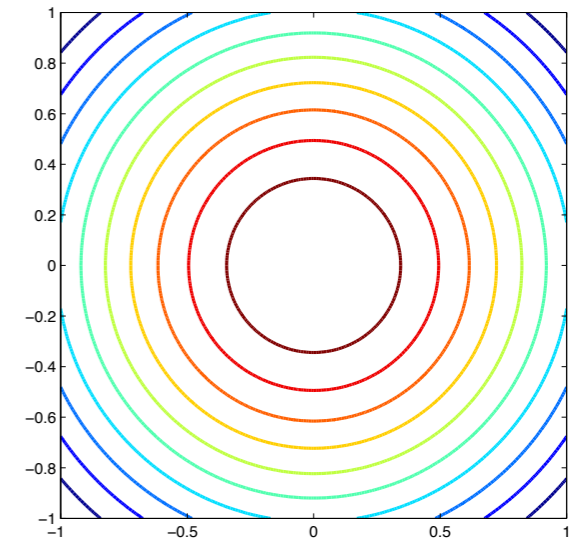


probability density of the 1-D standard normal distribution

2-D Normal Distribution



probability density of a 2-D normal distribution

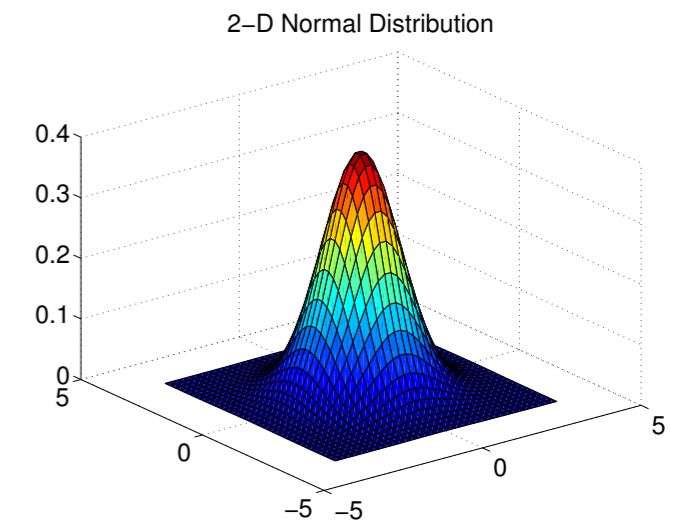


# The Multi-Variate ( $n$ -Dimensional) Normal Distribution

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



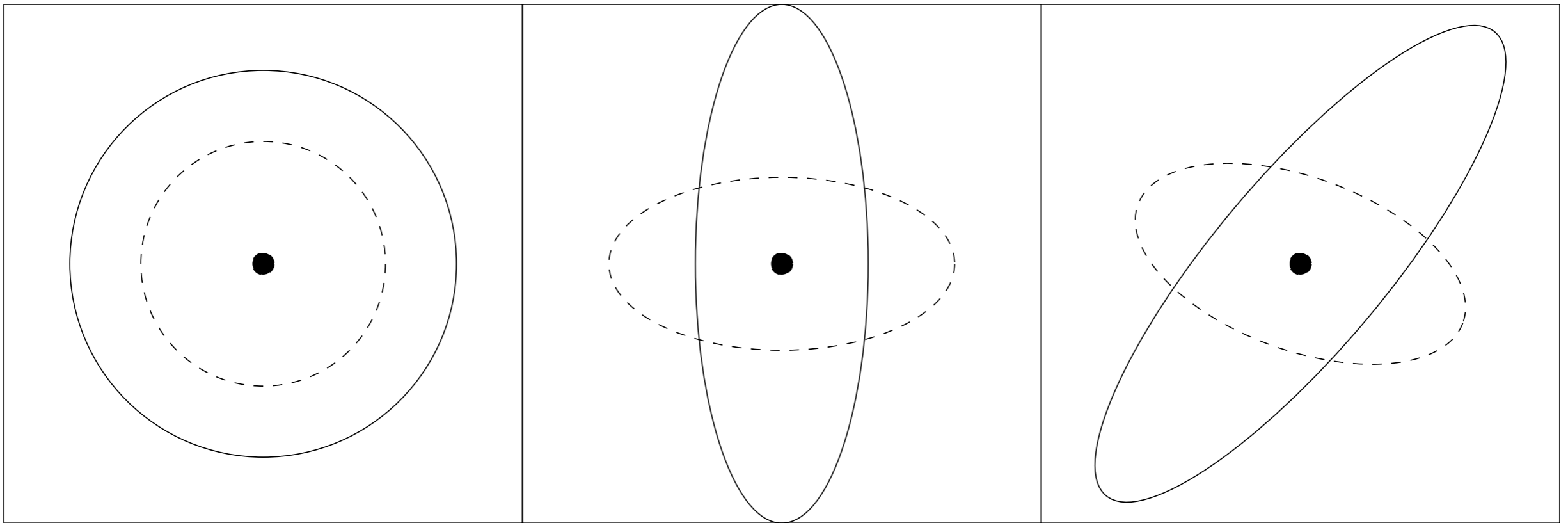
The **covariance matrix**  $\mathbf{C}$

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



... 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 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  $\mathbf{A}$ .

# Multivariate Normal Distribution and Eigenvalues

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

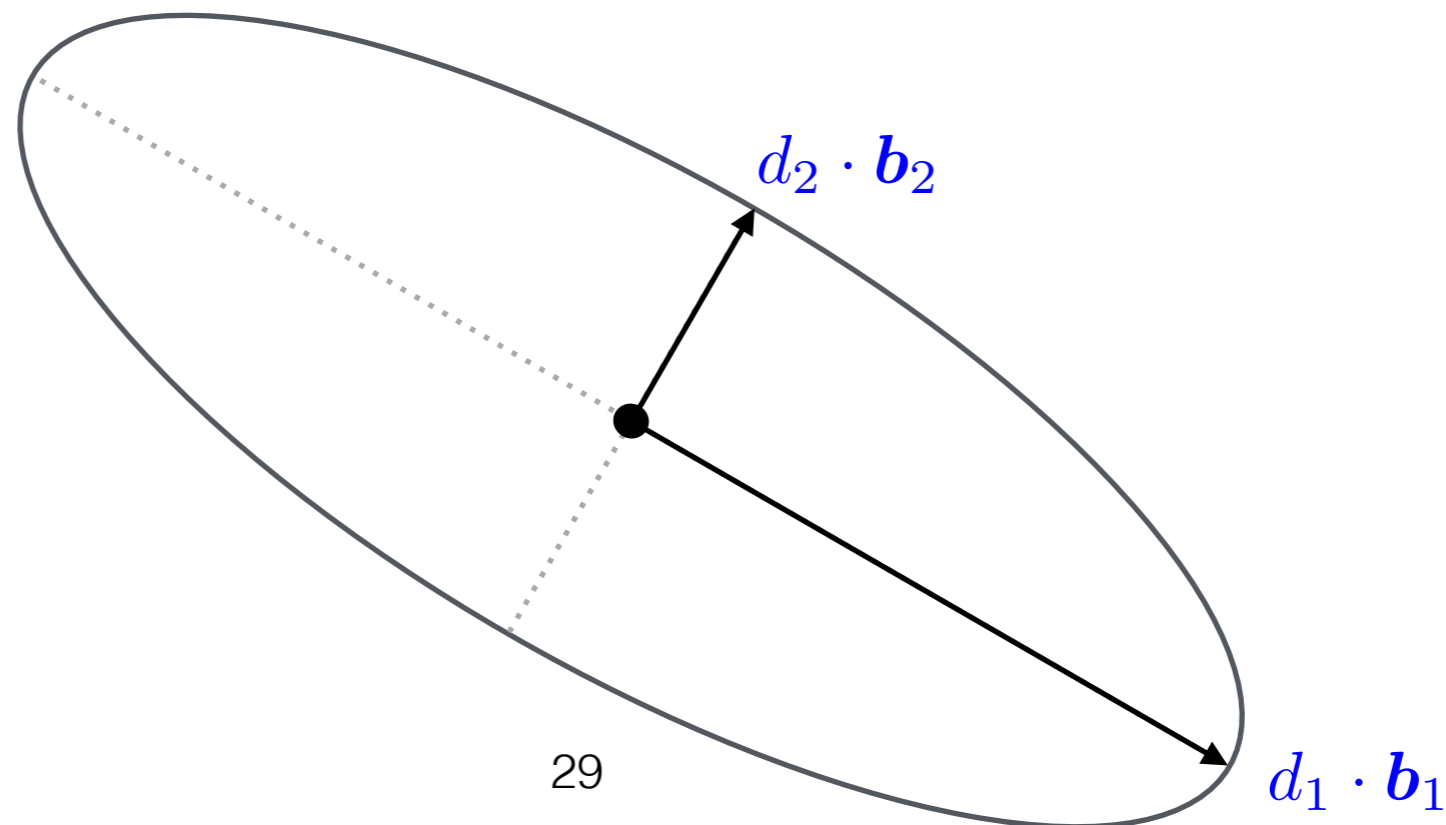
$$\mathbf{C} = d_1^2 \mathbf{b}_1 \mathbf{b}_1^T + \dots + d_N^2 \mathbf{b}_N \mathbf{b}_N^T$$

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

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

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

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



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

Non-elitist selection and intermediate (weighted) recombination

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

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

The new mean reads

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

where

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

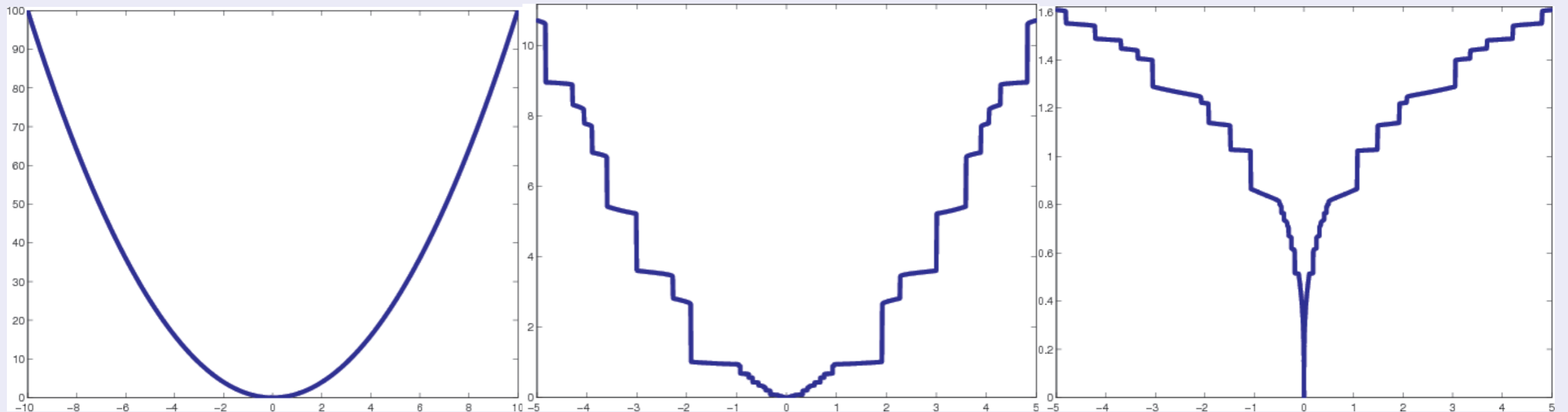
The best  $\mu$  points are selected from the new solutions (non-elitistic) and weighted intermediate recombination is applied.

# 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

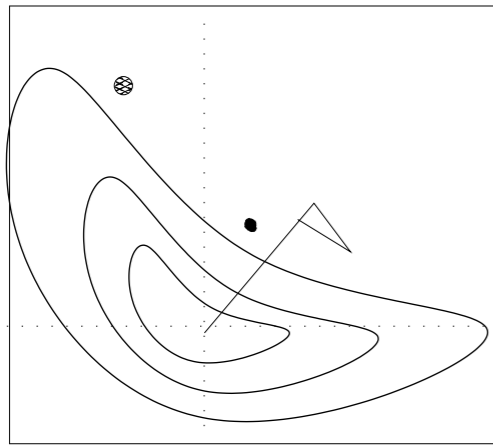
<sup>3</sup> Whitley 1989. The GENITOR algorithm and selection pressure: Why rank-based allocation of reproductive trials is best,

ICGA

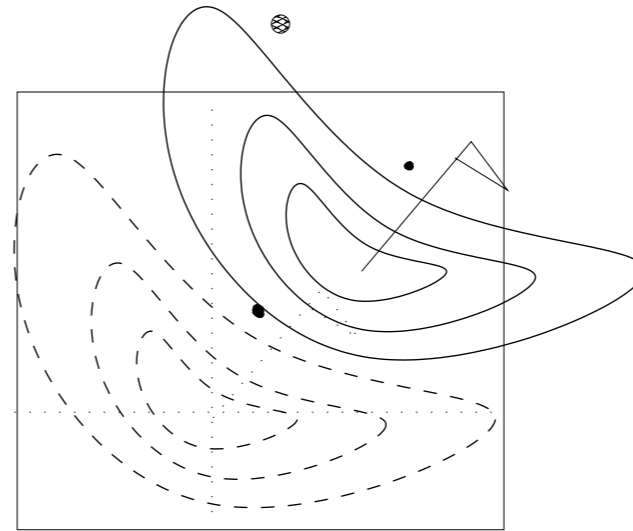
# Basic Invariance in Search Space

- translation invariance

is true for most optimization algorithms



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

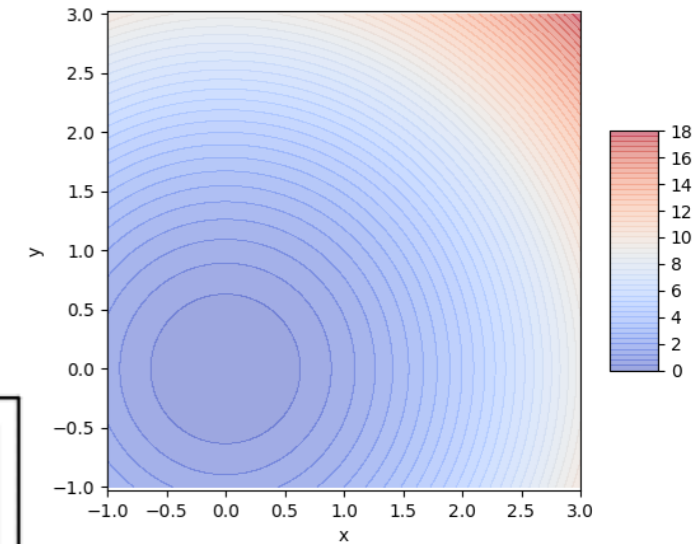
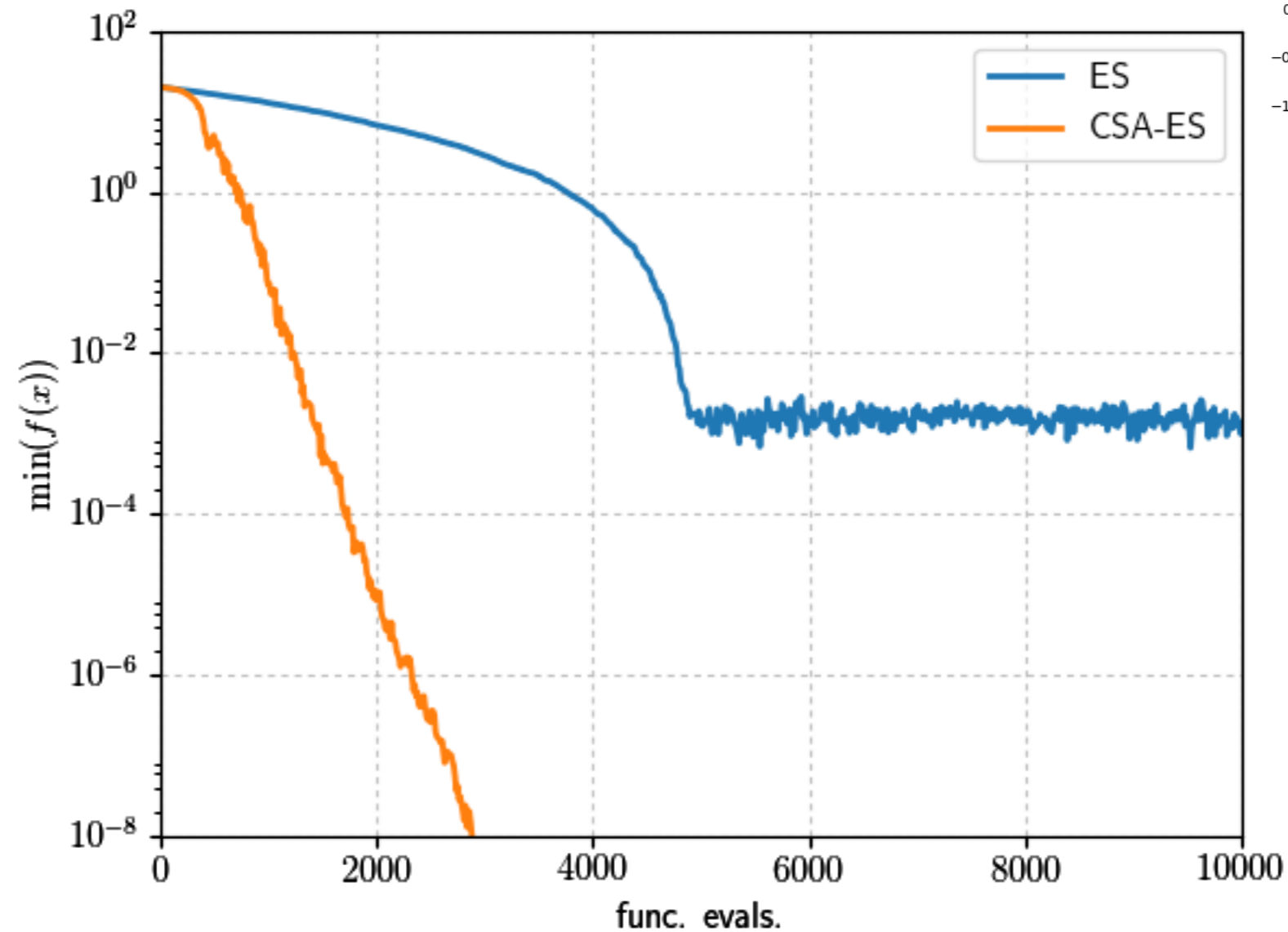


Identical behavior on  $f$  and  $f_a$

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

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

# Summary



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

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

# Evolution Strategies

Recalling

New search points are sampled normally distributed

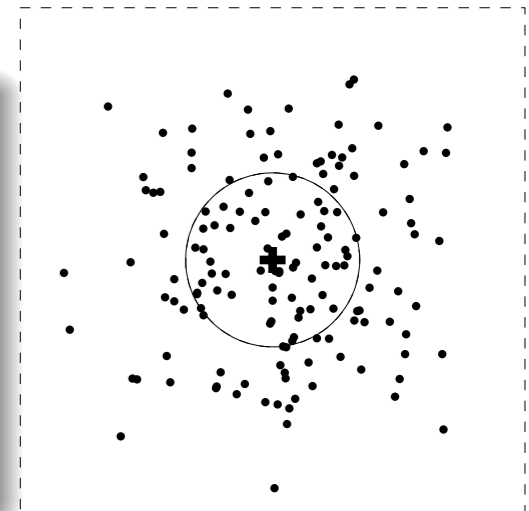
$$\mathbf{x}_i \sim \mathbf{m} + \sigma \mathcal{N}_i(\mathbf{0}, \mathbf{C}) \quad \text{for } i = 1, \dots, \lambda$$

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  $\mathbf{C}$ .



