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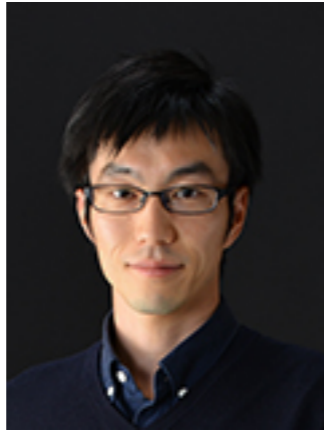
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CMA-ES and Advanced Adaptation Mechanisms

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We are happy to answer questions at any time.

Topics

1. What makes 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/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

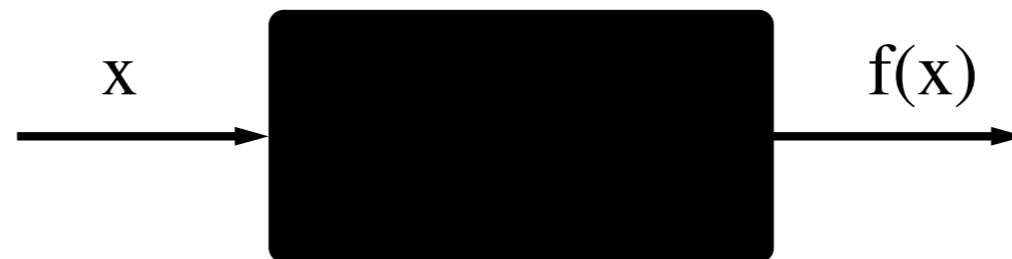
Problem Statement

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

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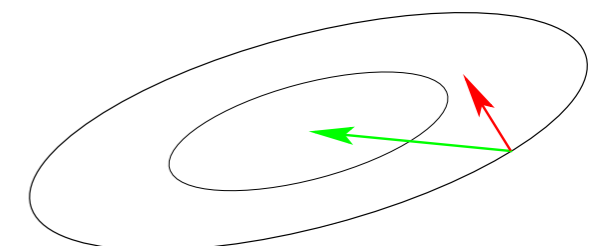
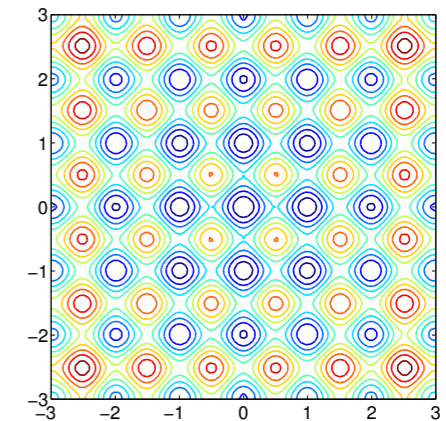
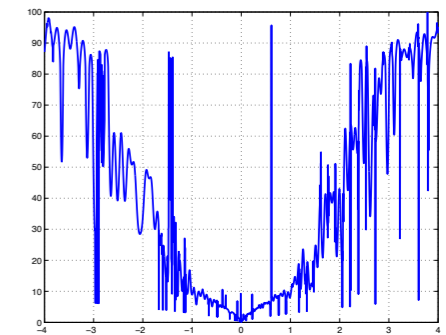
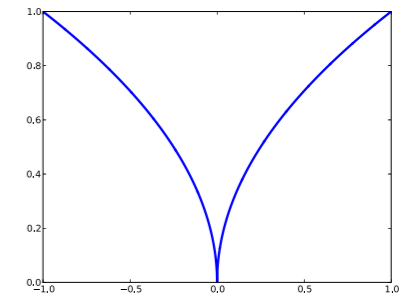
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What Makes a Function Difficult to Solve?

Why stochastic search?