# 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

---

<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*



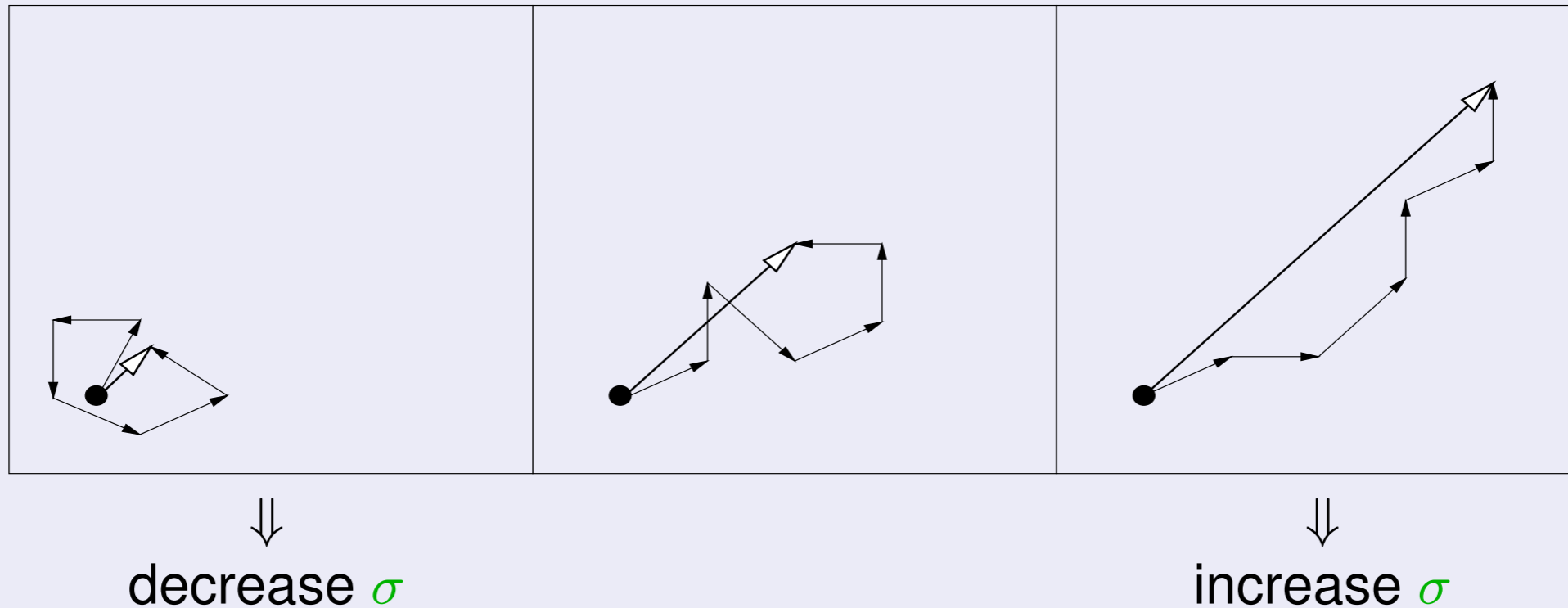
# Path Length Control (CSA)

## 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

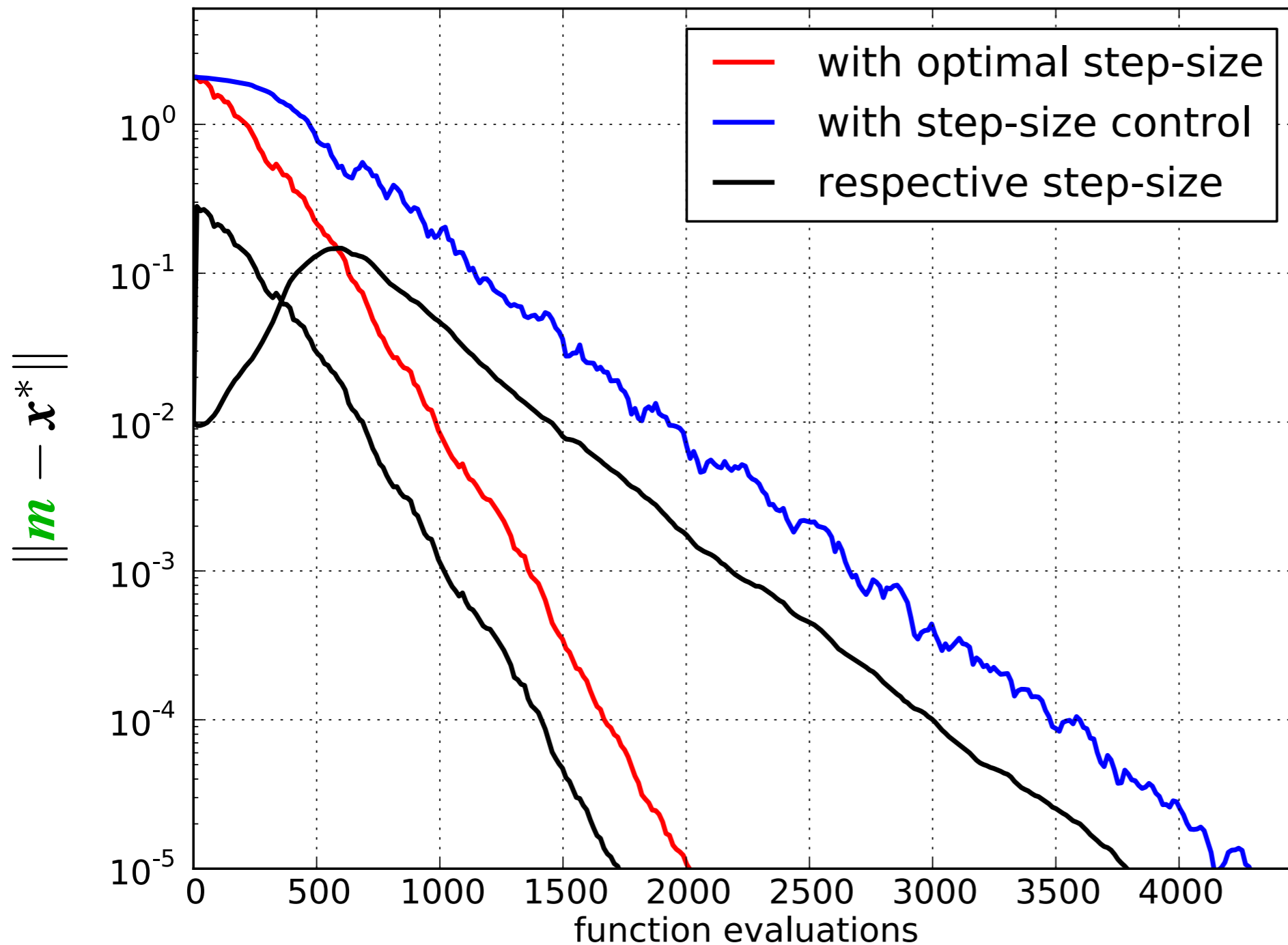
Initialize  $\mathbf{m} \in \mathbb{R}^n$ ,  $\sigma \in \mathbb{R}_+$ , evolution path  $\mathbf{p}_\sigma = \mathbf{0}$ ,  
set  $c_\sigma \approx 4/n$ ,  $d_\sigma \approx 1$ .

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

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

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

# (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

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

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

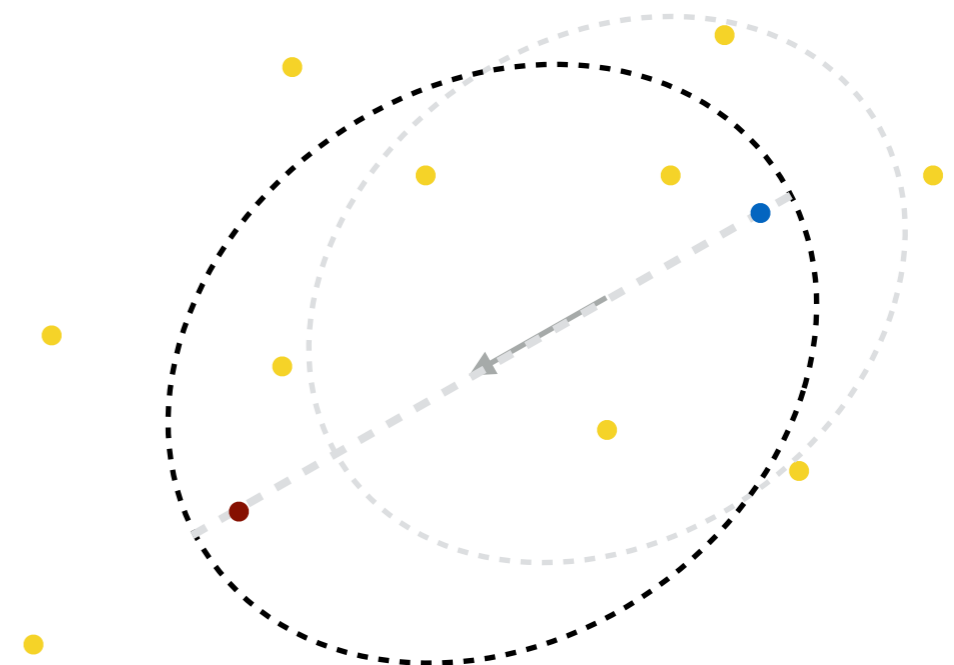
- Compare the ranking of  $\mathbf{x}_1$  and  $\mathbf{x}_2$  among  $\lambda$  current populations

$$s^{(g+1)} = (1 - c_s) s^{(g)} + c_s \underbrace{\frac{\text{rank}(\mathbf{x}_2) - \text{rank}(\mathbf{x}_1)}{\lambda - 1}}$$

>0 if the previous step still produces a promising solution

- Update the step-size

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



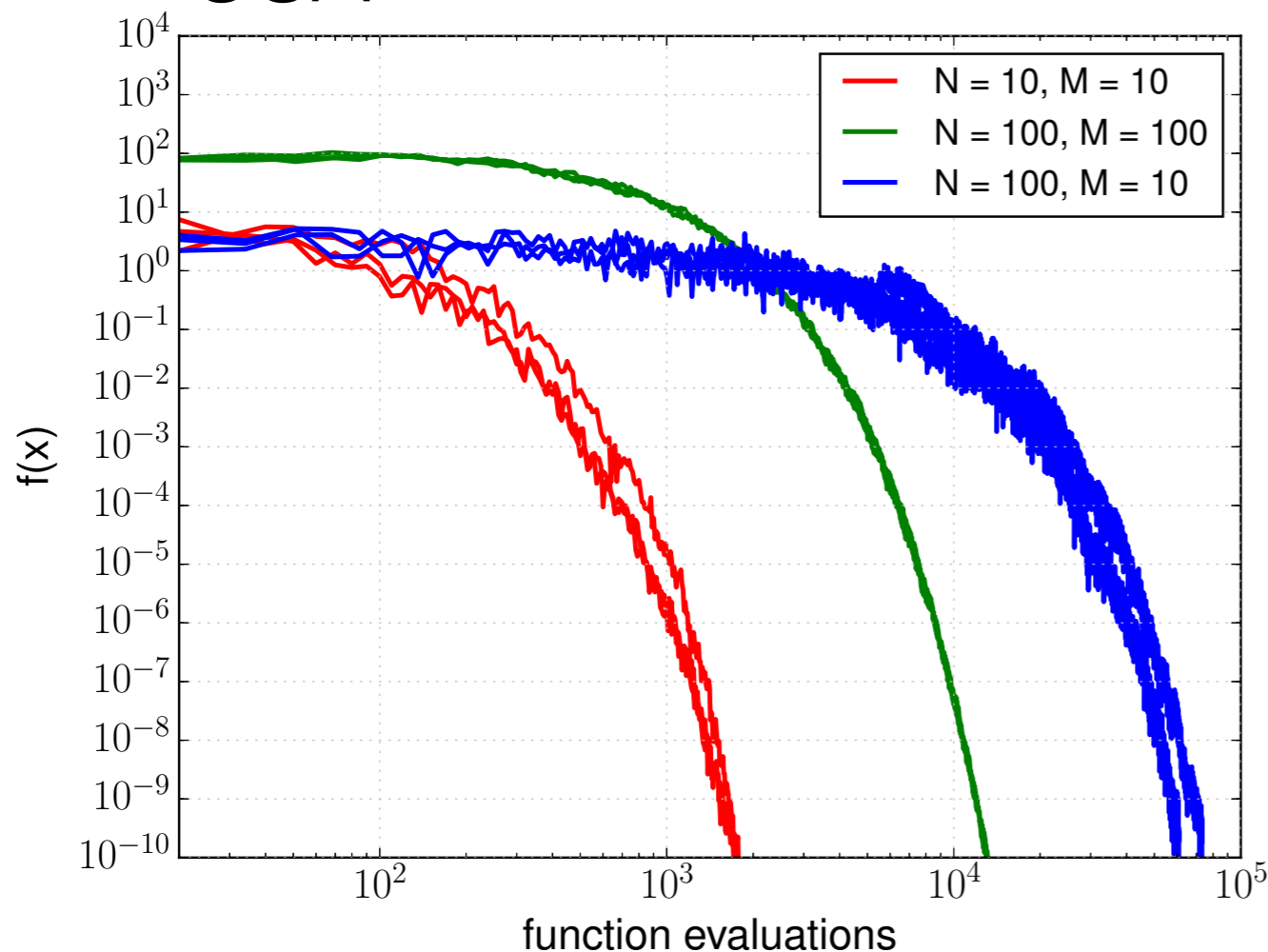
[Hansen, 2008] Hansen, N. (2008). CMA-ES with two-point step-size adaptation. [research report] rr-6527, 2008. Inria-00276854v5.  
 [Hansen et al., 2014] Hansen, N., Atamna, A., and Auger, A. (2014). How to assess step-size adaptation mechanisms in randomised search. In Parallel Problem Solving from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

# On Sphere with Low Effective Dimension

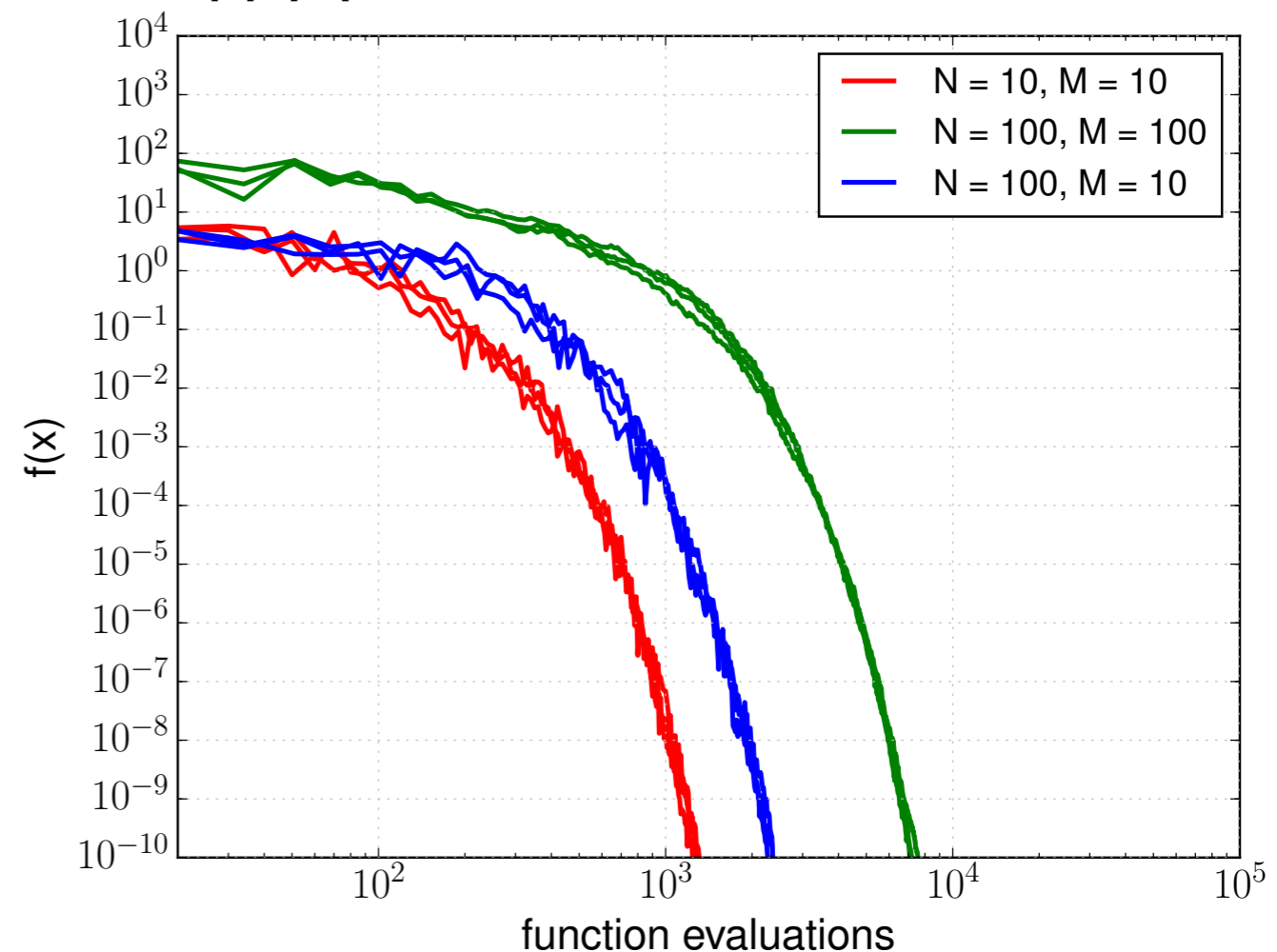
On a function with low effective dimension

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

## CSA



## TPA



# Alternatives: Success-Based Step-Size Control

comparing the fitness distributions of current and previous iterations

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

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

controls a *success probability*

An advantage over CSA and TPA: Cheap Computation

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

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

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

# Step-Size Control: Summary

## Why Step-Size Control?

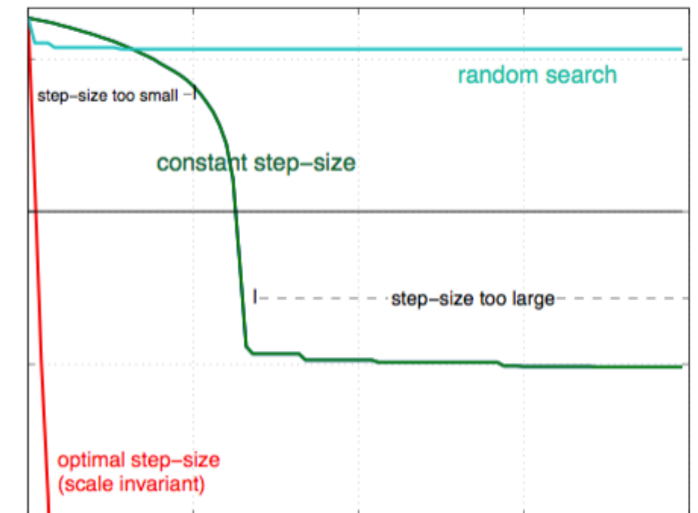
- to achieve linear convergence at near-optimal rate

## Cumulative Step-Size Adaptation

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

## Alternative Step-Size Adaptation Mechanisms

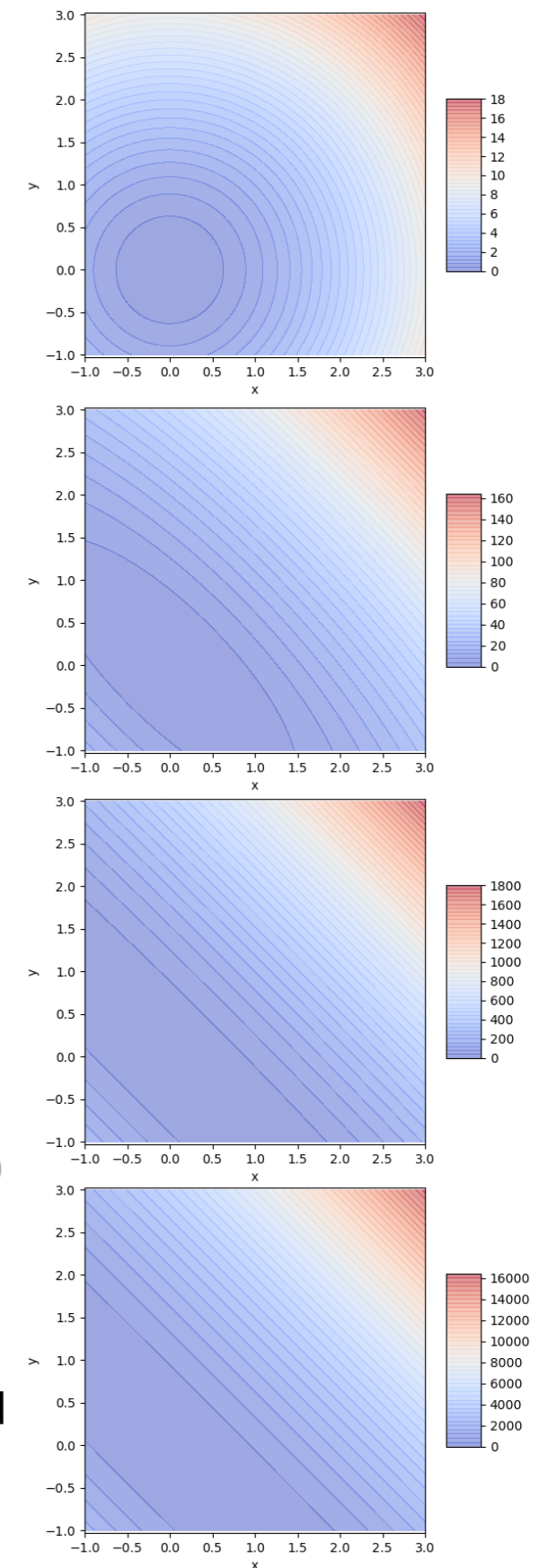
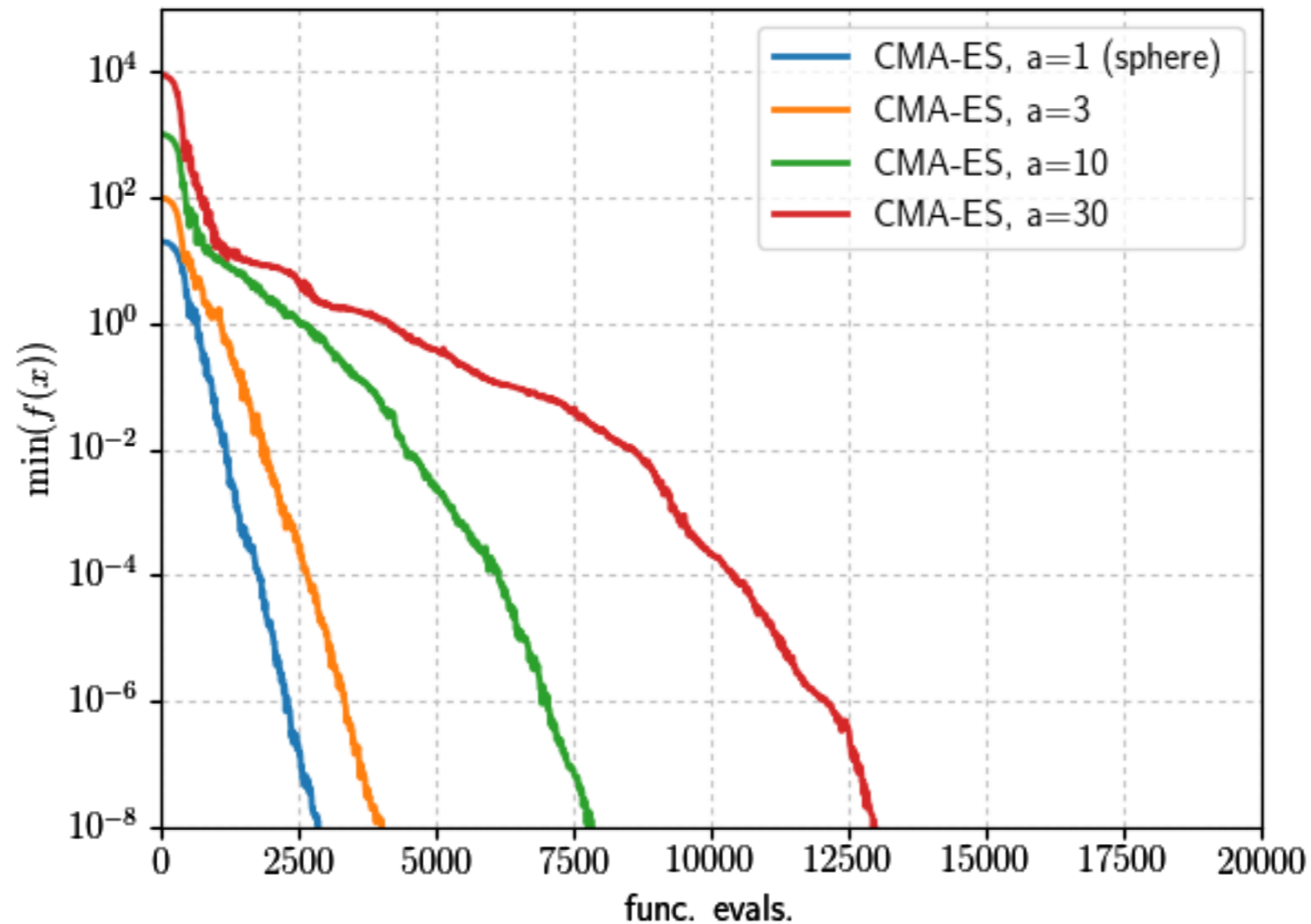
- Two-Point Step-Size Adaptation
- Median Success Rule, Population Success Rule



*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

# Step-Size Control: Summary



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

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



# Evolution Strategies

Recalling

New search points are sampled normally distributed

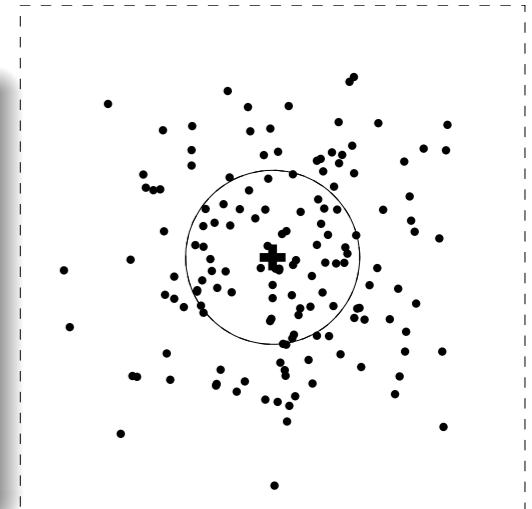
$$\mathbf{x}_i \sim \mathbf{m} + \sigma \mathcal{N}_i(\mathbf{0}, \mathbf{C}) \quad \text{for } i = 1, \dots, \lambda$$

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*
- the **covariance matrix**  $\mathbf{C} \in \mathbb{R}^{n \times n}$  determines the **shape** of the distribution ellipsoid

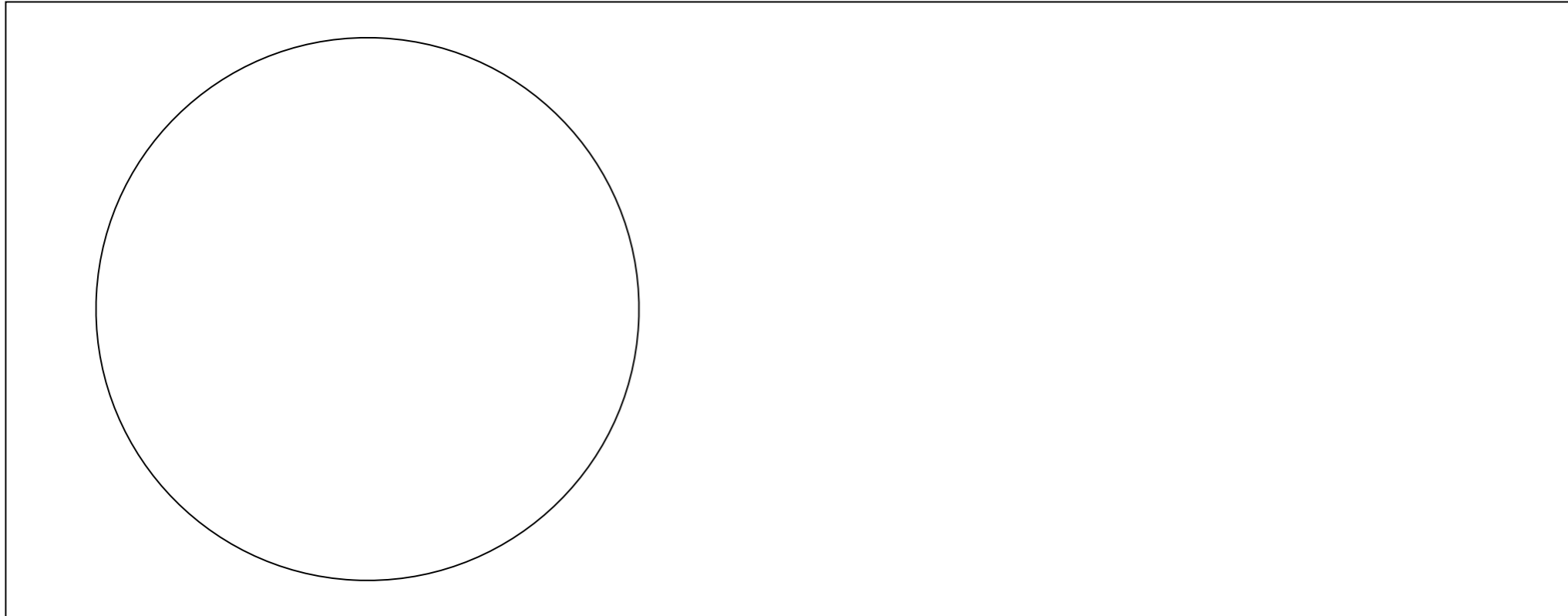
The remaining question is how to update  $\mathbf{C}$ .



# Covariance Matrix Adaptation

## Rank-One Update

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



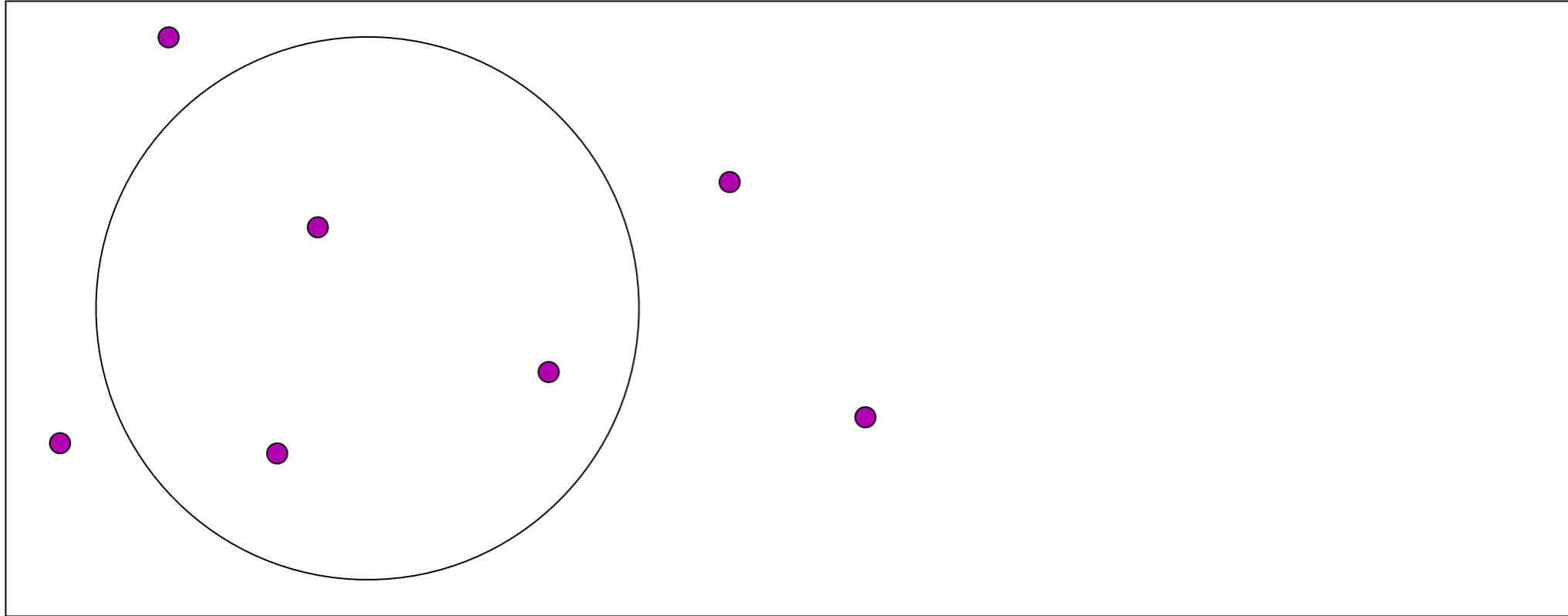
initial distribution,  $\mathbf{C} = \mathbf{I}$

... equations

# Covariance Matrix Adaptation

## Rank-One Update

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



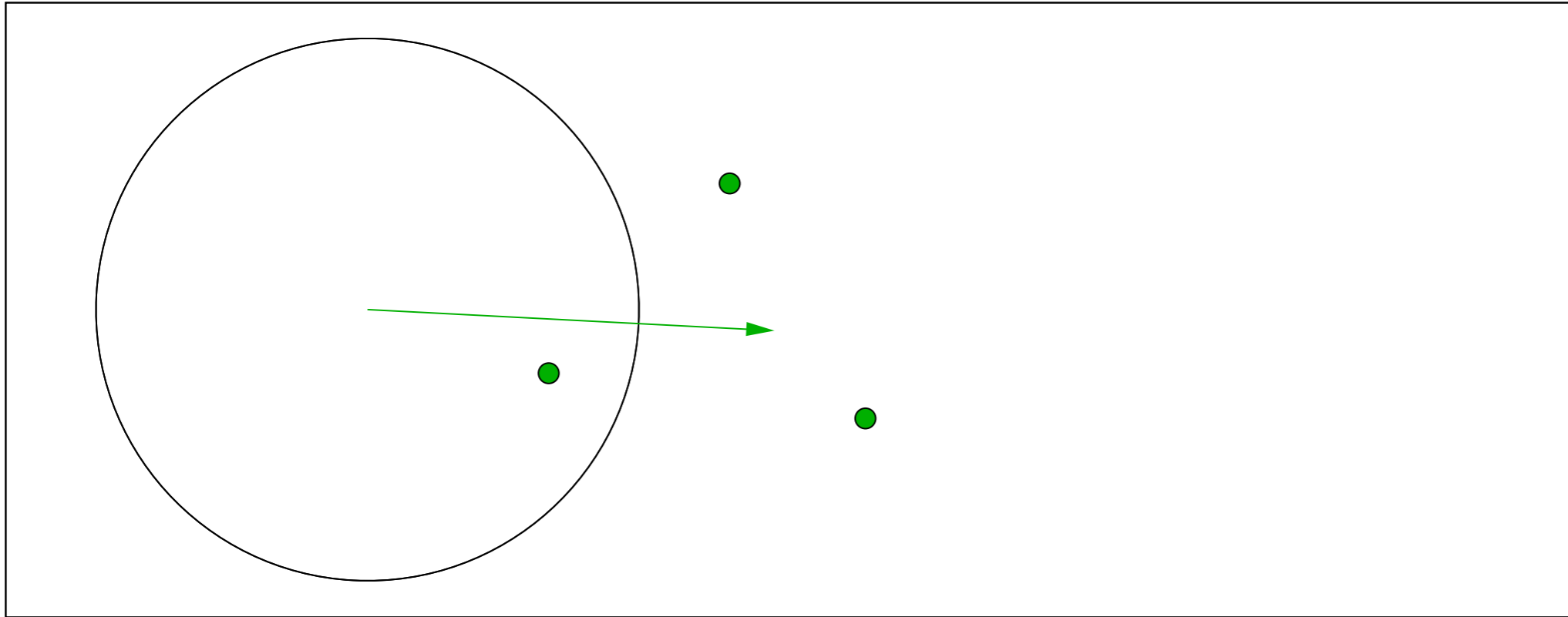
initial distribution,  $\mathbf{C} = \mathbf{I}$

... equations

# Covariance Matrix Adaptation

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



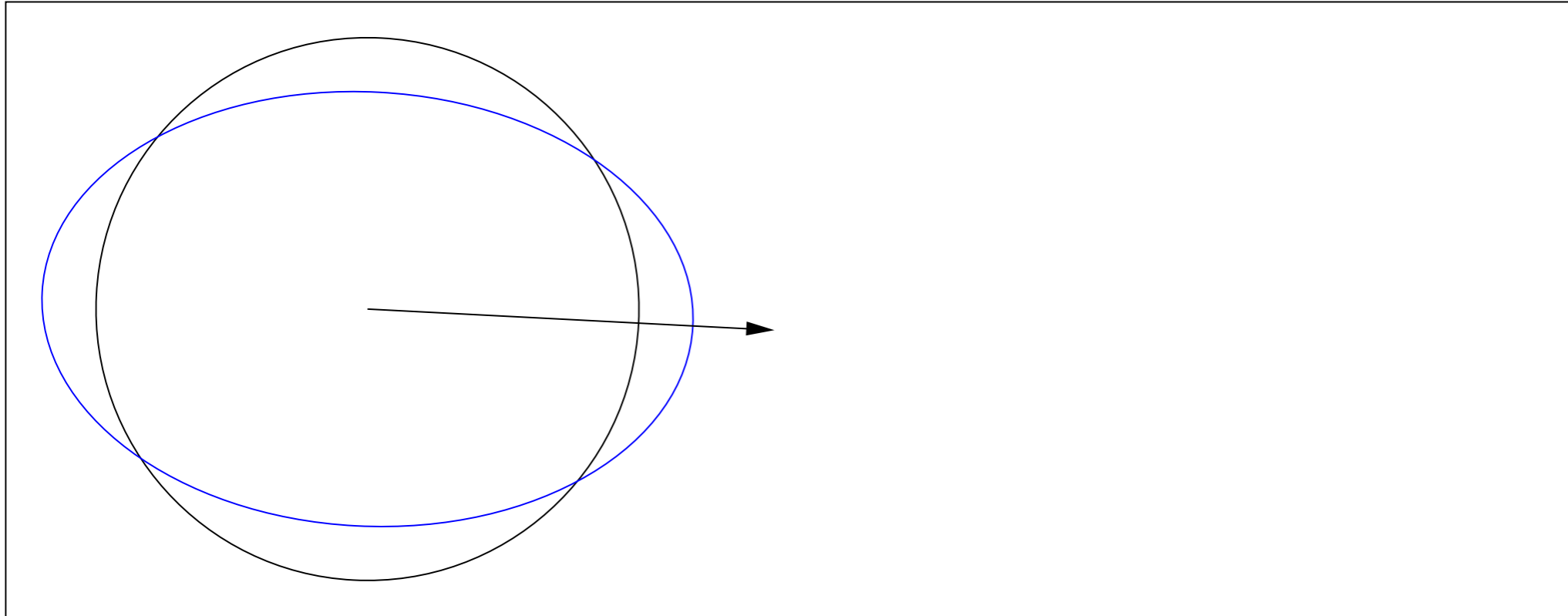
$\mathbf{y}_w$ , movement of the population mean  $\mathbf{m}$  (disregarding  $\sigma$ )

... equations

# Covariance Matrix Adaptation

## Rank-One Update

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

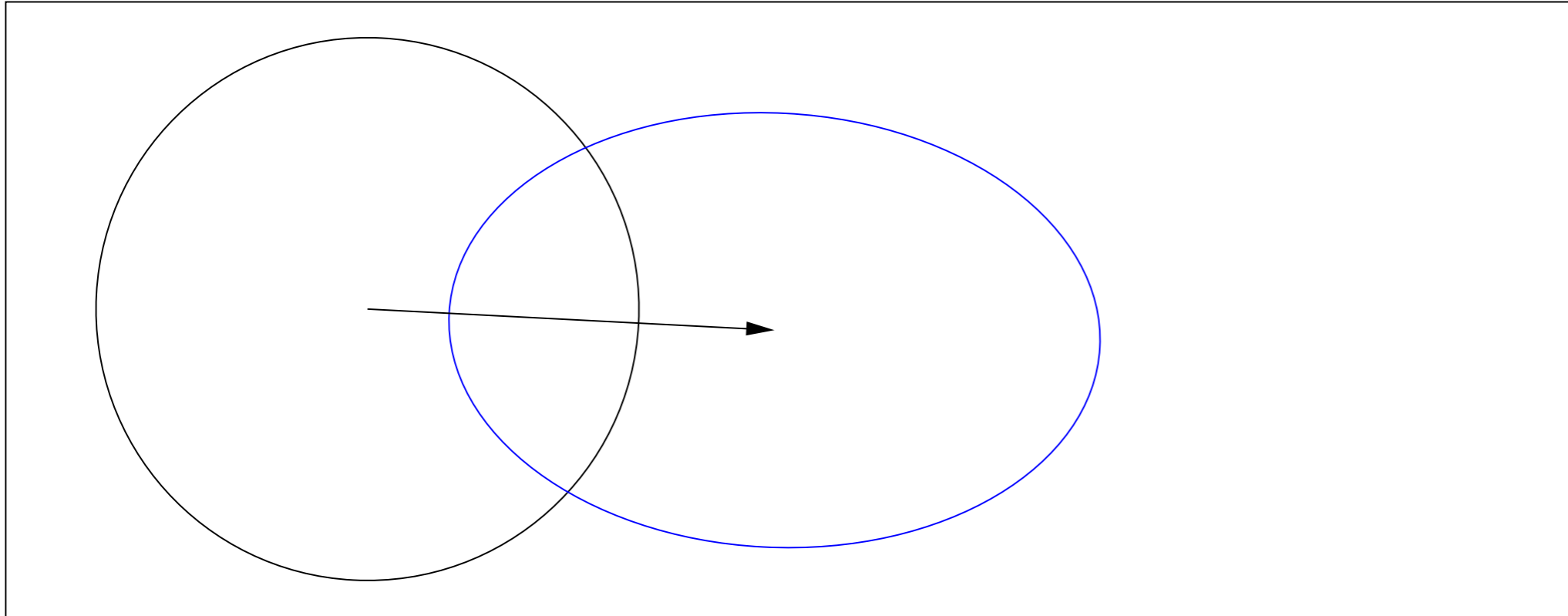
$$\mathbf{C} \leftarrow 0.8 \times \mathbf{C} + 0.2 \times \mathbf{y}_w \mathbf{y}_w^T$$

... equations

# Covariance Matrix Adaptation

## Rank-One Update

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



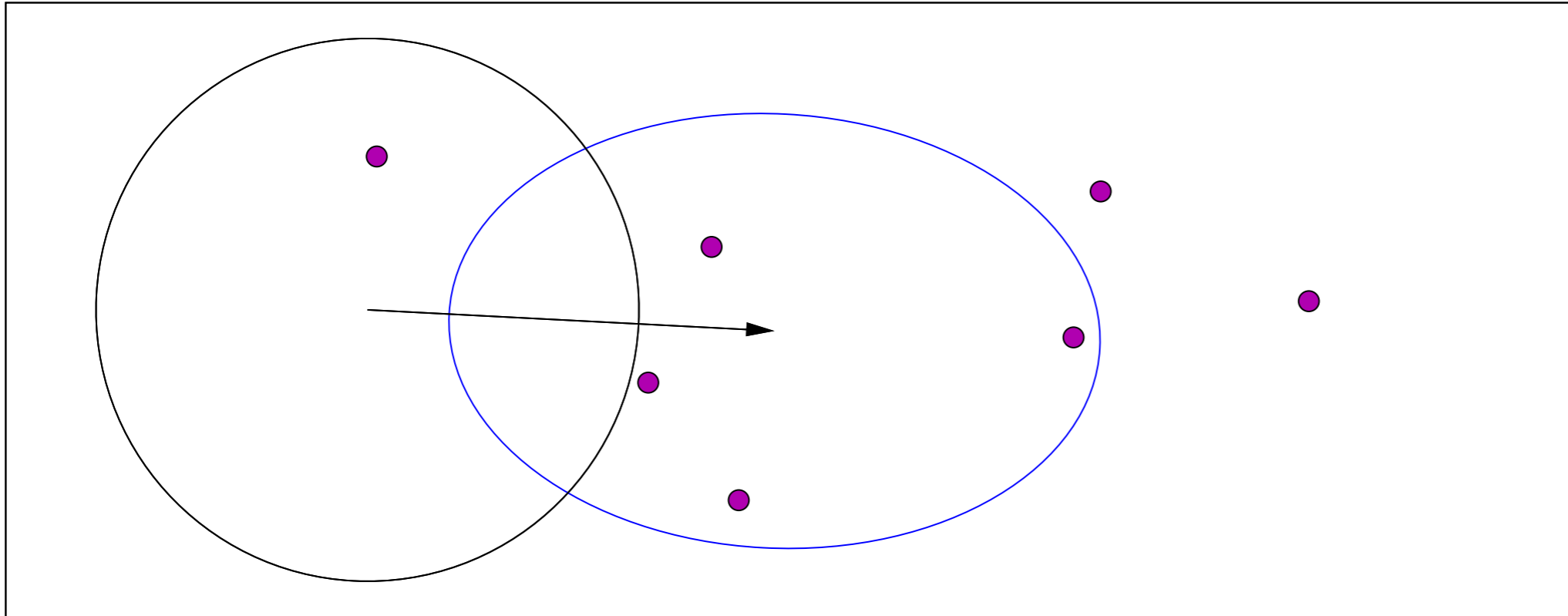
new distribution (disregarding  $\sigma$ )

... equations

# Covariance Matrix Adaptation

## Rank-One Update

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



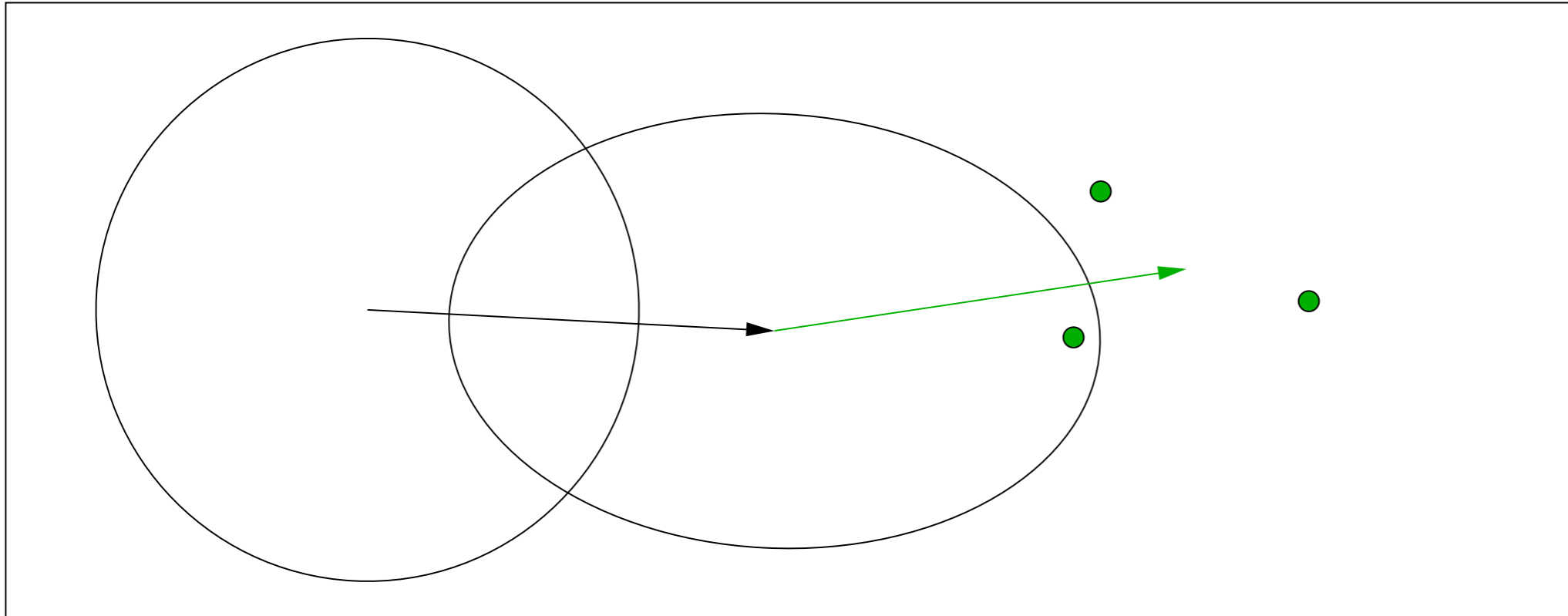
new distribution (disregarding  $\sigma$ )