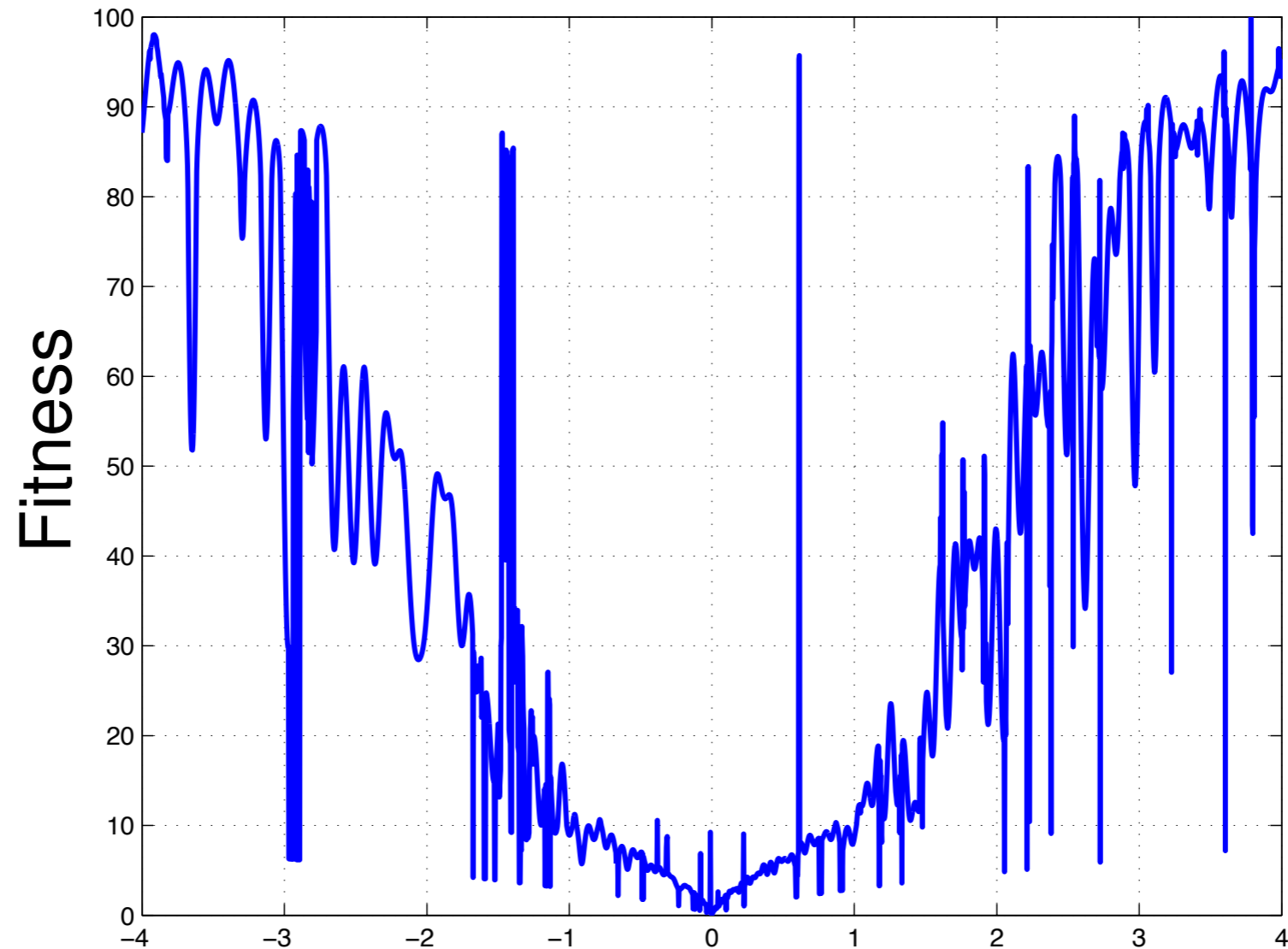
- non-linear, non-quadratic, non-convex
on linear and quadratic functions much better search policies are available
- ruggedness
non-smooth, discontinuous, multimodal, and/or noisy function
- dimensionality (size of search space)
(considerably) larger than three
- non-separability
dependencies between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

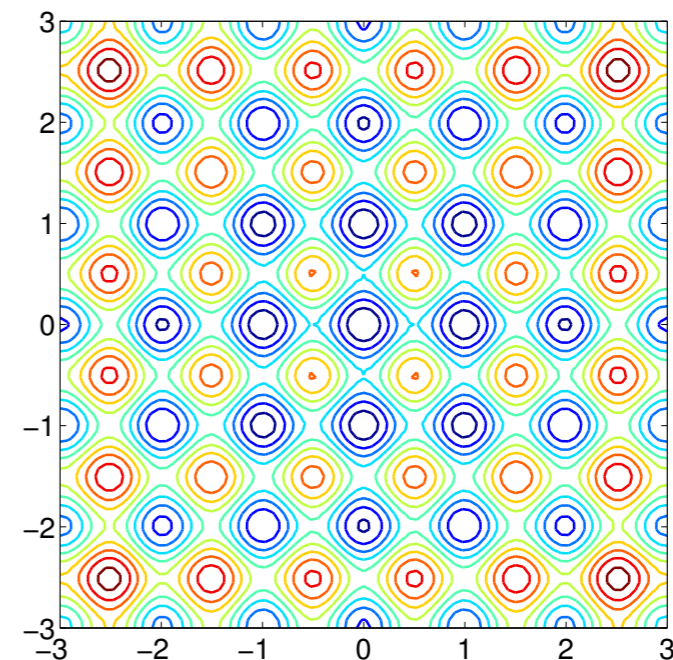
$$\arg \min_{(x_1, \dots, x_n)} f(x_1, \dots, x_n) = \left(\arg \min_{x_1} f(x_1, \dots), \dots, \arg \min_{x_n} f(\dots, x_n) \right)$$