... equations

# Covariance Matrix Adaptation

## Rank-One Update

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

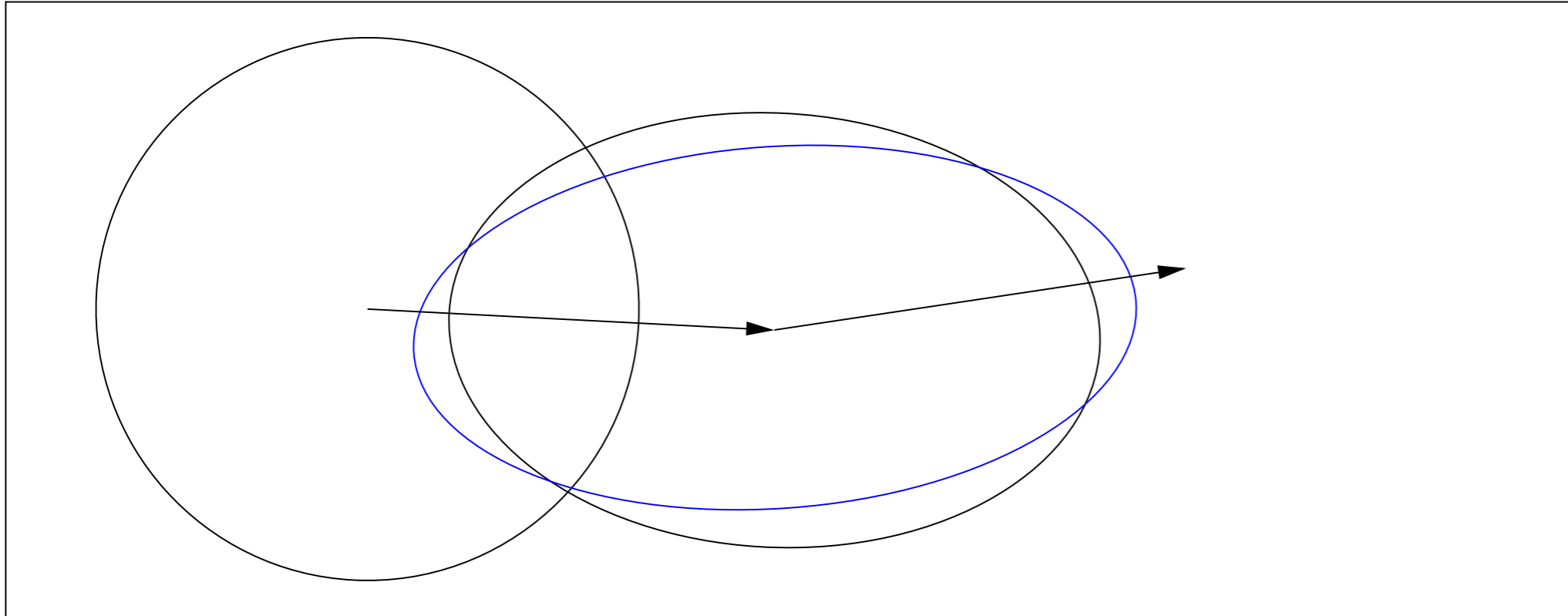
... equations



# Covariance Matrix Adaptation

## Rank-One Update

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

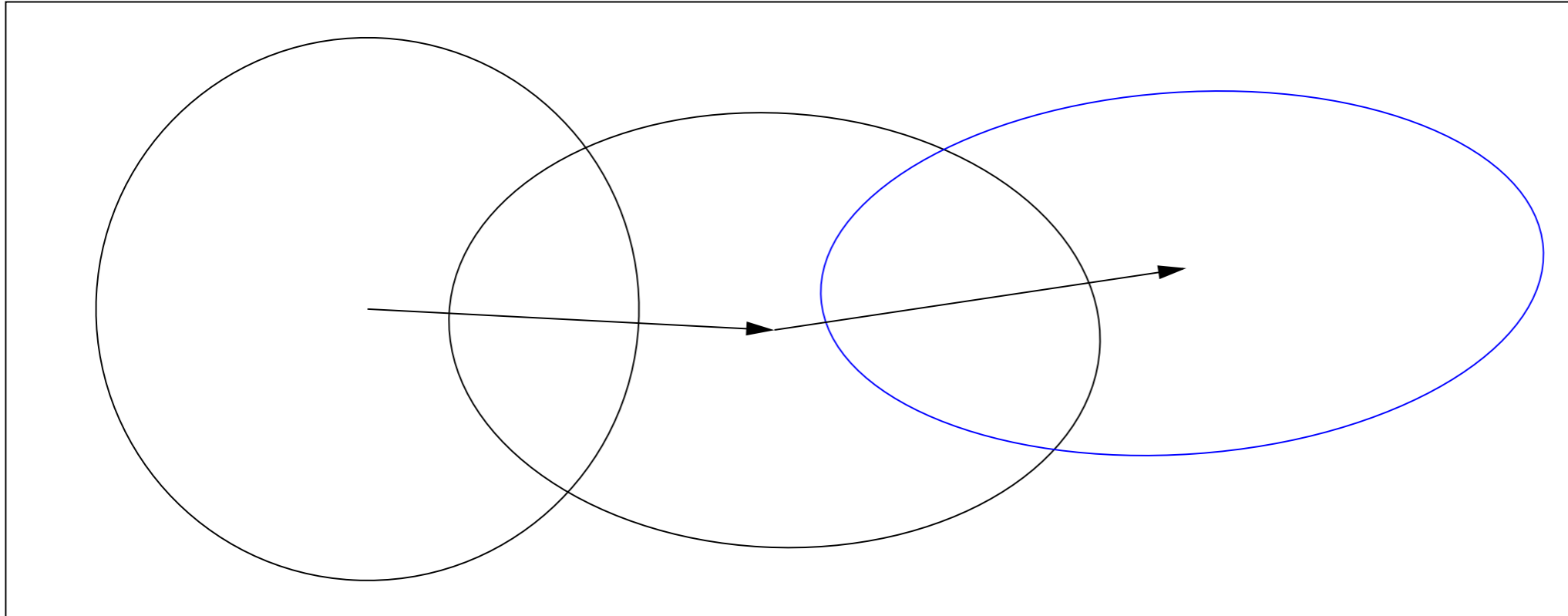
$$\mathbf{C} \leftarrow 0.8 \times \mathbf{C} + 0.2 \times \mathbf{y}_w \mathbf{y}_w^T$$

... equations

# Covariance Matrix Adaptation

## 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 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

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

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

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

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

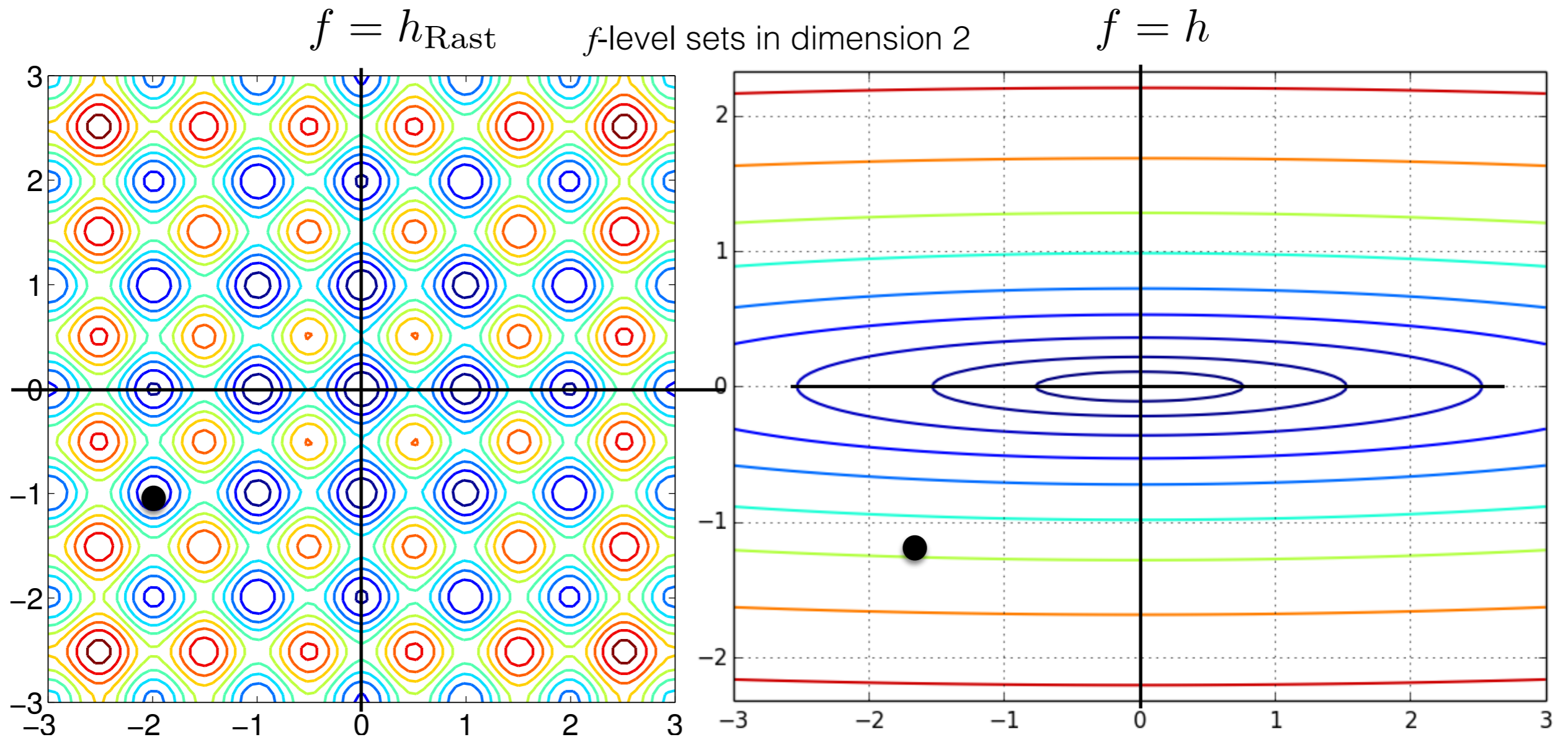
<sup>9</sup> Haario et al 2001. An adaptive Metropolis algorithm, JSTOR

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

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

# Invariance Under Rigid Search Space Transformation



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

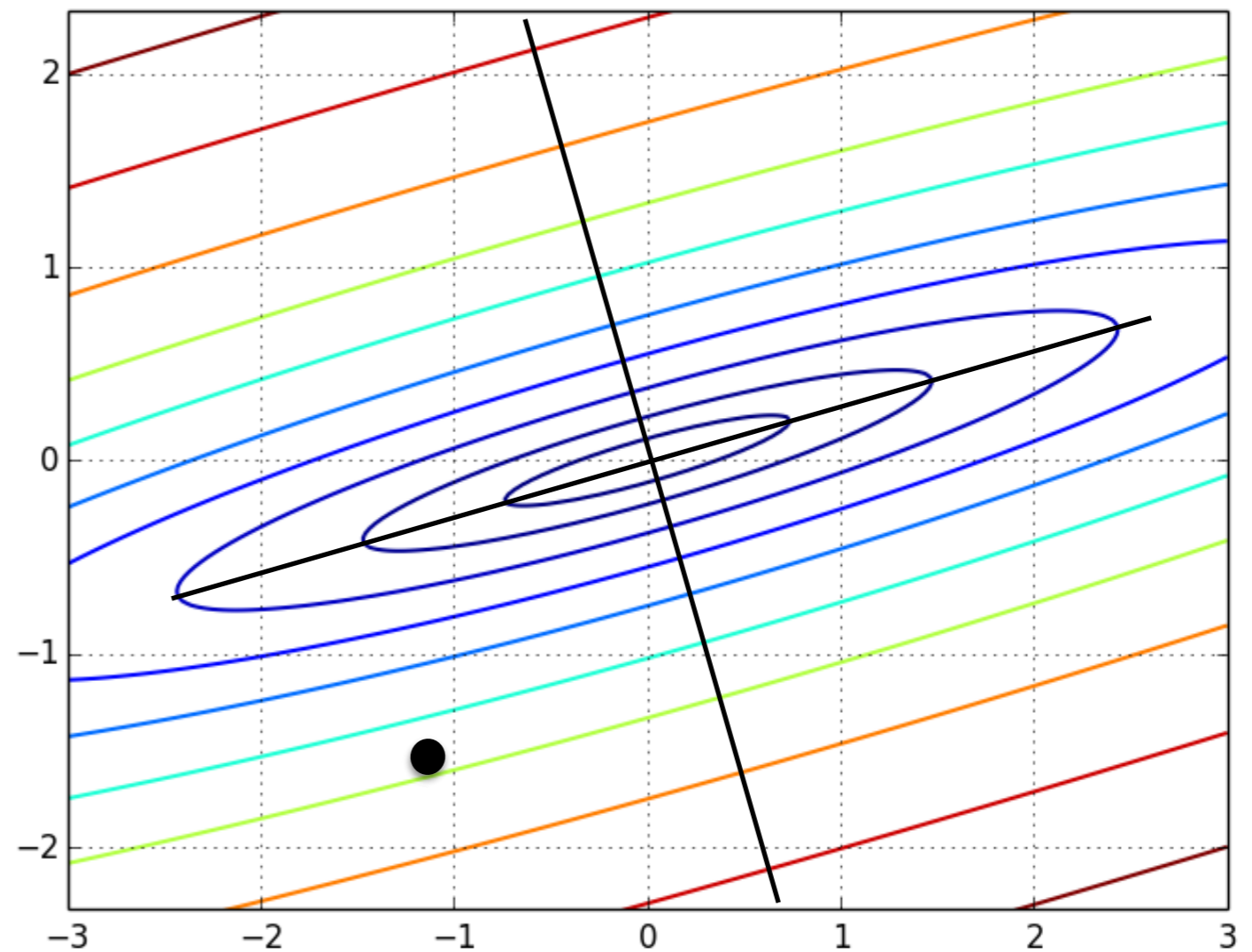
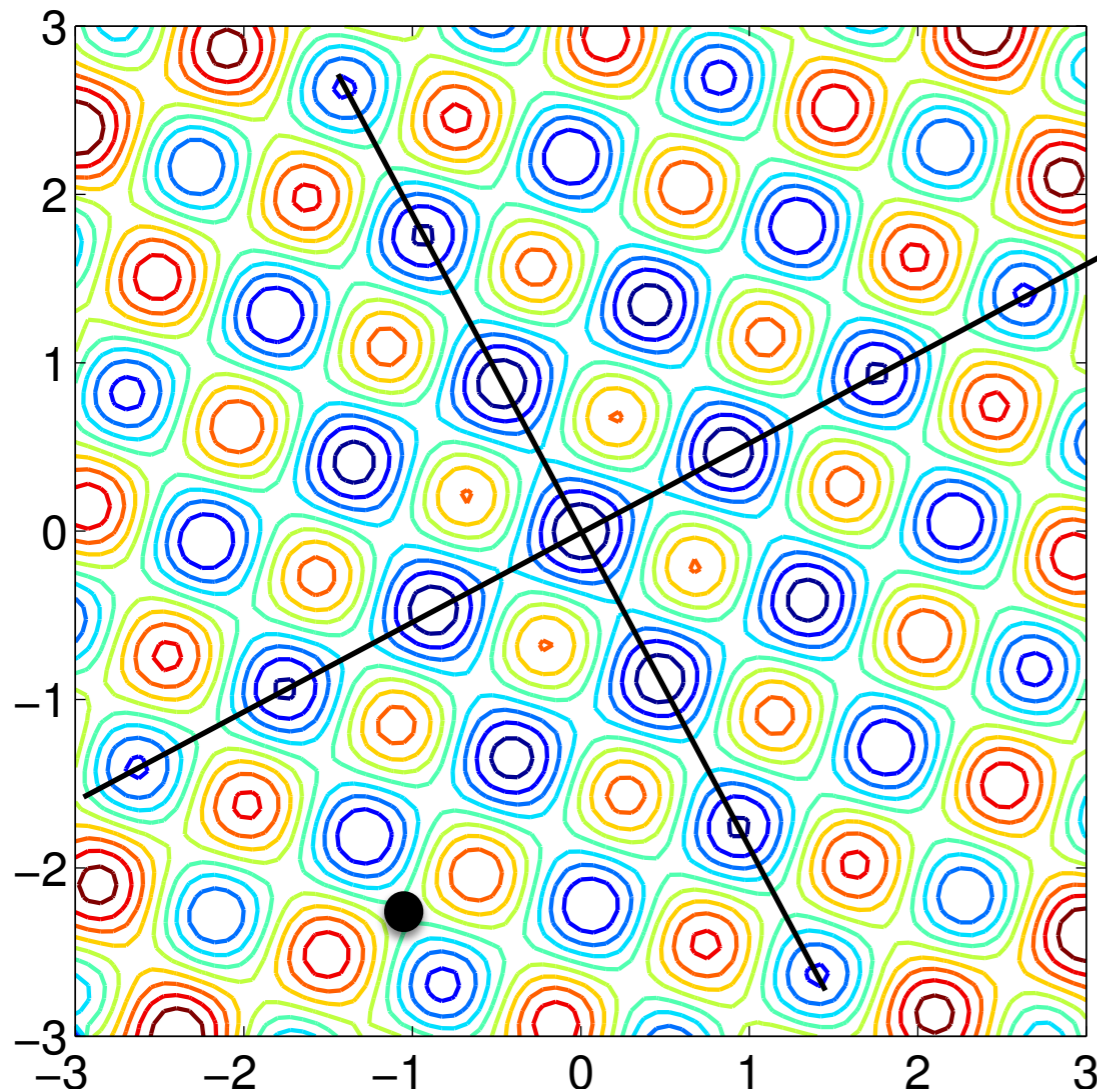


# Invariance Under Rigid Search Space Transformation

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

$f$ -level sets in dimension 2

$$f = h \circ R$$



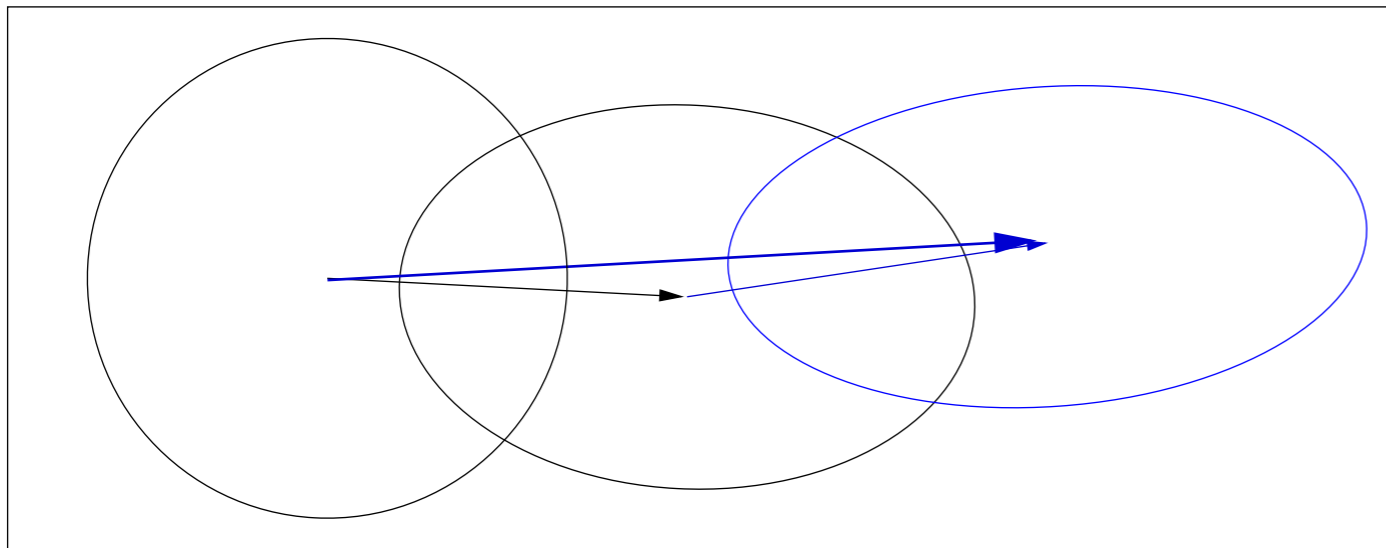
for example, invariance under search space rotation  
(separable  $\Leftrightarrow$  **non-separable**)

# 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):

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

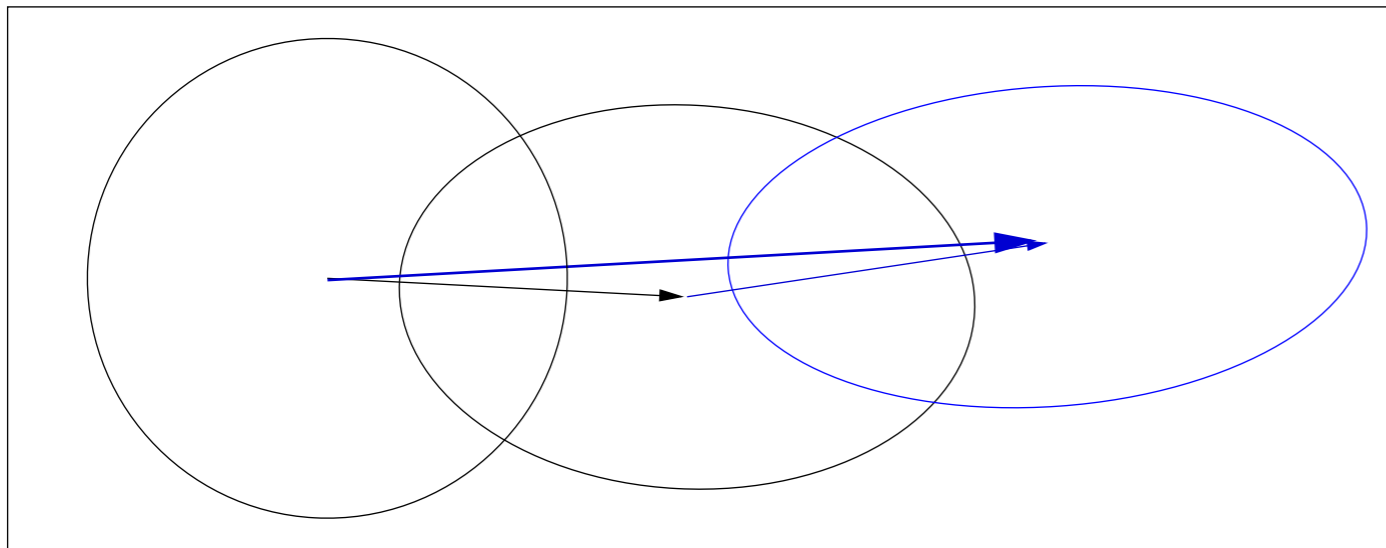
where  $\mu_w = \frac{1}{\sum w_i^2}$ ,  $c_c \ll 1$ . **History information** is accumulated in the evolution path.

# Cumulation

## 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  $m$ .



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

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...

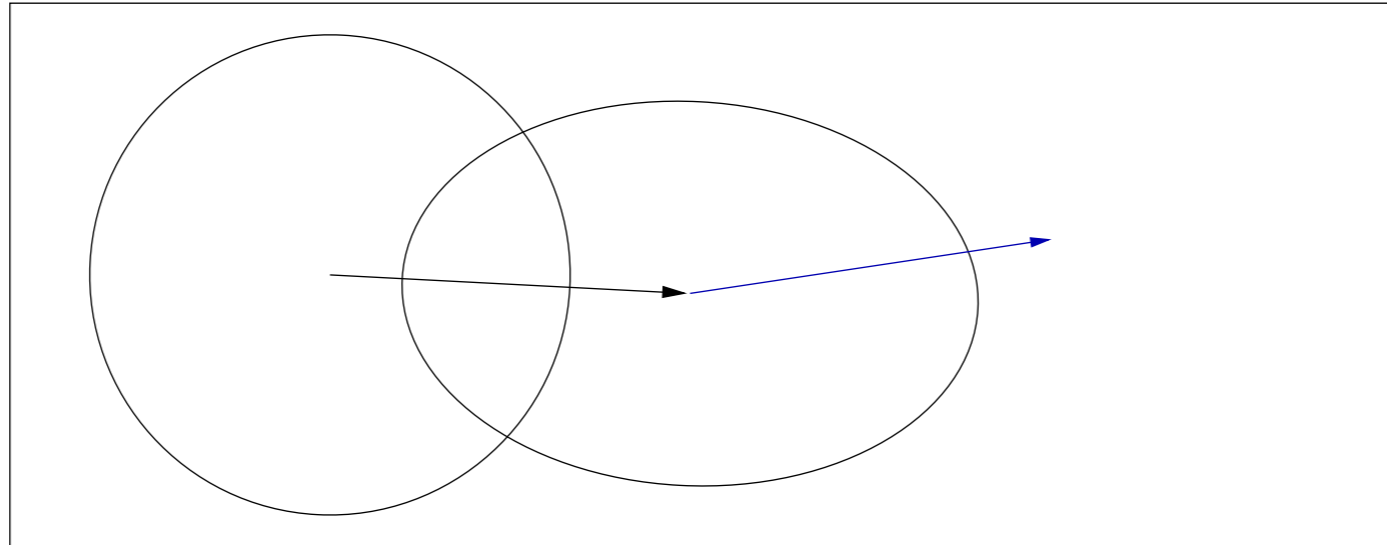
...why?

# 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*.

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

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

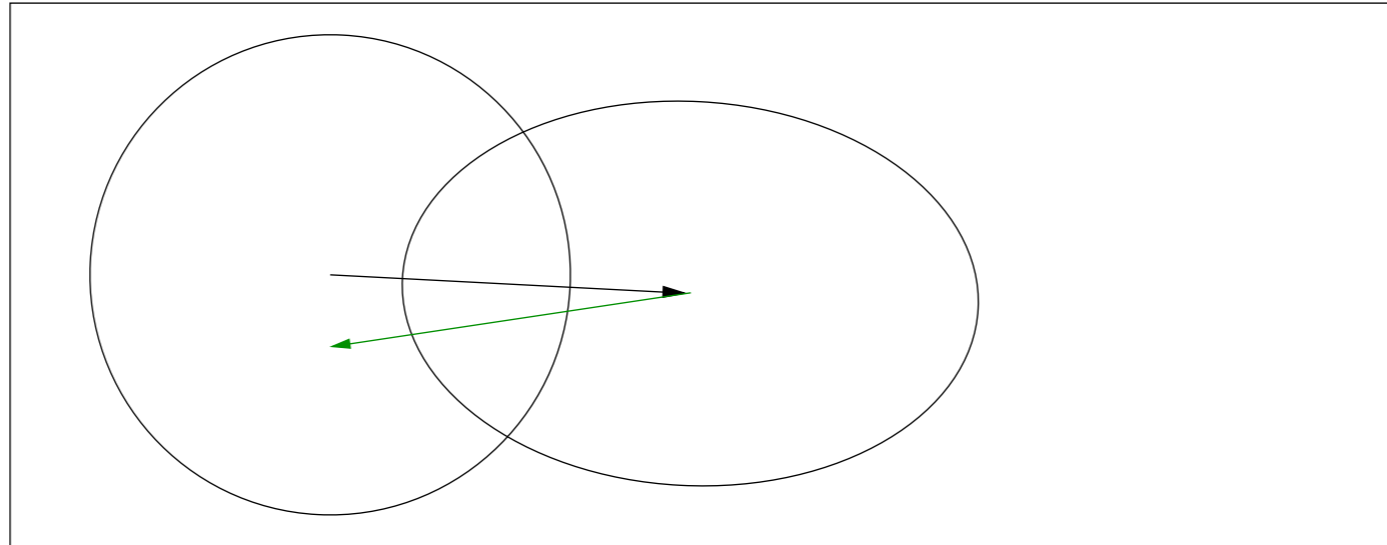
where  $\mu_w = \frac{1}{\sum w_i^2}$ ,  $c_{\text{cov}} \ll c_c \ll 1$  such that  $1/c_c$  is the “backward time horizon”.

# Cumulation

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

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

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

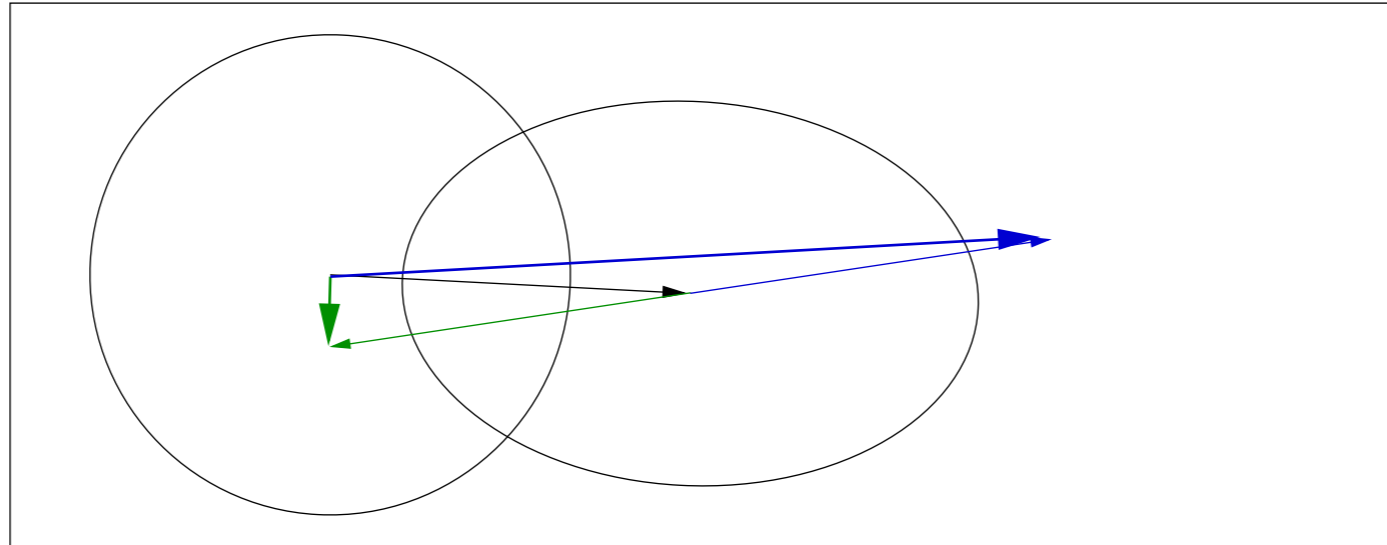
where  $\mu_w = \frac{1}{\sum w_i^2}$ ,  $c_{\text{cov}} \ll c_e \ll 1$  such that  $1/c_e$  is the “backward time horizon”.

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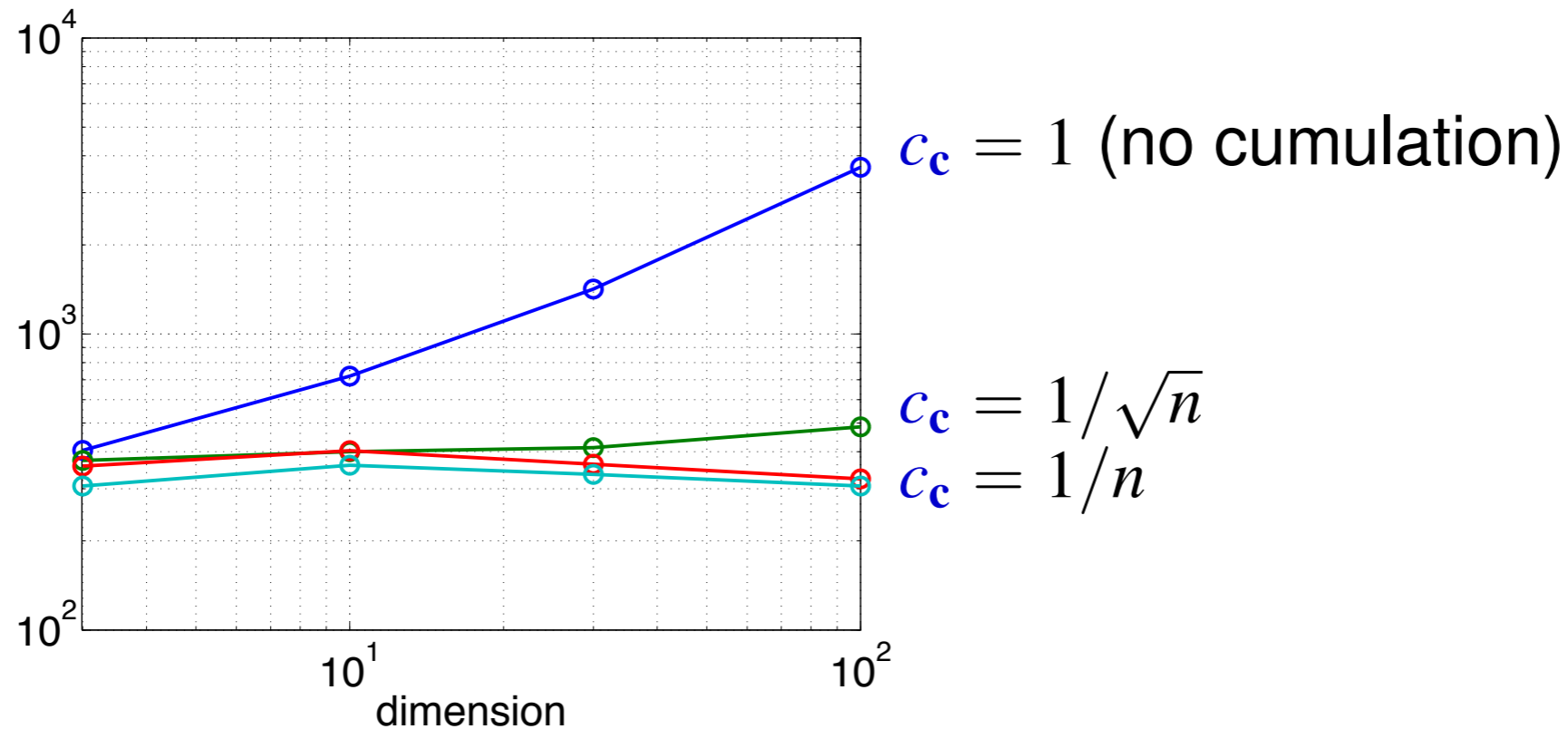
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where  $\mu_w = \frac{1}{\sum w_i^2}$ ,  $c_{\text{cov}} \ll c_c \ll 1$  such that  $1/c_c$  is the “backward time horizon”.

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  $f(\mathbf{x}) = x_1^2 + 10^6 \sum_{i=2}^n x_i^2$



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

# 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.

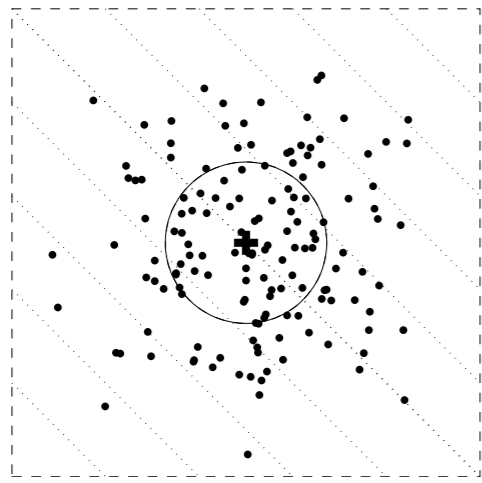
with  $\mu = \lambda$  weights can be negative <sup>10</sup>

The rank- $\mu$  update then reads

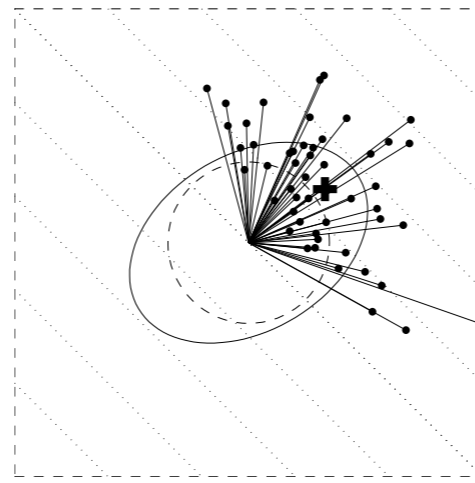
$$\mathbf{C} \leftarrow (1 - c_{\text{cov}}) \mathbf{C} + c_{\text{cov}} \mathbf{C}_\mu$$

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

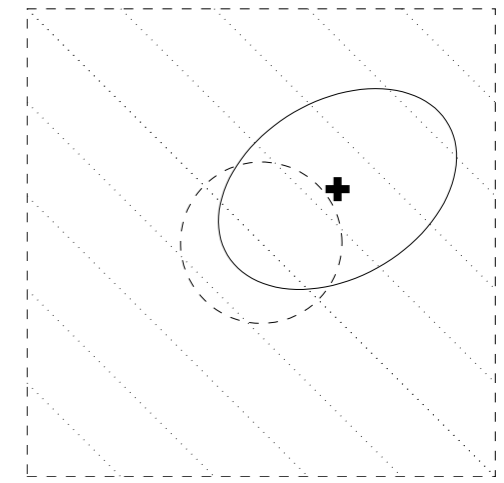
<sup>10</sup>Jastrebski and Arnold (2006). Improving evolution strategies through active covariance matrix adaptation. CEC.



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



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

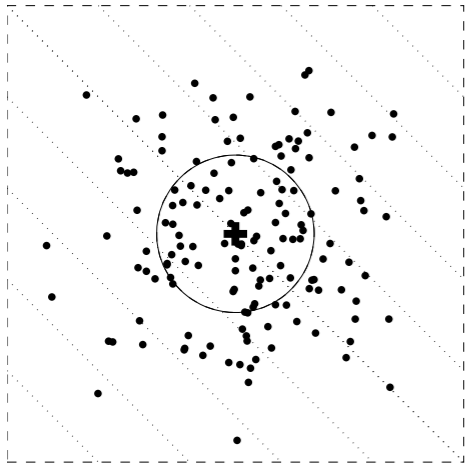


$$m_{\text{new}} \leftarrow m + \frac{1}{\mu} \sum y_{i:\lambda}$$

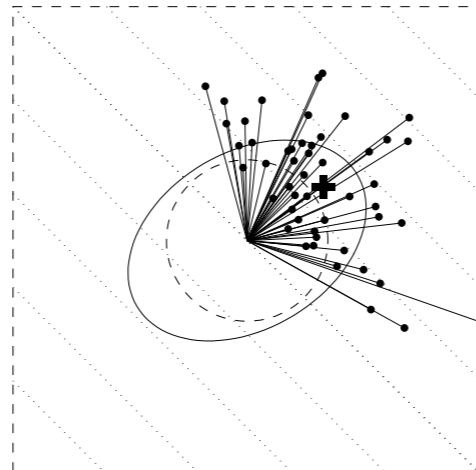
new distribution

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

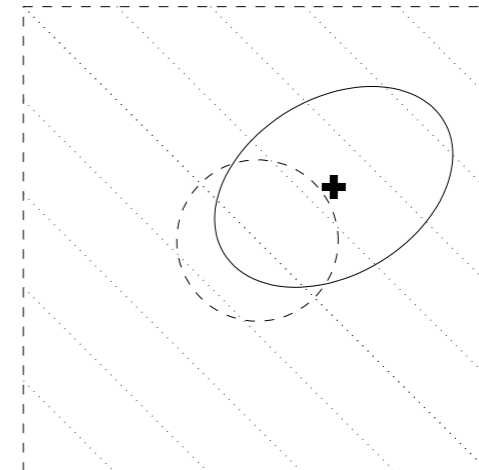
calculating  $\mathbf{C}$  where  
 $\mu = 50$ ,  
 $w_1 = \dots = w_\mu = \frac{1}{\mu}$ ,  
and  $c_{\text{cov}} = 1$

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

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

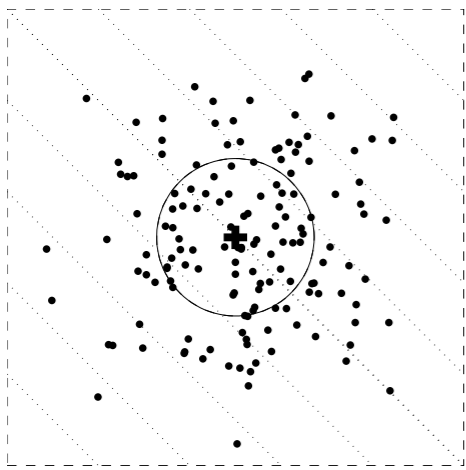


$$\mathbf{C} \leftarrow \frac{1}{\mu} \sum (x_{i:\lambda} - m_{\text{old}})(x_{i:\lambda} - m_{\text{old}})^T$$

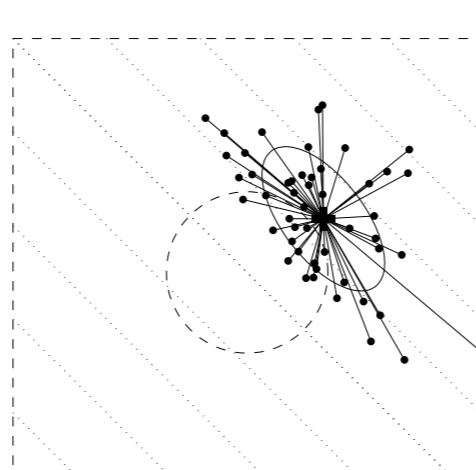


$$m_{\text{new}} = m_{\text{old}} + \frac{1}{\mu} \sum y_{i:\lambda}$$

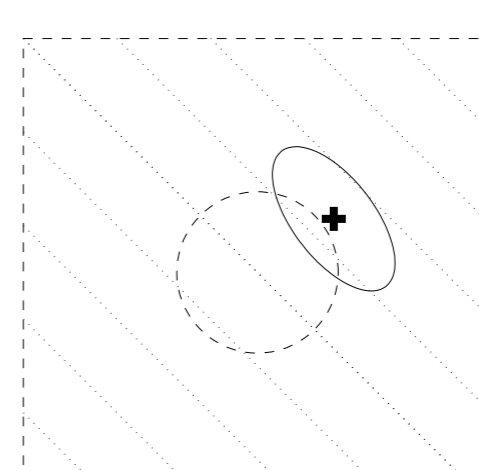
rank- $\mu$  CMA  
conducts a  
PCA of  
steps