\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



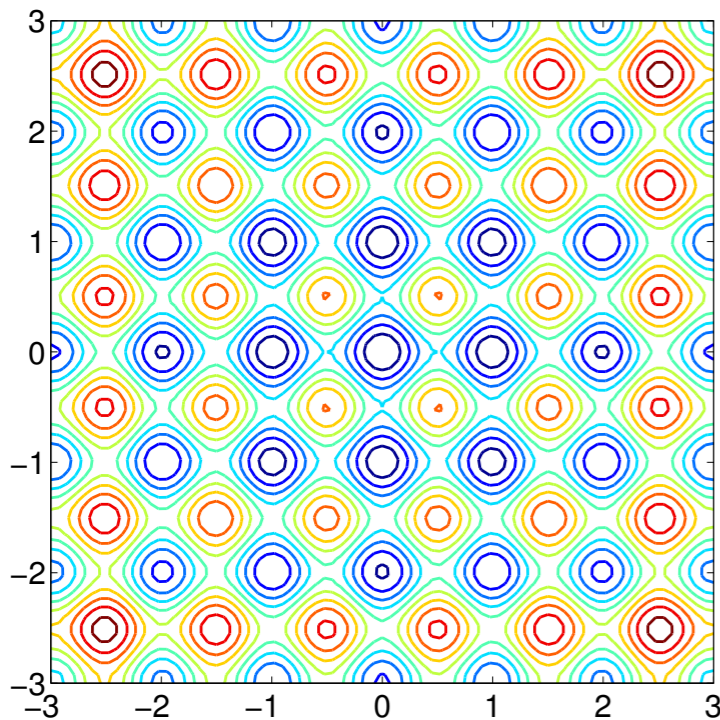
Non-Separable Problems

Building a non-separable problem from a separable one ^(1,2)