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



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



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

EMNA<sub>global</sub>  
conducts a  
PCA of  
points

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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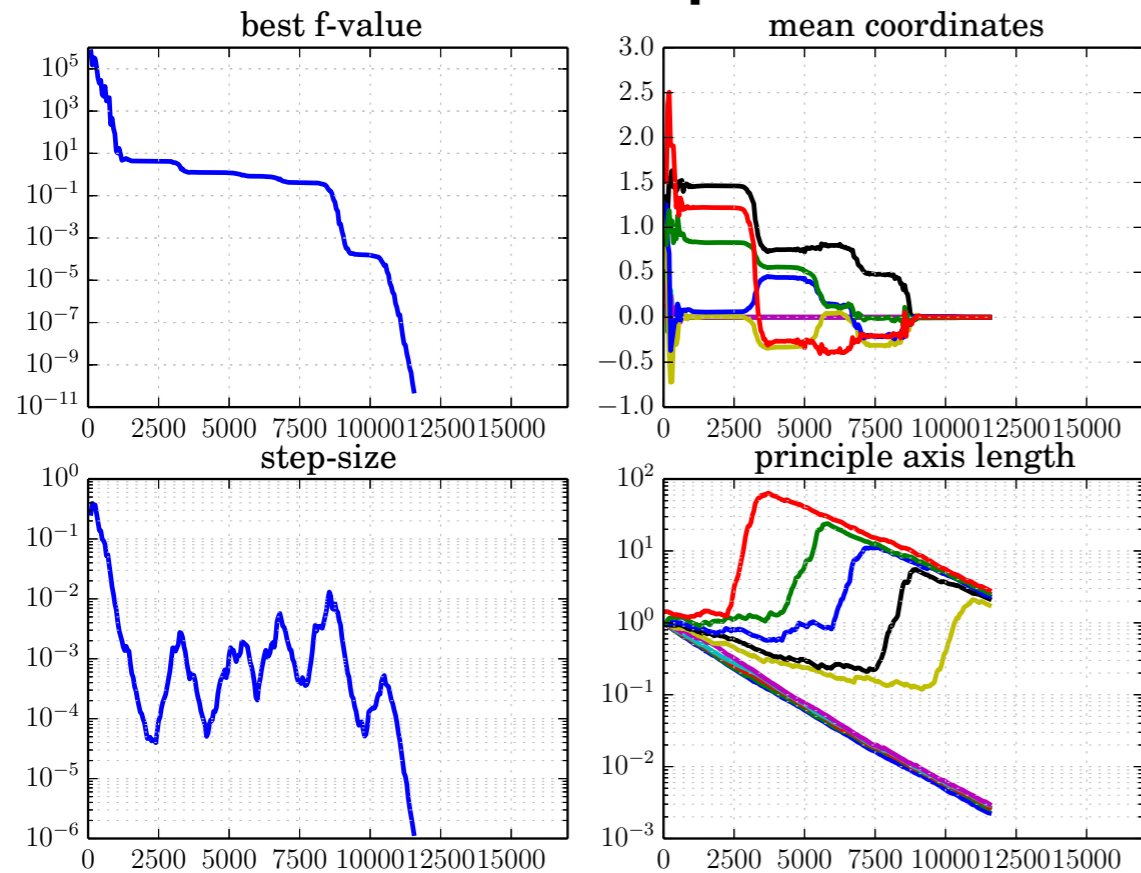
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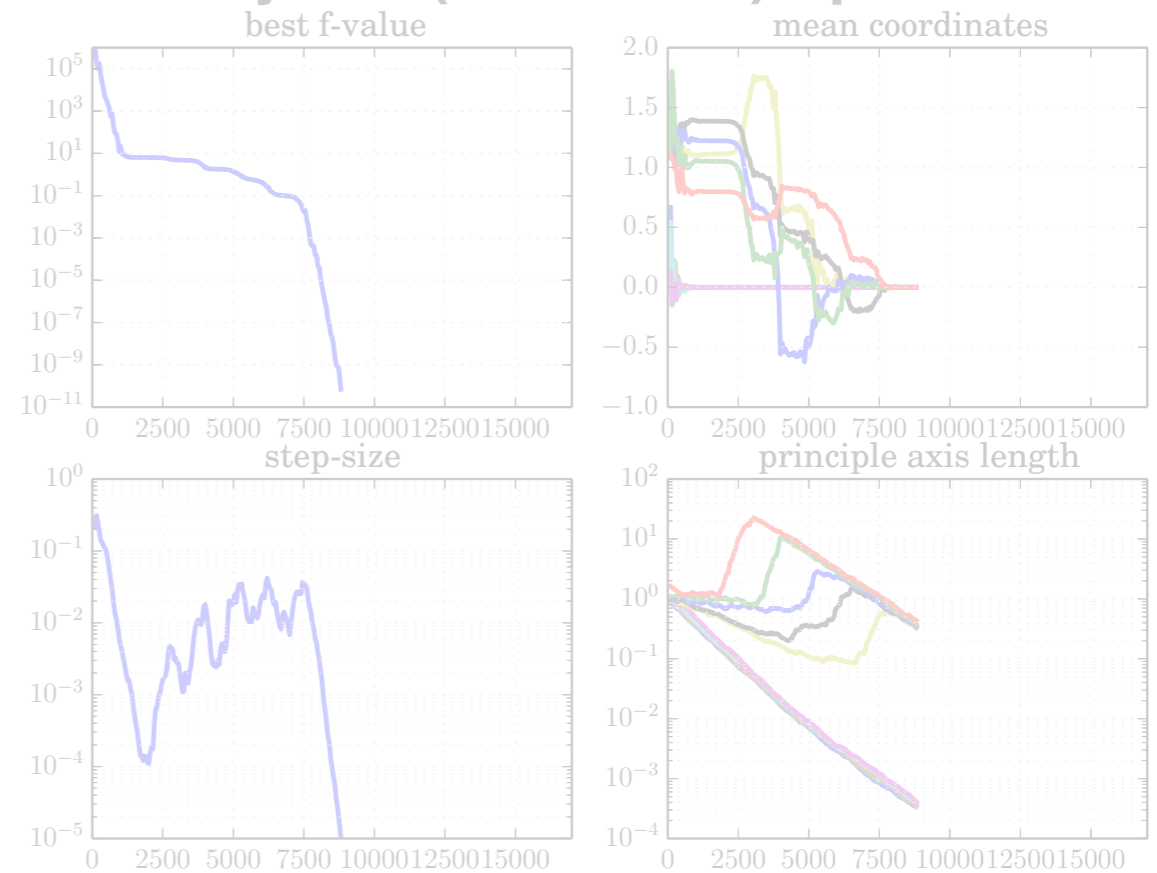
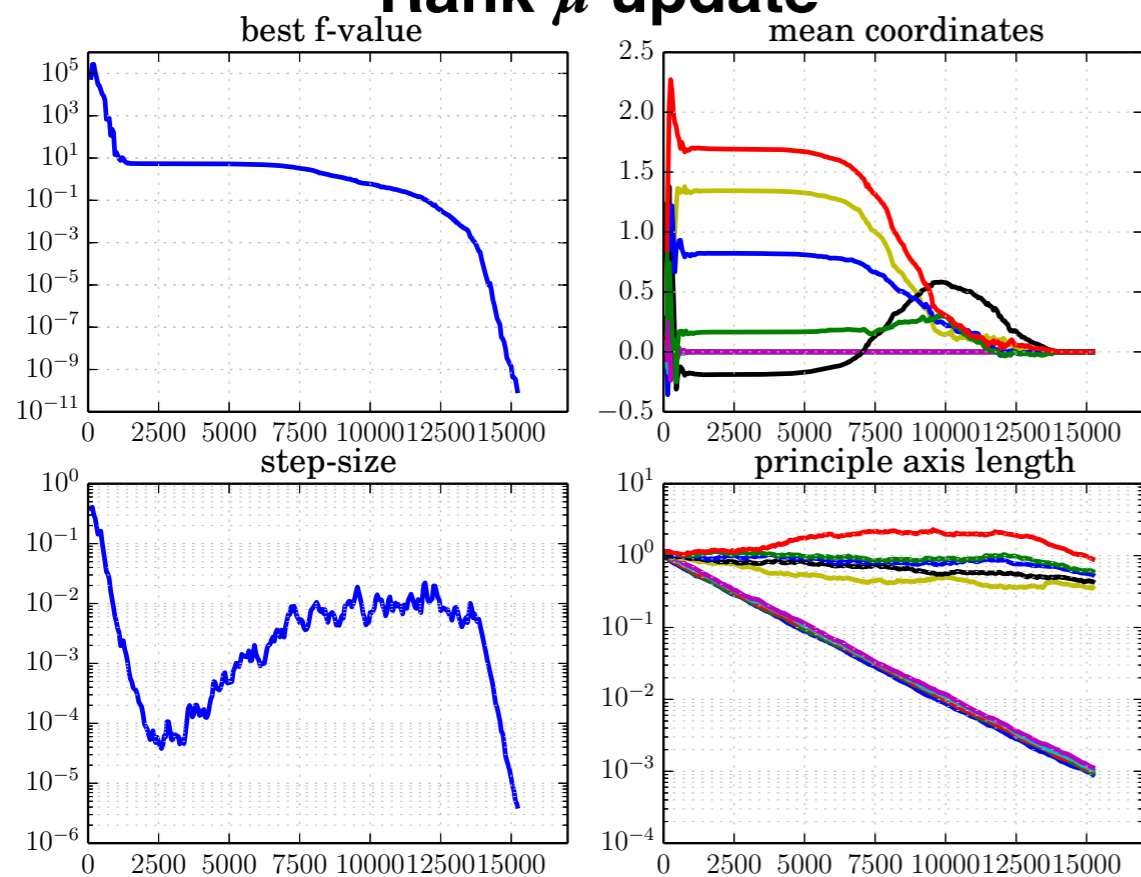
... all equations

<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

## Rank-one update



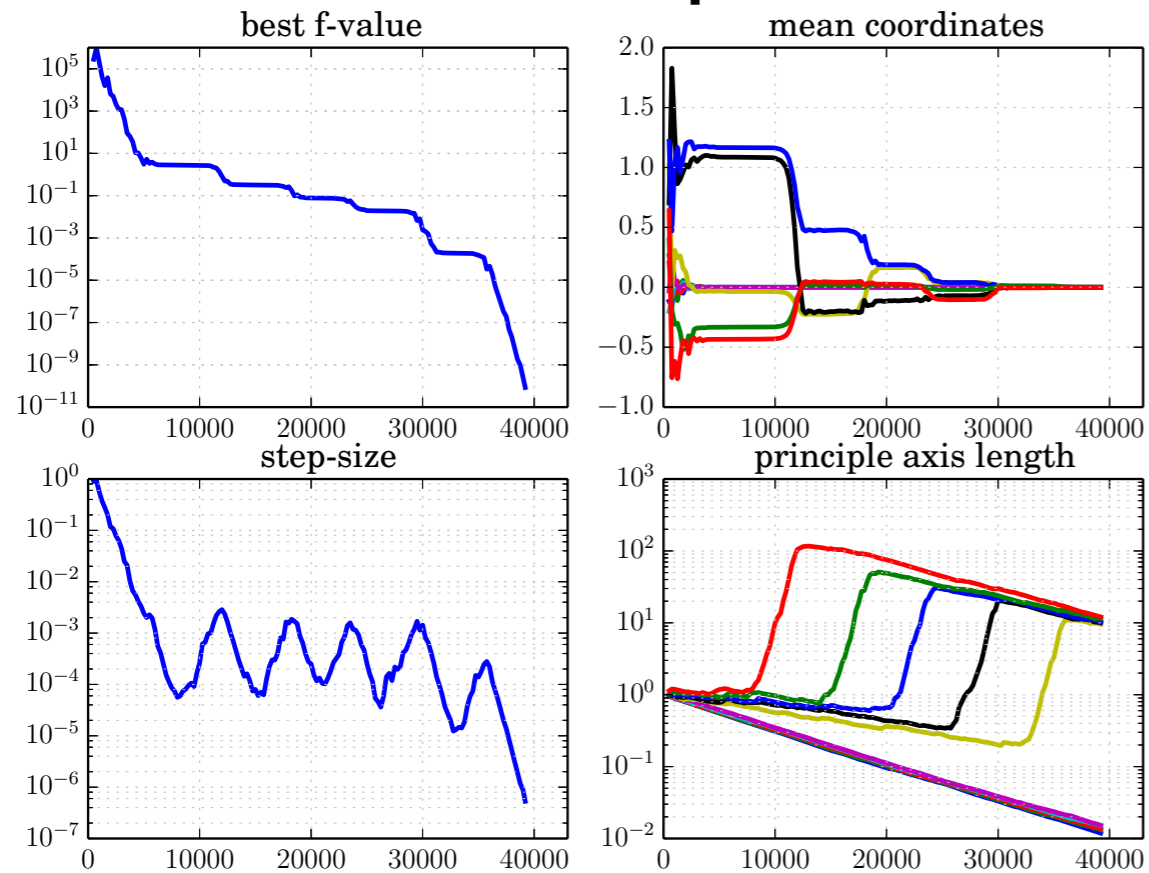
## Hybrid (combined) update

Rank- $\mu$  update

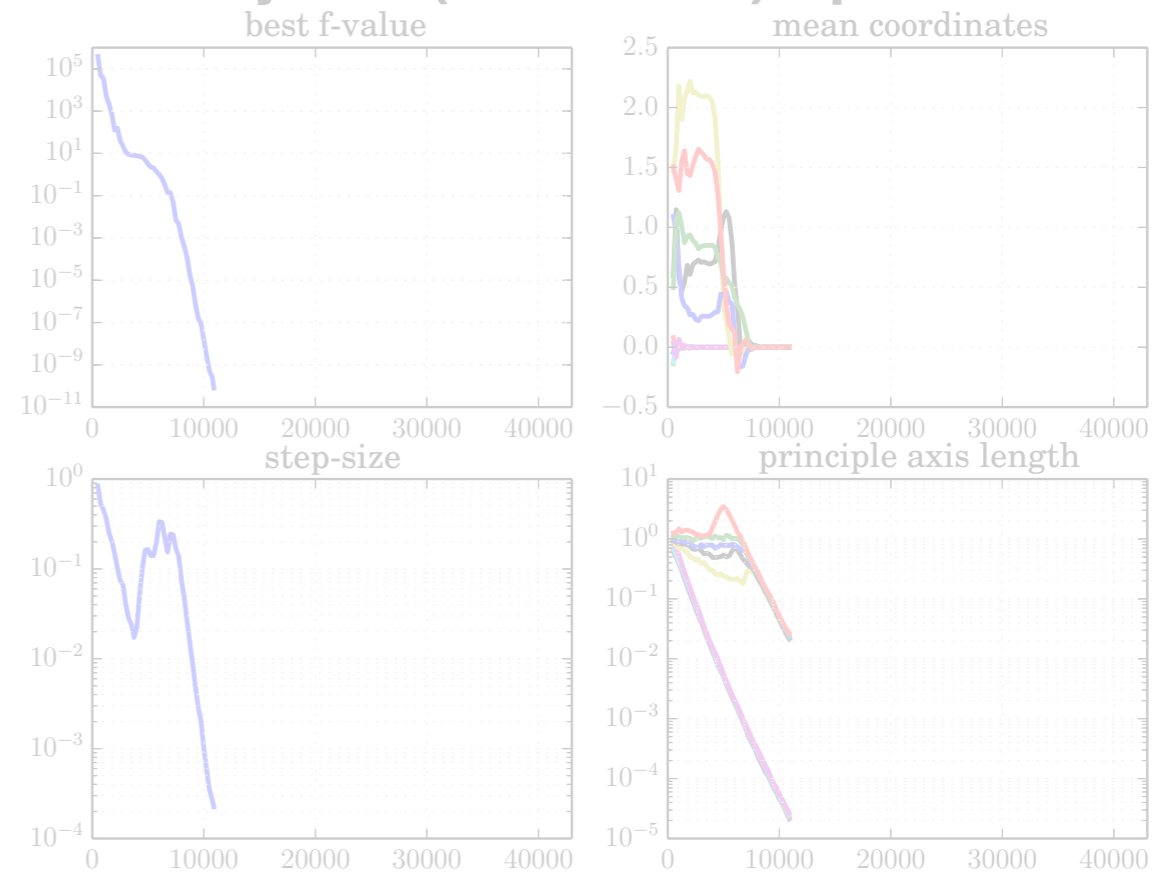
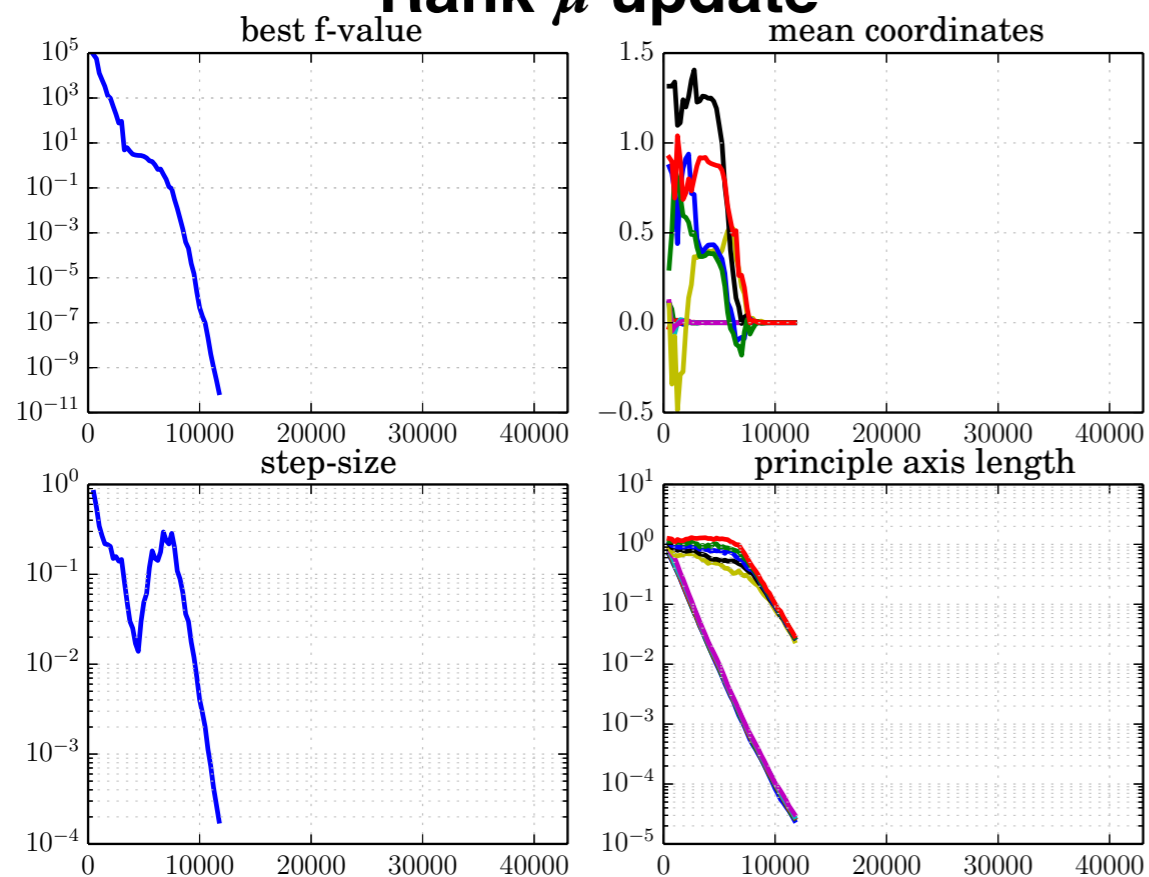
$$f_{\text{TwoAxes}}(x) = \sum_{i=1}^5 x_i^2 + 10^6 \sum_{i=6}^{10} x_i^2$$

$$\lambda = 10 \text{ (default for } N = 10\text{)}$$

## Rank-one update



## Hybrid (combined) update

Rank- $\mu$  update

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

$$\lambda = 50$$

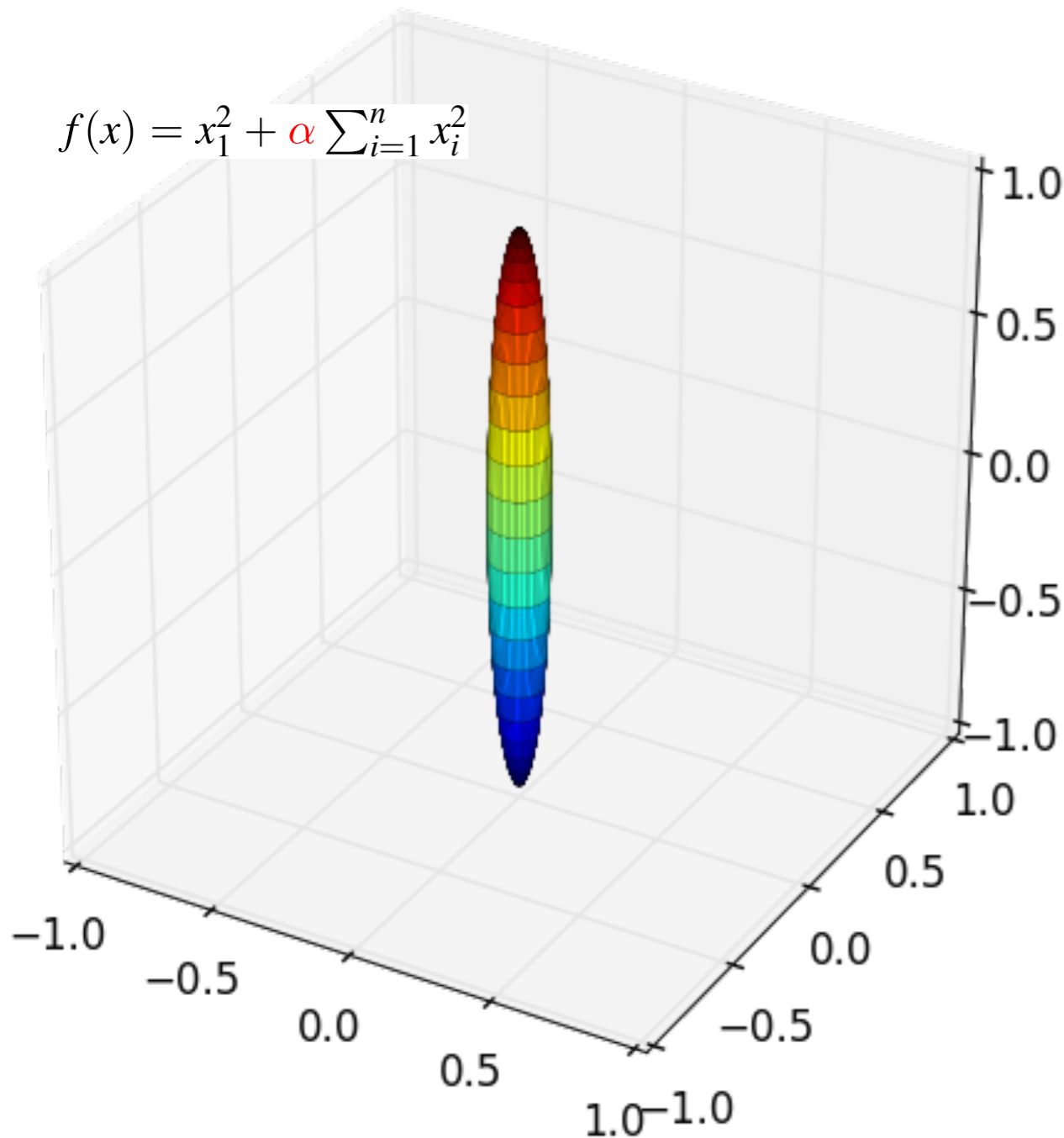
# Different Types of Ill-Conditioning

( $\alpha$ : Axes Ratio = 10)

Cigar Type:

1 **long** axis = n-1 **short** axes

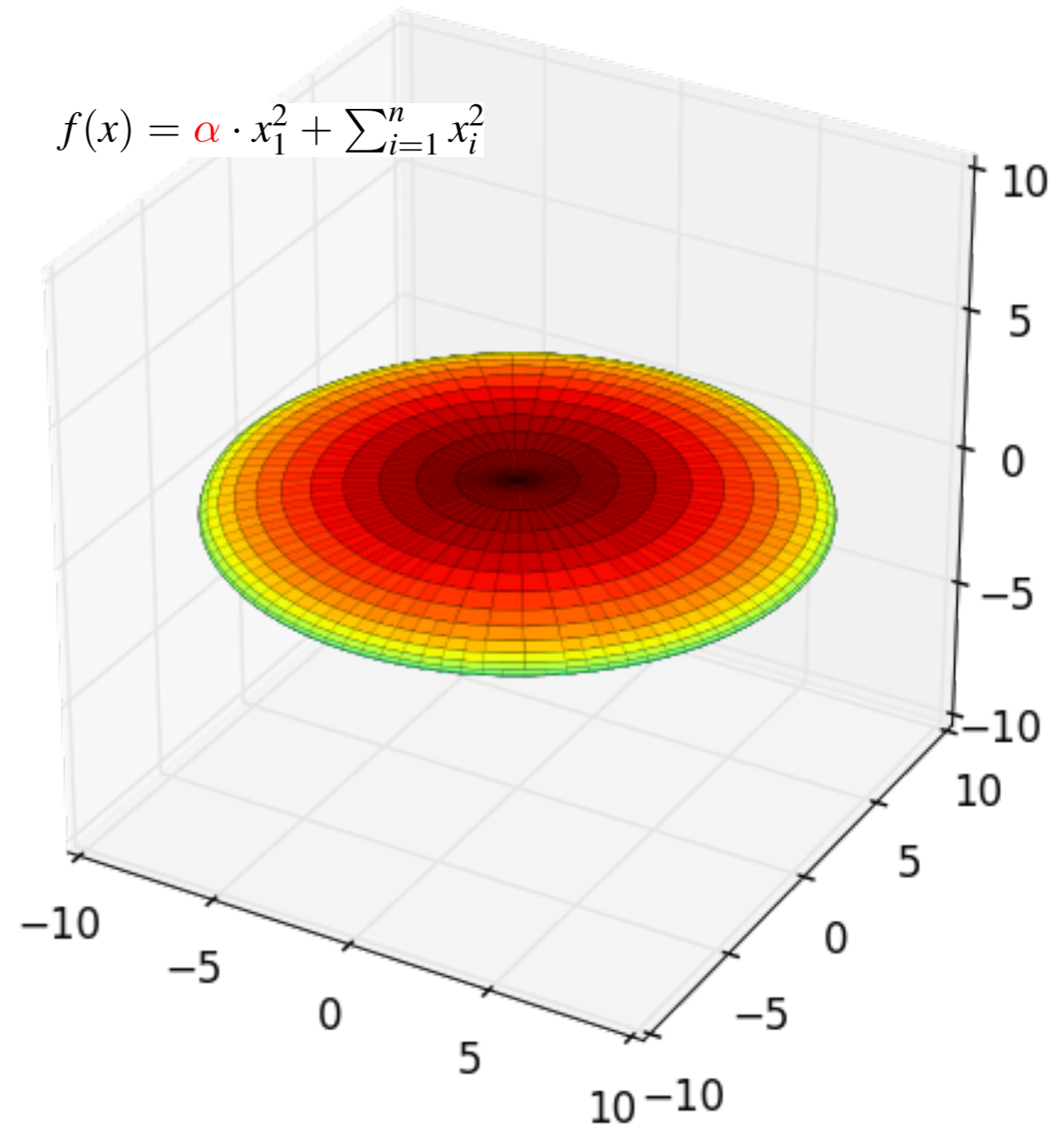
$$f(x) = x_1^2 + \alpha \sum_{i=1}^n x_i^2$$



Discus Type:

1 **short** axis = n-1 **long** axes

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





# Active Update

utilize negative weights [Jastrebski and Arnold, 2006]

## Active Update (rewriting)

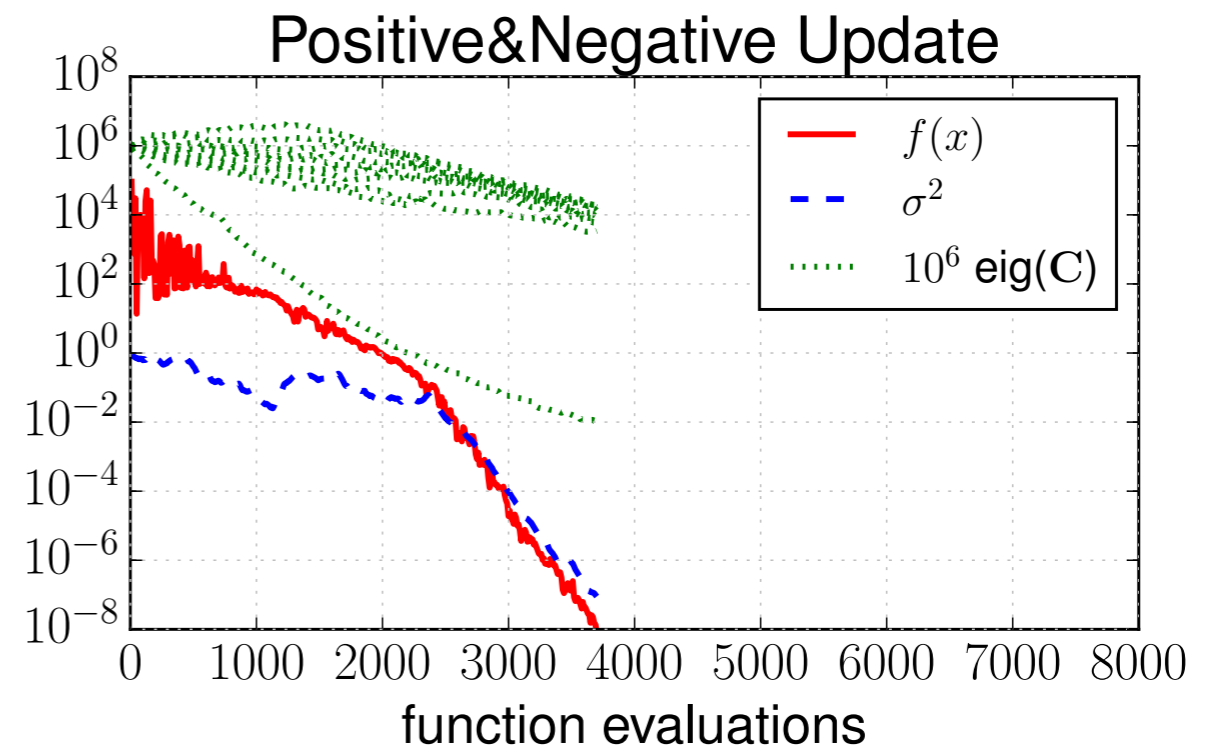
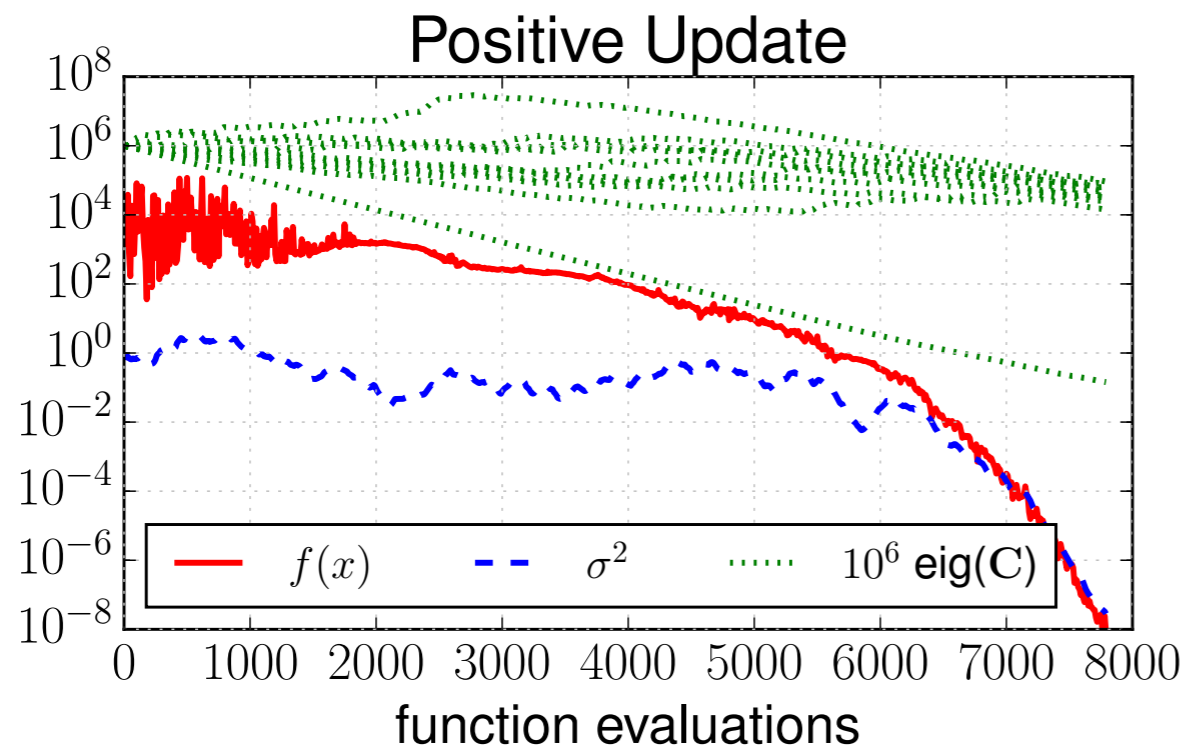
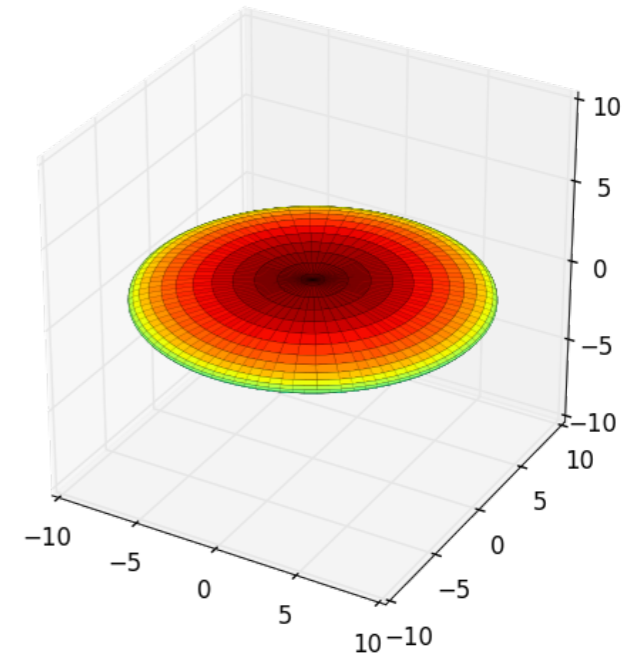
$$\mathbf{C} \leftarrow \underbrace{\mathbf{C} + c_1 \mathbf{p}_c \mathbf{p}_c^T + c_\mu \sum_{i=1}^{\lfloor \lambda/2 \rfloor} w_i \mathbf{y}_{i:\lambda} \mathbf{y}_{i:\lambda}^T}_{\text{increasing the variances in promising directions}} - \underbrace{c_\mu \sum_{i=\lambda - \lfloor \lambda/2 \rfloor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

- 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

# On 10D Discus Function

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

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



- Positive: wait for the smallest  $\text{eig}(\mathbf{C})$  decreasing
- Active: decrease the smallest  $\text{eig}(\mathbf{C})$  actively



# Summary

## Active Covariance Matrix Adaptation + Cumulation

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

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

These components complement each other

- cumulation: excels to learn a long axis, but inefficient for a large  $\lambda$
- rank- $\mu$  update: efficient for a large  $\lambda$
- active update: effective to learn short axes

An important yet solvable issue of active update

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

**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  $\mathbf{y}_w = \sum_{i=1}^\mu w_{\text{rk}(i)} \mathbf{y}_i$  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  $\lambda$

# Topics

1. What makes the problem difficult to solve?

2. How does the CMA-ES work?

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

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

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

# Default Parameter Values

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

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

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

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

# Parameters to be set depending on the problem

## Initialization and termination conditions

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

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

### *Practical Hints:*

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

# Python CMA-ES Implementation

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

## pycma

---

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

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

Useful links:

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

## Installation of the [latest release](#)

---

Type

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

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

# Python CMA-ES Demo

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

## Optimizing 10D Rosenbrock Function

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

```
(5_w,10)-aCMA-ES (mu_w=3.2,w_1=45%) in dimension 10 (seed=909490, Mon Apr 16 13:39:57 2018)
```

Iterat	#Fevals	function value	axis ratio	sigma	min&max	std	t[m:s]
1	10	1.169928472214858e+01	1.0e+00	9.12e-02	9e-02	9e-02	0:00.0
2	20	1.363303277917634e+01	1.1e+00	8.33e-02	8e-02	8e-02	0:00.0
3	30	1.232089008099892e+01	1.2e+00	7.55e-02	7e-02	8e-02	0:00.0
100	1000	5.724977739870999e+00	9.1e+00	1.65e-02	7e-03	2e-02	0:00.1
200	2000	2.550841127554589e+00	1.5e+01	3.97e-02	1e-02	4e-02	0:00.2
300	3000	3.674986141687857e-01	1.5e+01	2.76e-02	3e-03	2e-02	0:00.4
400	4000	1.266345464781239e-03	5.0e+01	1.18e-02	8e-04	2e-02	0:00.5
420	4200	7.039461687999381e-05	5.5e+01	4.04e-03	2e-04	5e-03	0:00.5

```
termination on ftarget=0.0001 (Mon Apr 16 13:39:58 2018)
```

```
final/bestever f-value = 2.804423e-05 2.804423e-05
```

```
incumbent solution: [ 0.9998542  0.99996219  0.9999681  1.00000445  0.99998977  0.99968537
```

```
0.99954974  0.99918266 ...]
```

```
std deviations: [ 0.00023937  0.00022203  0.00024836  0.00024782  0.00031258  0.00043481
```

```
0.00078261  0.0014964 ...]
```

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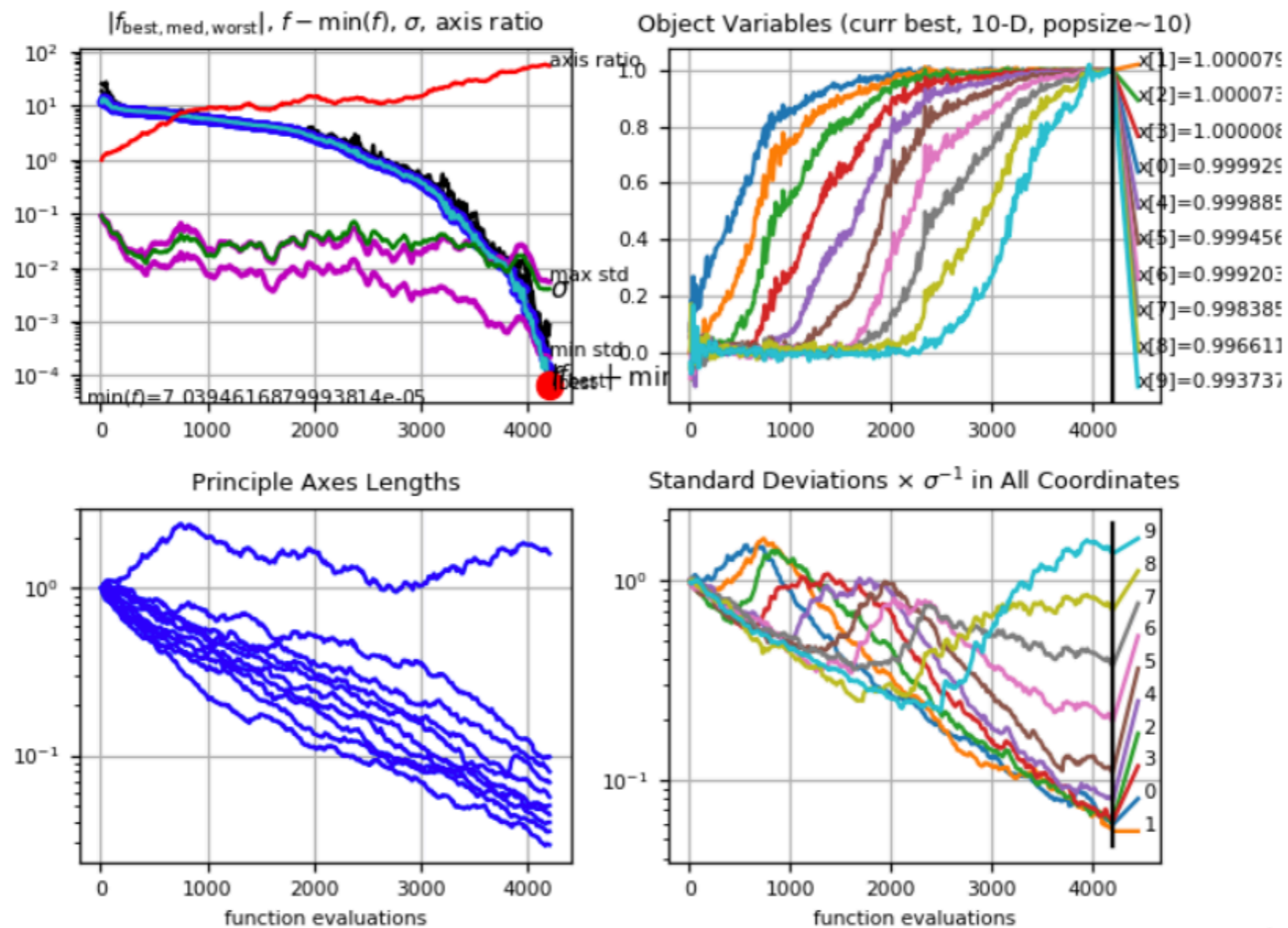
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## Optimizing 10D Rosenbrock Function

```
cma.plot()
```

Figure 325





# Multimodality

Two approaches for multimodal functions: Try again with

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

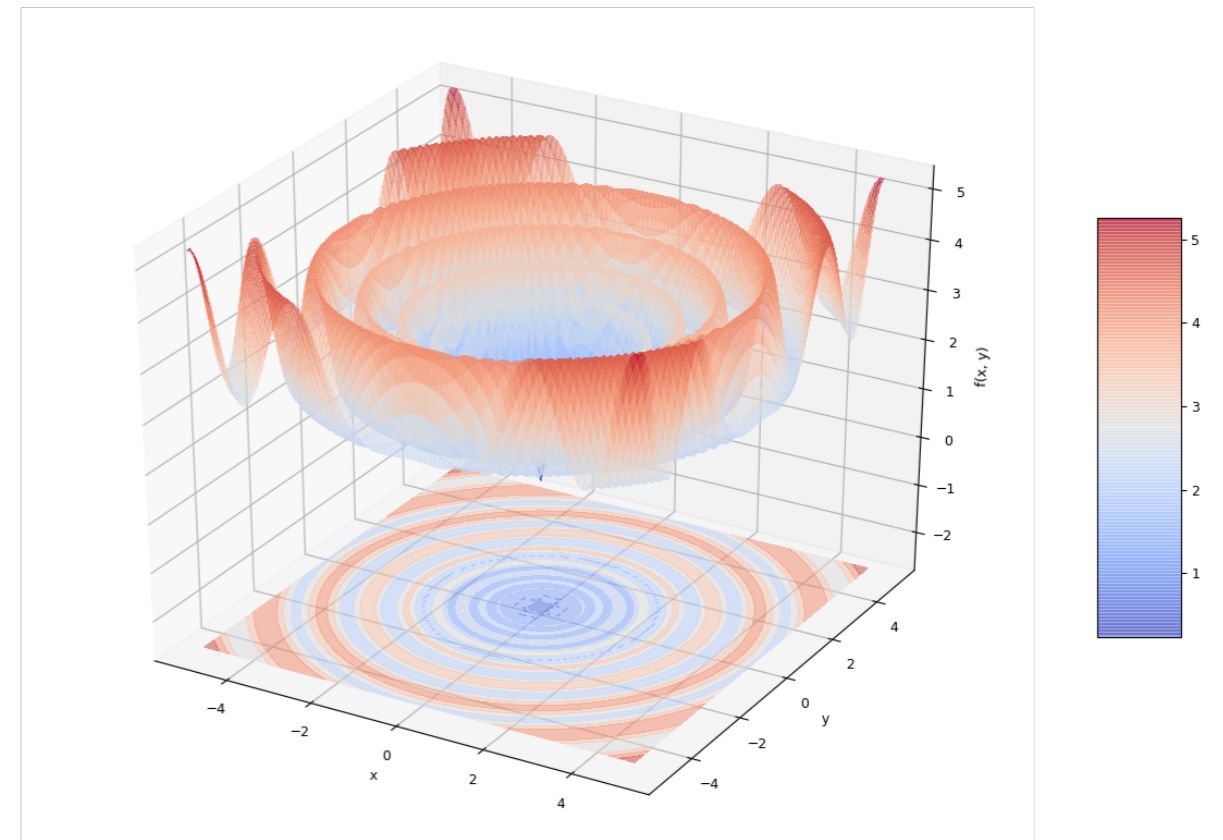
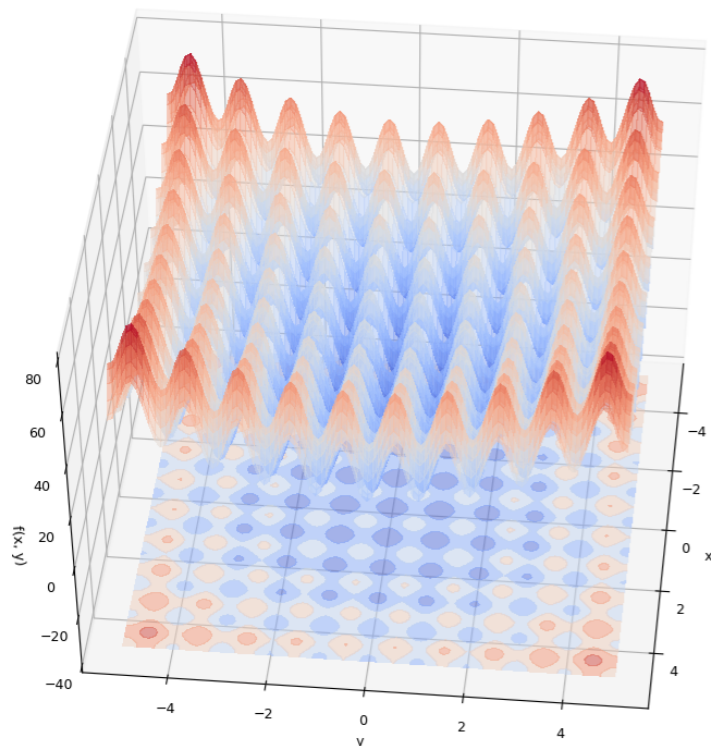
# Multimodality