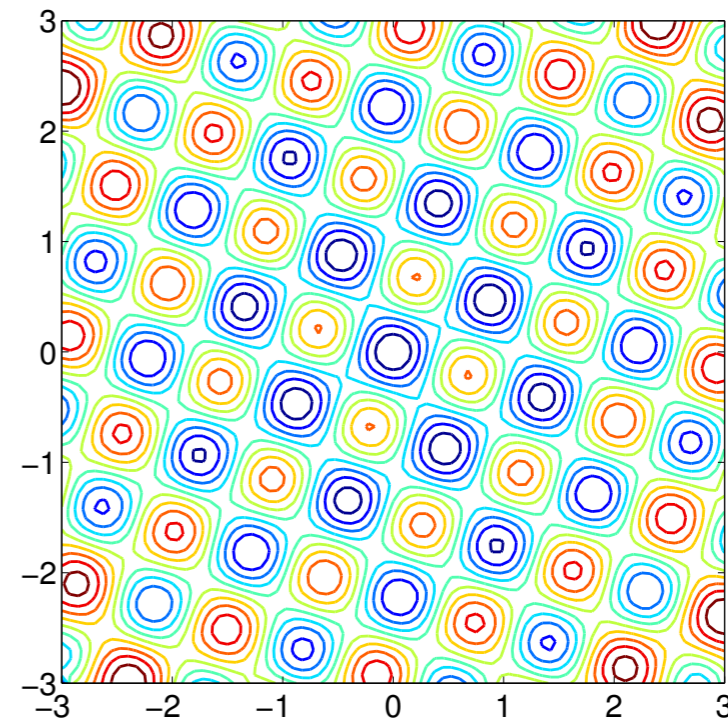
Rotating the coordinate system

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

R rotation matrix



R
→



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

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

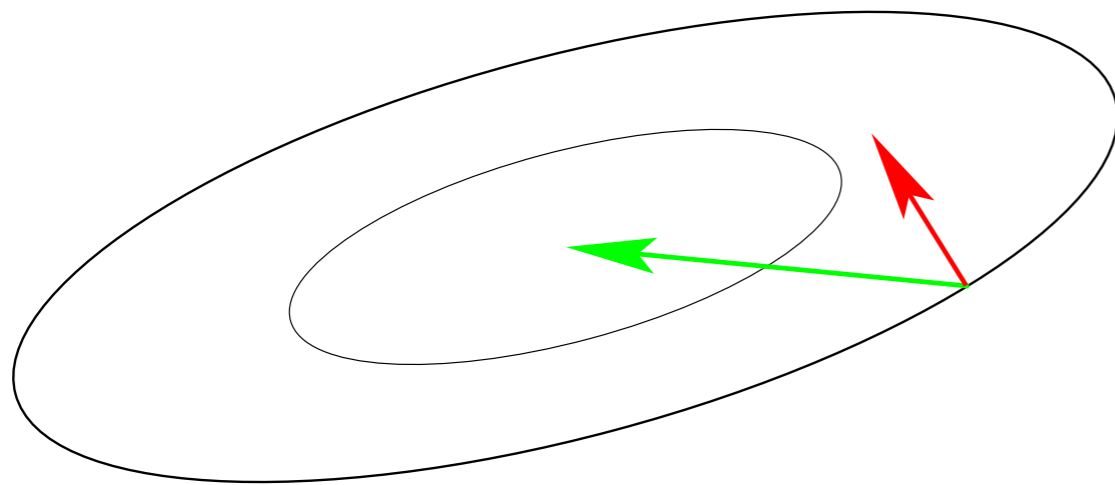
III-Conditioned Problems

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