Approaches for multimodal functions: Try again with

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

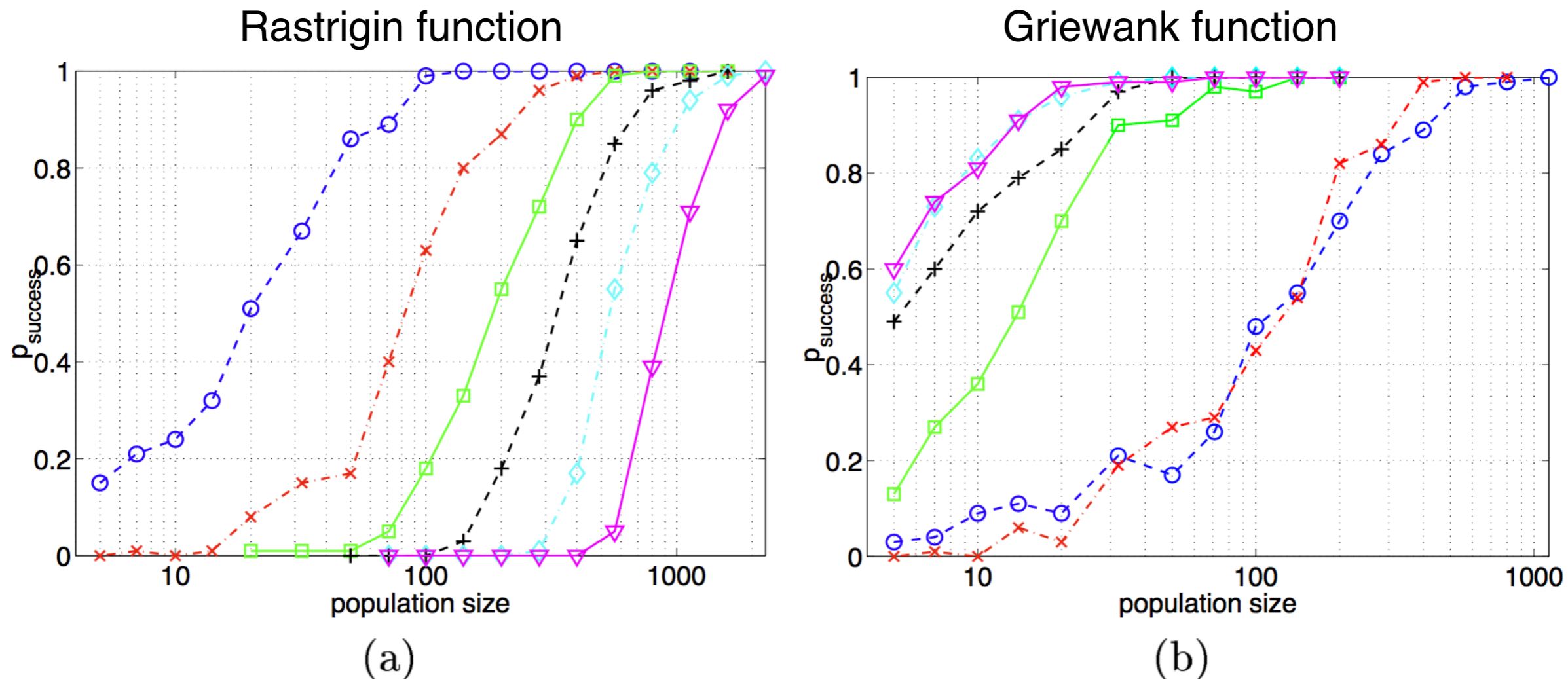
A restart with a **large population size** helps if the objective function has a **well global structure**

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



# Multimodality

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



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

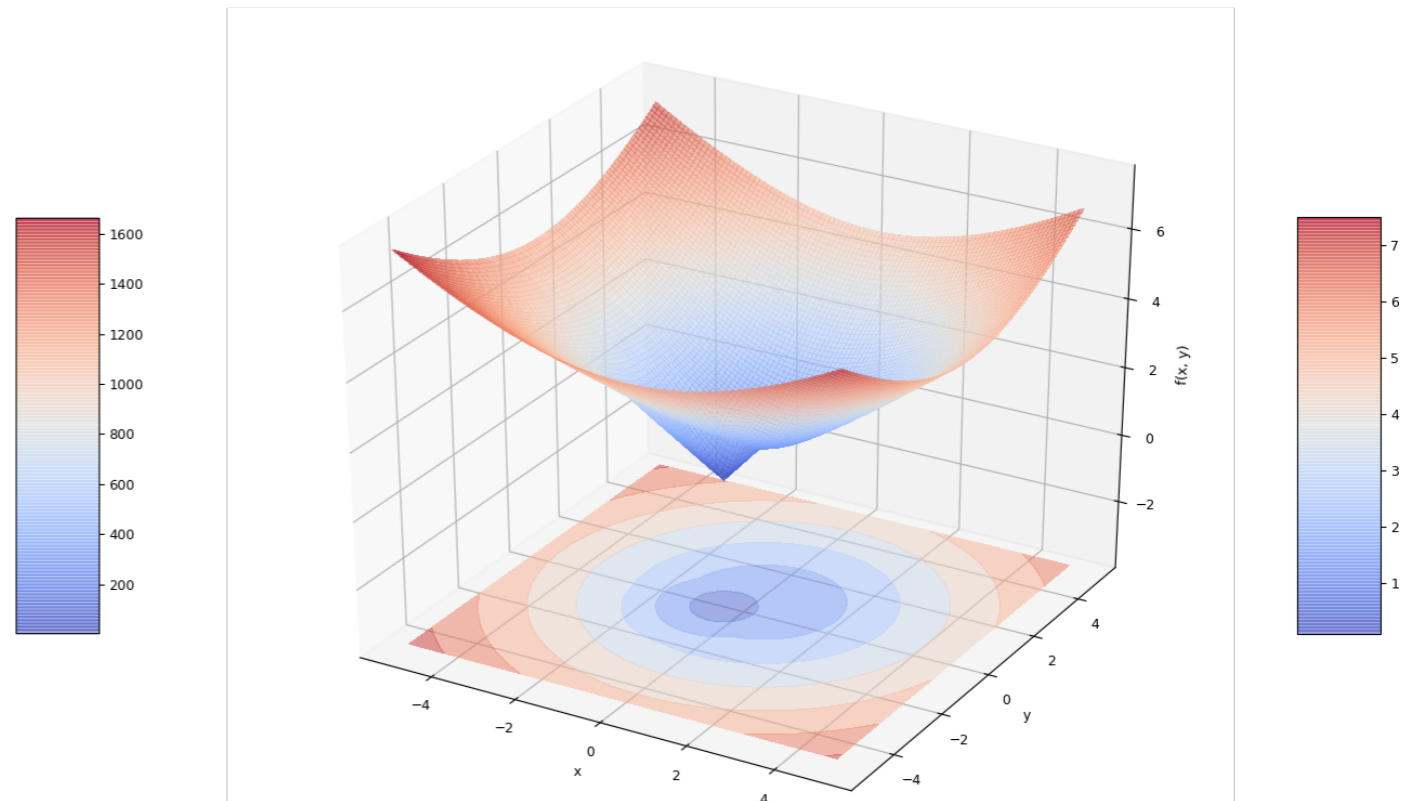
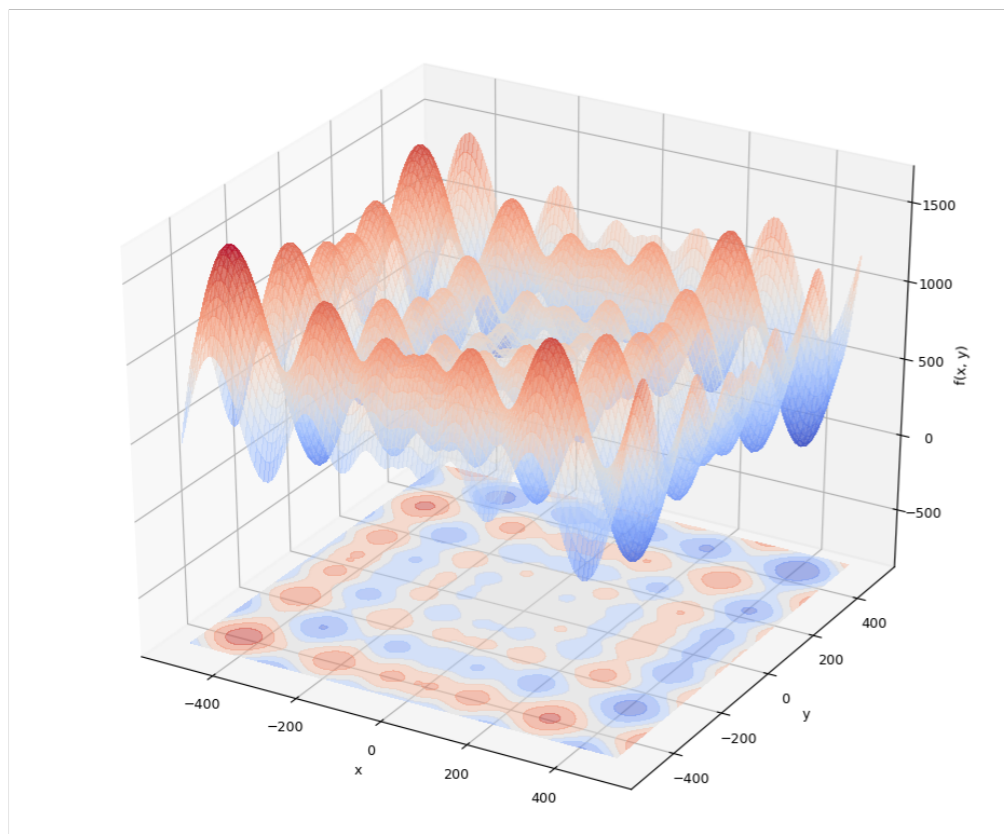
# Multimodality

Approaches for multimodal functions: Try again with

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

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

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



a large population size has a negative effect

# Restart Strategy

It makes the CMA-ES parameter free

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

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

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

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

# Topics

1. What makes the problem difficult to solve?

2. How does the CMA-ES work?

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

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

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



# Motivation of the Restricted Covariance Matrix

Bottlenecks of the CMA-ES on high dimensional problems

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

Exploit prior knowledge on the problem structure such as separability

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

# Variants with Restricted Covariance Matrix

## CMA-ES Variants with Restricted Covariance Matrices

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

[Ros and Hansen, 2008] Ros, R. and Hansen, N. (2008). A simple modification in CMA-ES achieving linear time and space complexity. In Parallel Problem Solving from Nature - PPSN X, pages 296–305. Springer.

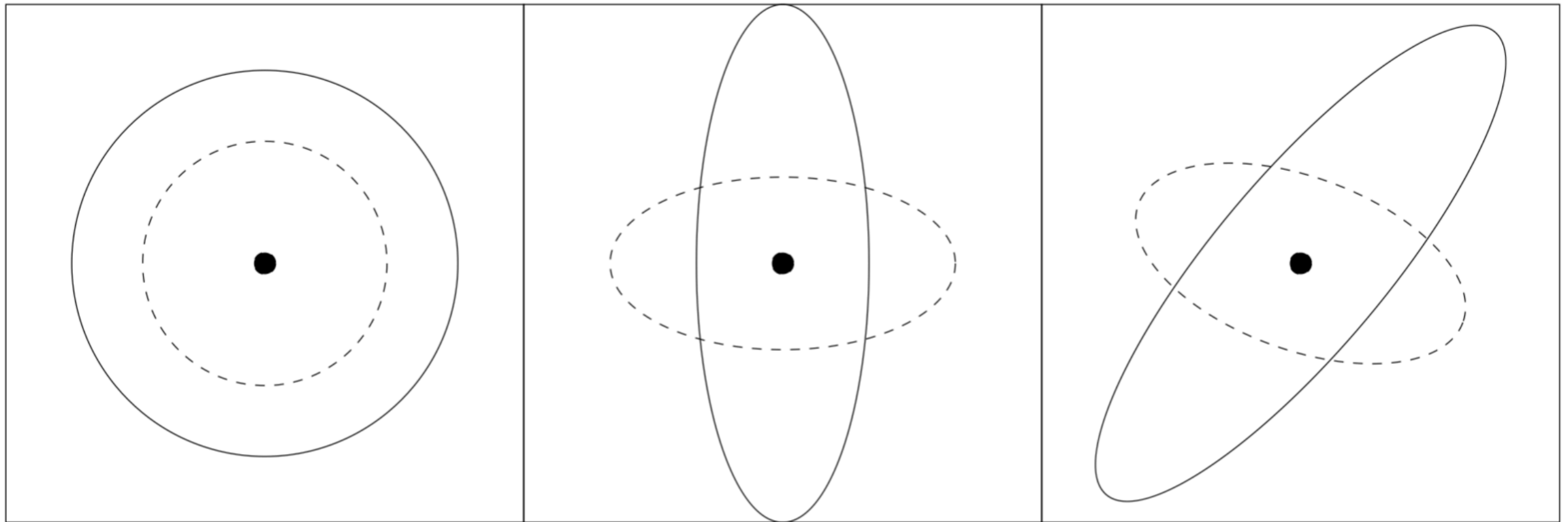
[Akimoto et al., 2014] Akimoto, Y., Auger, A., and Hansen, N. (2014). Comparison-based natural gradient optimization in high dimension. In Proceedings of Genetic and Evolutionary Computation Conference, pages 373–380, Vancouver, BC, Canada.

[Loshchilov, 2014] Loshchilov, I. (2014). A computationally efficient limited memory cma-es for large scale optimization. In Proceedings of Genetic and Evolutionary Computation Conference, pages 397–404.

[Akimoto and Hansen, 2016] Akimoto, Y. and Hansen, N. (2016). Projection-based restricted covariance matrix adaptation for high dimension. In Genetic and Evolutionary Computation Conference, GECCO 2016, Denver, Colorado, USA, July 20-24, 2016, page (accepted). ACM.



# Separable CMA (Sep-CMA)



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

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

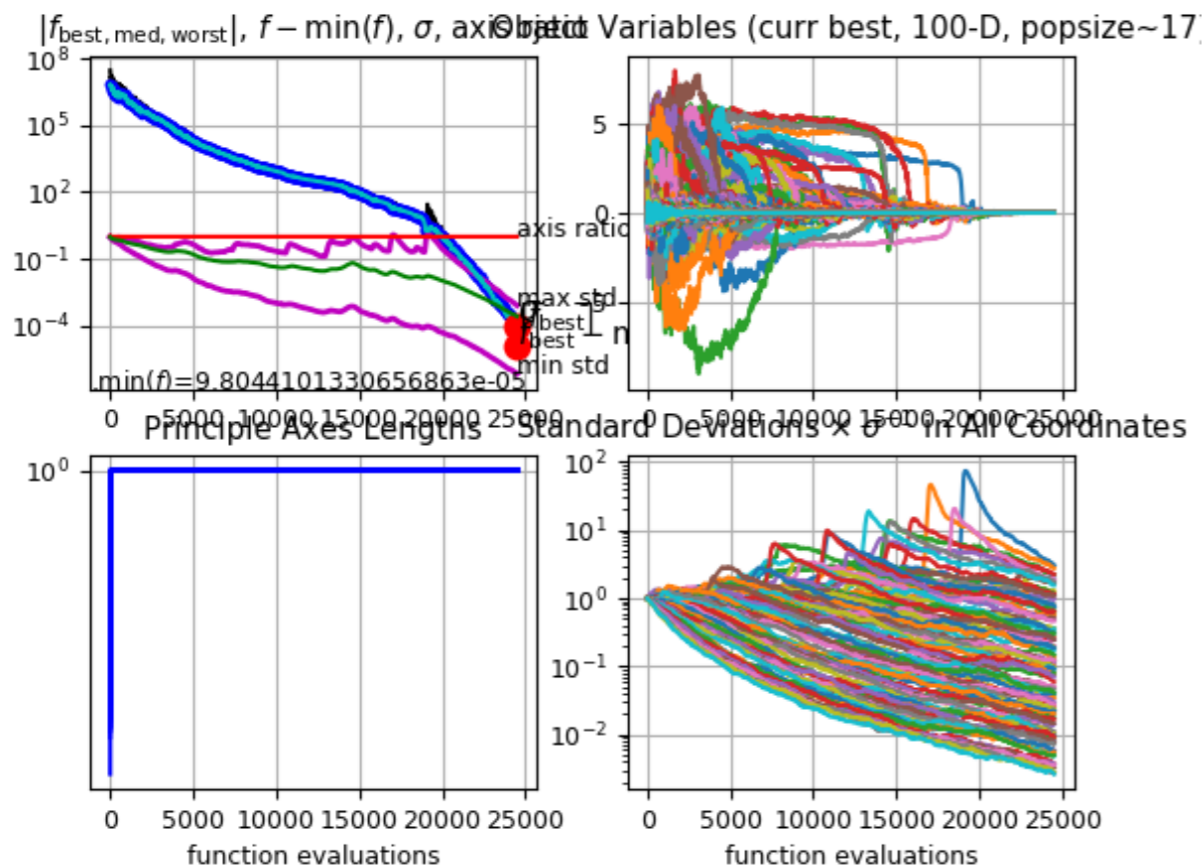
$\mathcal{N}(\mathbf{m}, \mathbf{C}) \sim \mathbf{m} + \mathbf{C}^{\frac{1}{2}} \mathcal{N}(\mathbf{0}, \mathbf{I})$   
 $(n^2 + n)/2$  degrees of freedom

CMA 
$$\mathbf{C}_{\text{cma}}^{(t+1)} = \mathbf{C}^{(t)} + c_1 (\mathbf{p}_c \mathbf{p}_c^T - \mathbf{C}^{(t)}) + c_\mu \sum_{i=1}^{\mu} w_i \left( (\mathbf{x}_i - \mathbf{m}^{(t)}) (\mathbf{x}_i - \mathbf{m}^{(t)})^T - \mathbf{C}^{(t)} \right)$$

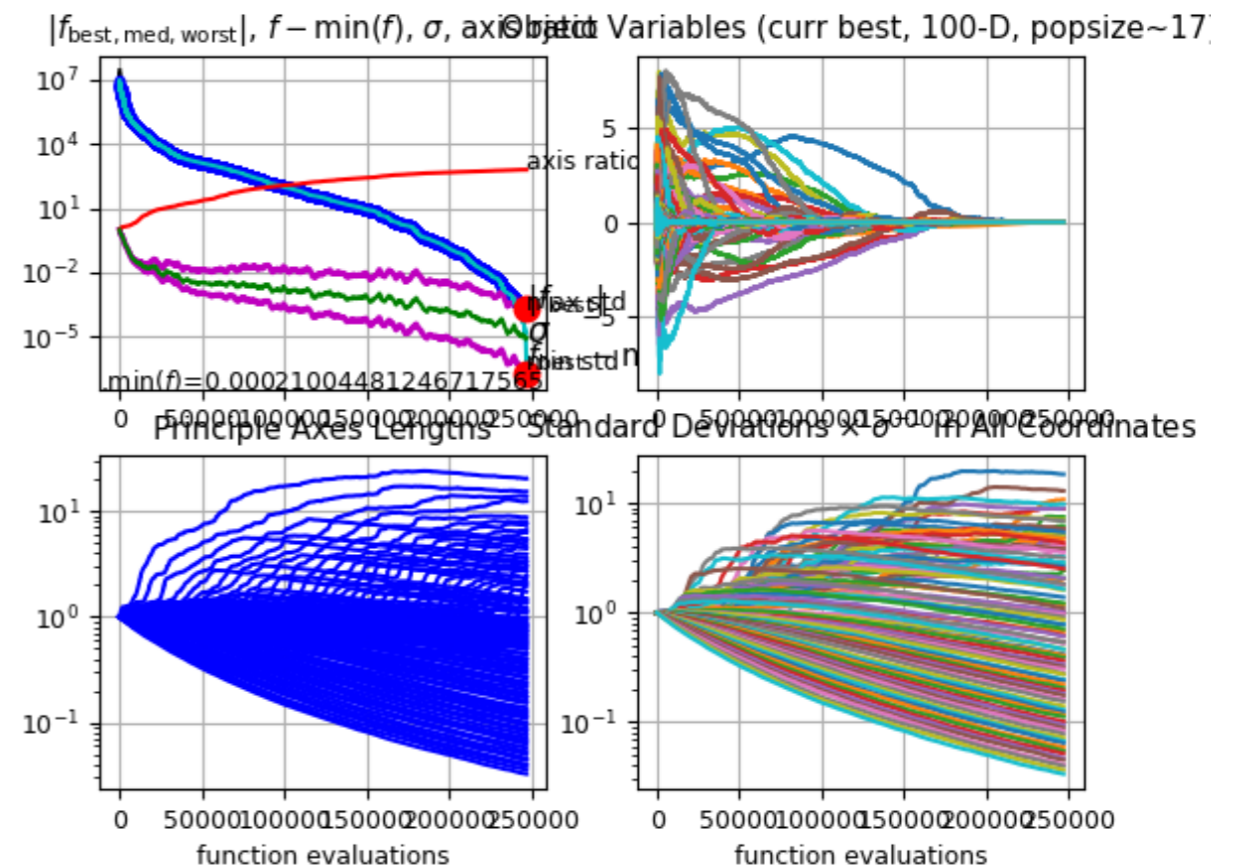
SEP 
$$[\mathbf{C}_{\text{sep}}^{(t+1)}]_{k,k} = [\mathbf{C}^{(t)}]_{k,k} + c_1 \left( [p_c]_k^2 - [\mathbf{C}^{(t)}]_{k,k} \right) + c_\mu \sum_{i=1}^{\mu} w_i \left( [\mathbf{x}_i - \mathbf{m}^{(t)}]_k^2 - [\mathbf{C}^{(t)}]_{k,k} \right)$$

→  $(N + 2)/3$  times greater than CMA

# Demo: On 100D Separable Ellipsoid Function



Separable-CMA



CMA

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

# Summary and Final Remarks

# Main Characteristics of (CMA) Evolution Strategies

- 1 Multivariate normal distribution to generate new search points  
follows the maximum entropy principle
- 2 Rank-based selection  
implies invariance, same performance on  $g(f(\mathbf{x}))$  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

[http://cma.gforge.inria.fr/cmaes\\_sourcecode\\_page.html](http://cma.gforge.inria.fr/cmaes_sourcecode_page.html)

# Comparison during BBOB at GECCO 2010

24 functions and 20+ algorithms in 20-D