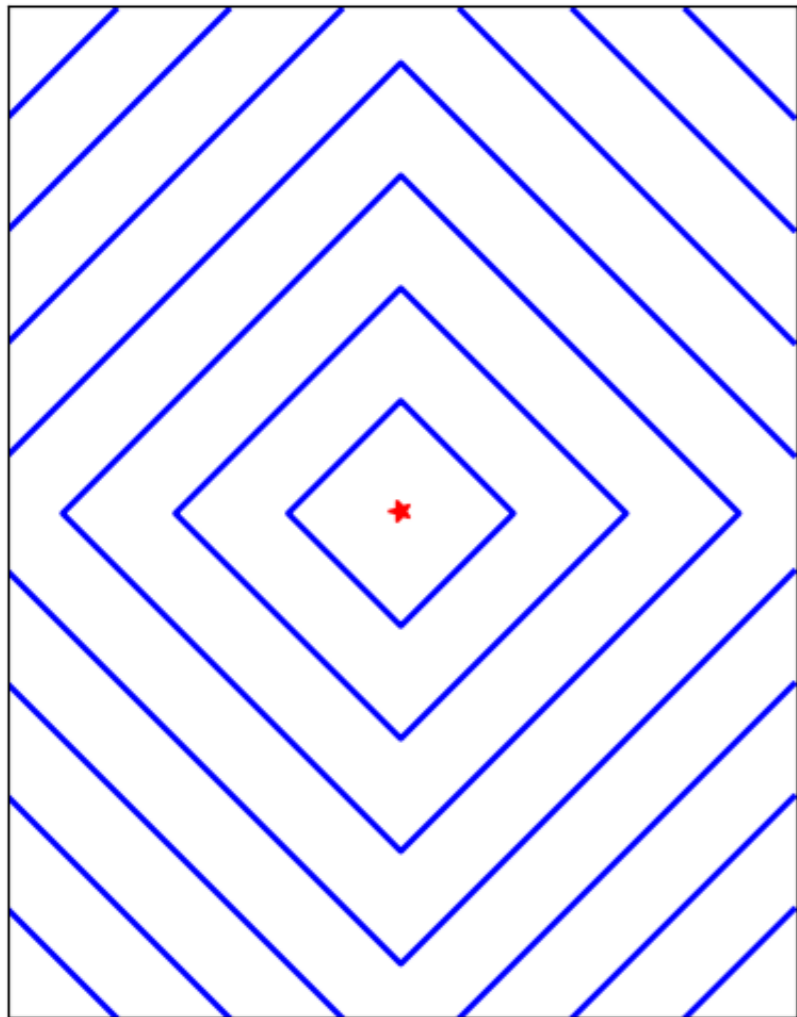
Newton direction $-\mathbf{H}^{-1}f'(\mathbf{x})^T$

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.

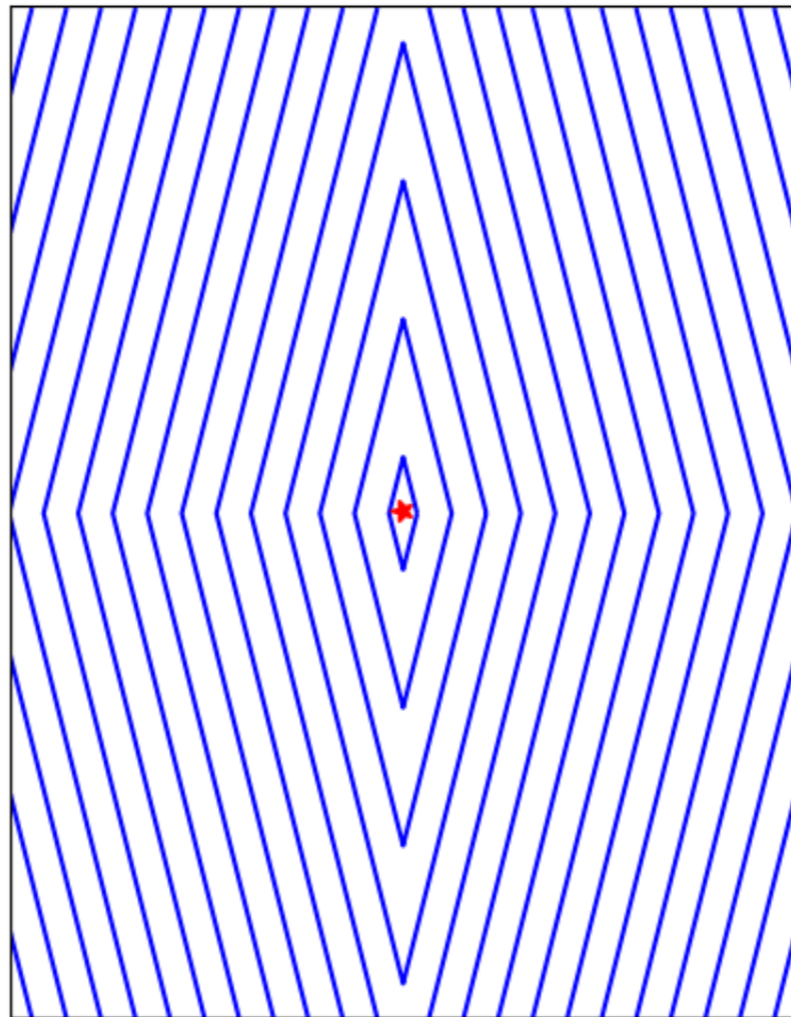
If $\mathbf{H} \approx \mathbf{I}$ (small condition number of \mathbf{H}) first order information (e.g. the gradient) is sufficient. Otherwise **second order information** (estimation of \mathbf{H}^{-1}) **is necessary**.

Non-smooth level sets (sharp ridges)

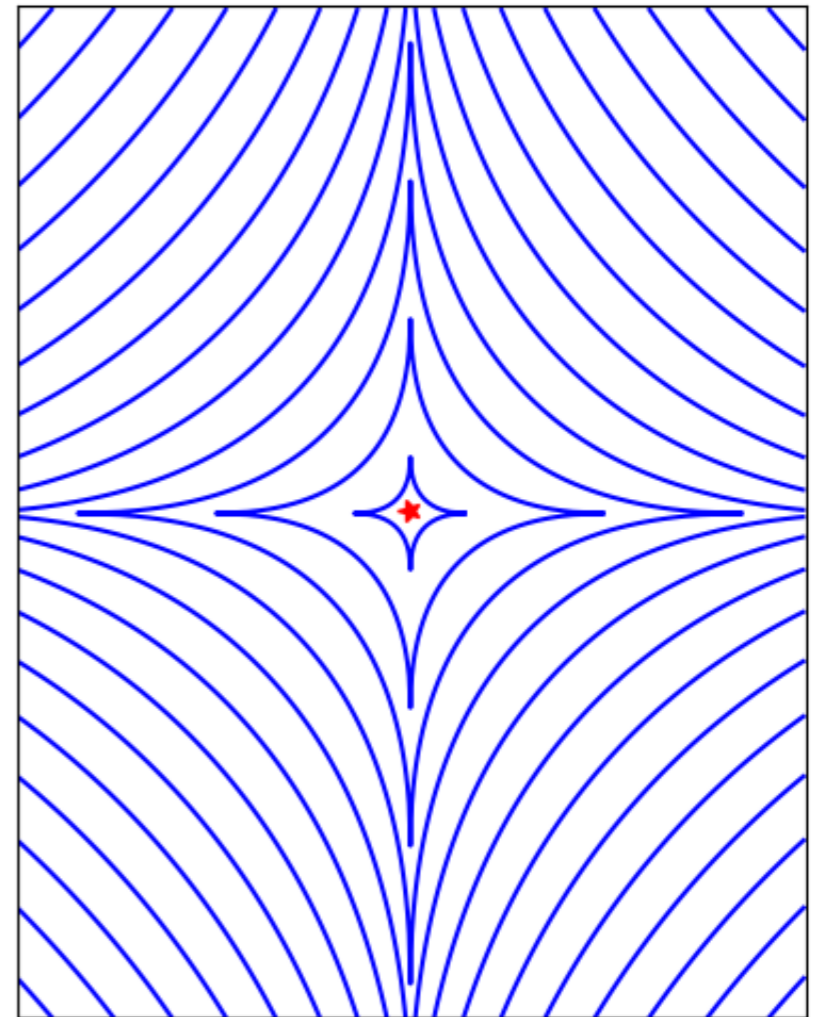
Similar difficulty **but worse** than ill-conditioning



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	non-local policy, large sampling width (step-size) as large as possible while preserving a reasonable convergence speed population-based 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 θ , 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_θ

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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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 σ

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

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

Not covered: termination, restarts, useful output, search boundaries and encoding, corrections for: positive definiteness guaranty, \mathbf{p}_c variance loss, c_σ and d_σ for large λ

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Evolution Strategies

New search points are sampled normally distributed

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

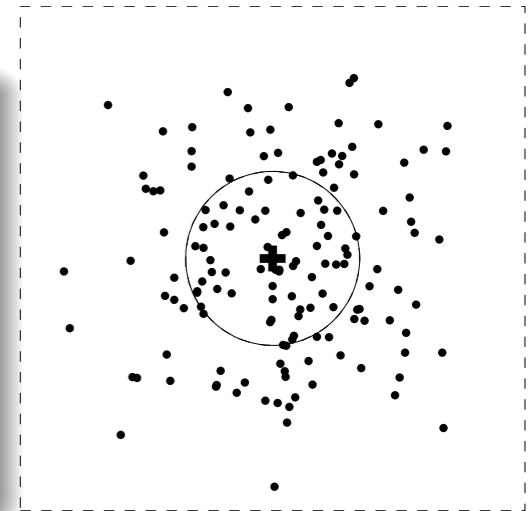
as perturbations of \mathbf{m} , where $\mathbf{x}_i, \mathbf{m} \in \mathbb{R}^n$, $\sigma \in \mathbb{R}_+$, $\mathbf{C} \in \mathbb{R}^{n \times n}$

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 σ .



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

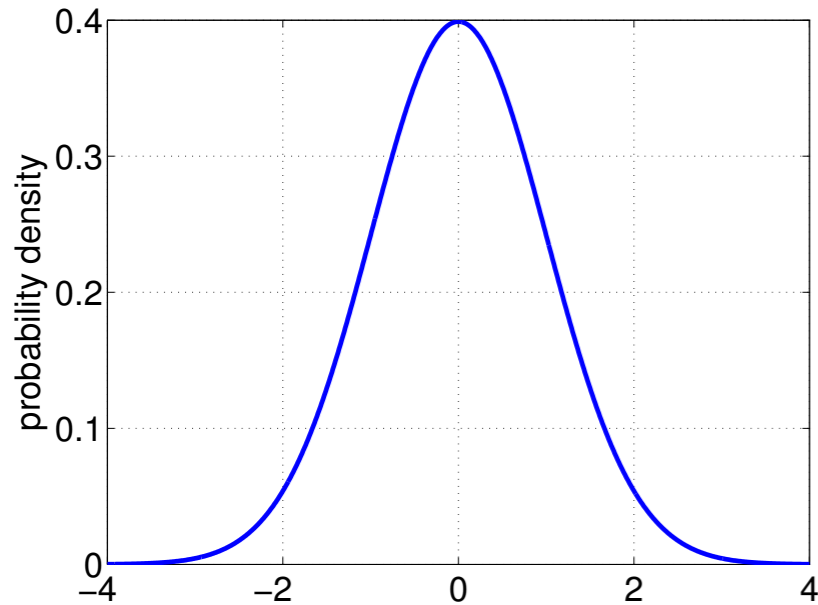
the isotropic distribution does **not favor any direction**, rotational
invariant

4 maximum entropy distribution with finite variance

the least possible assumptions on f in the distribution shape

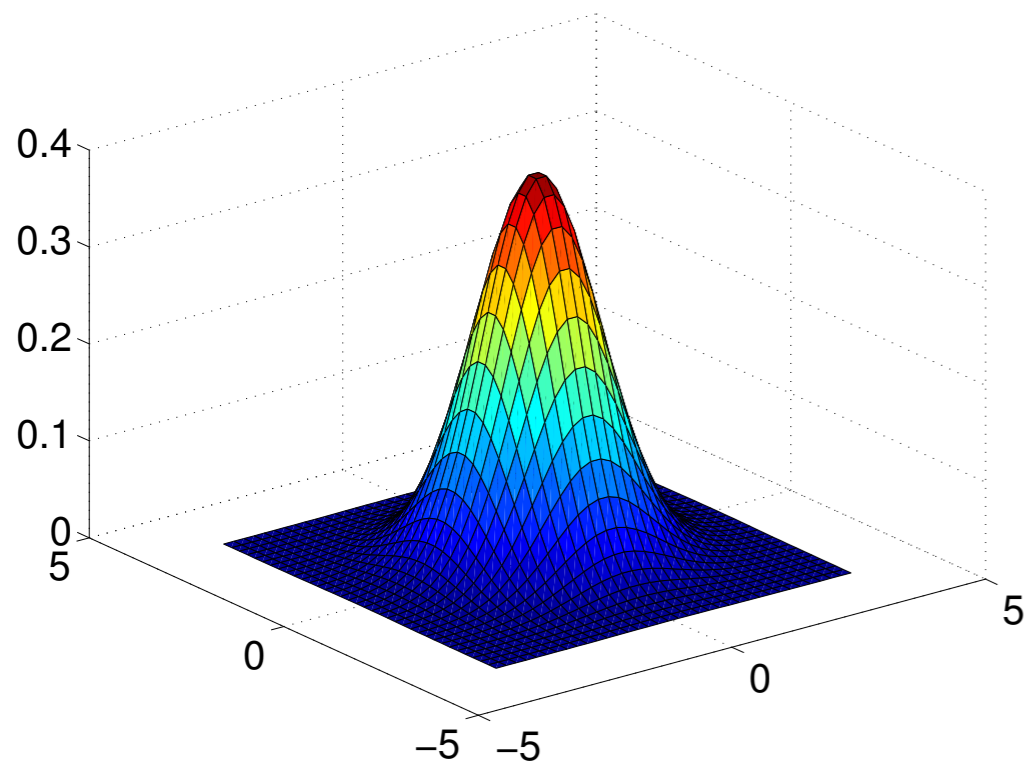
Normal Distribution

Standard Normal Distribution

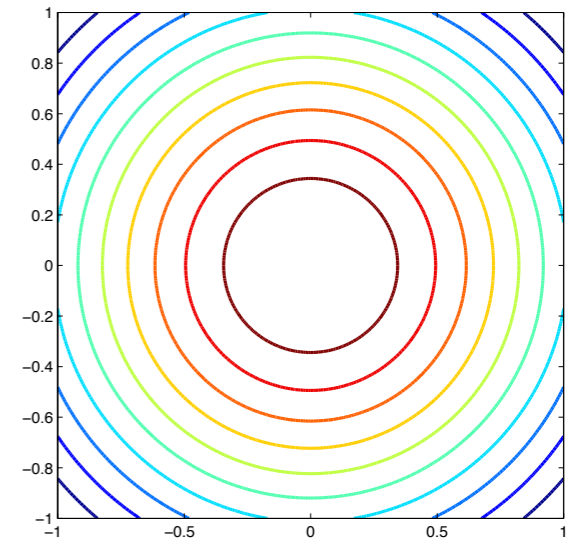


probability density of the 1-D standard normal distribution

2-D Normal Distribution



probability density of a 2-D normal distribution

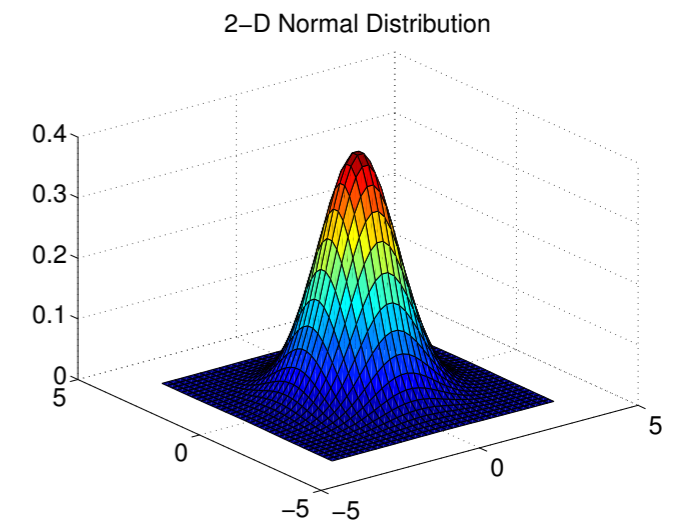


The Multi-Variate (n -Dimensional) Normal Distribution

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

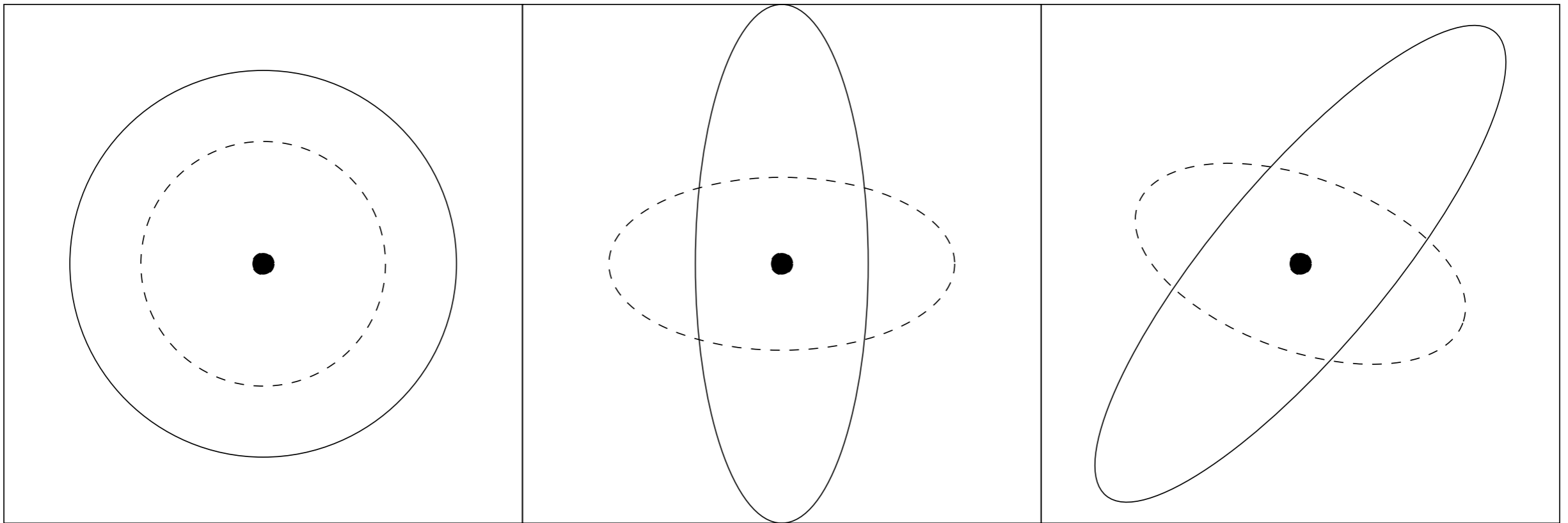


The **covariance matrix** \mathbf{C}

- 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 σ
 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} ,

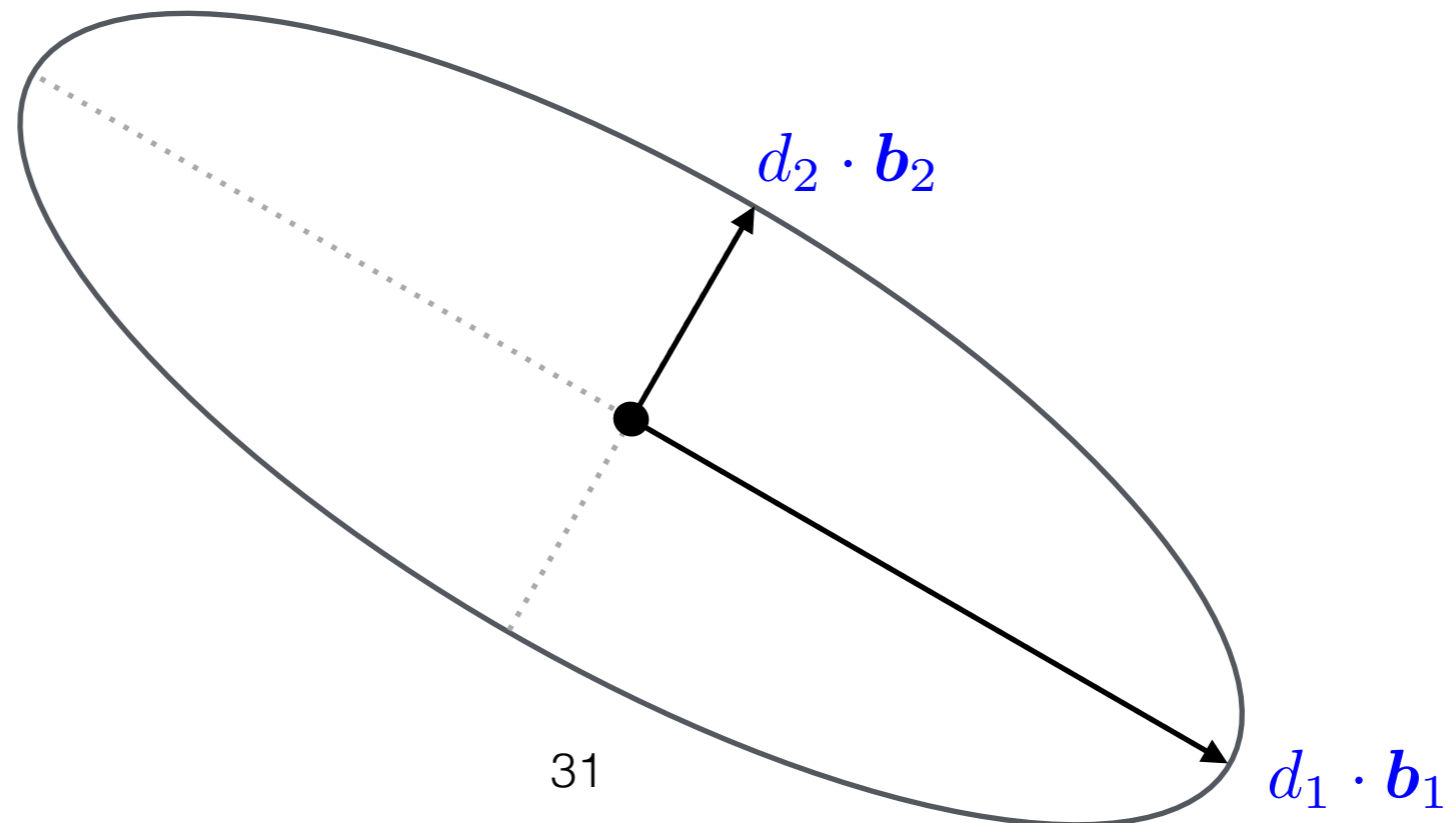
$$\mathbf{C} = d_1^2 \mathbf{b}_1 \mathbf{b}_1^T + \dots + d_N^2 \mathbf{b}_N \mathbf{b}_N^T$$

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

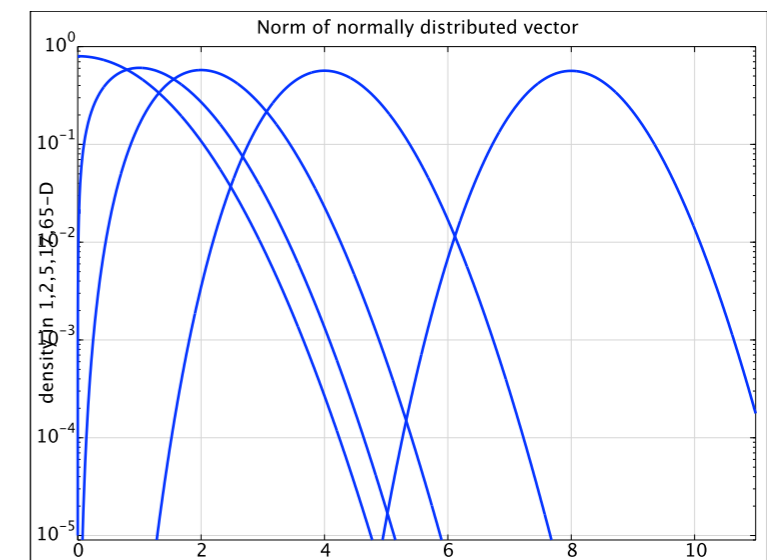
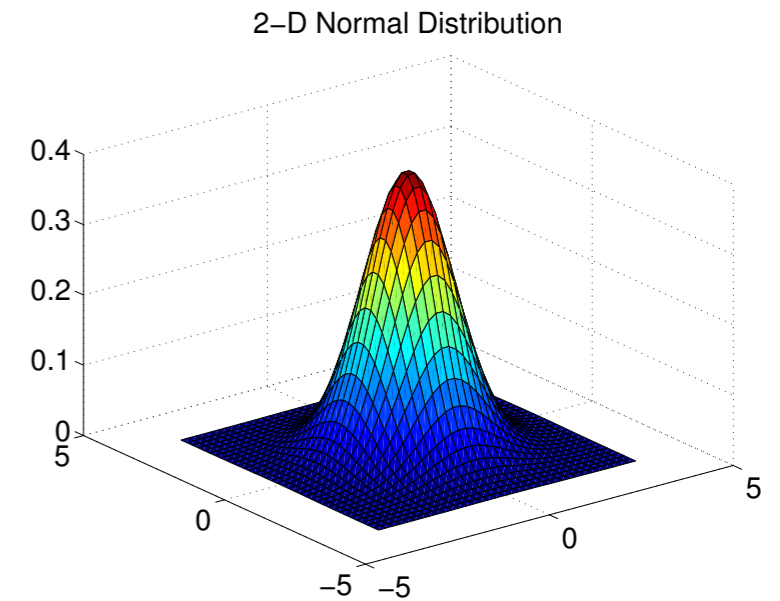
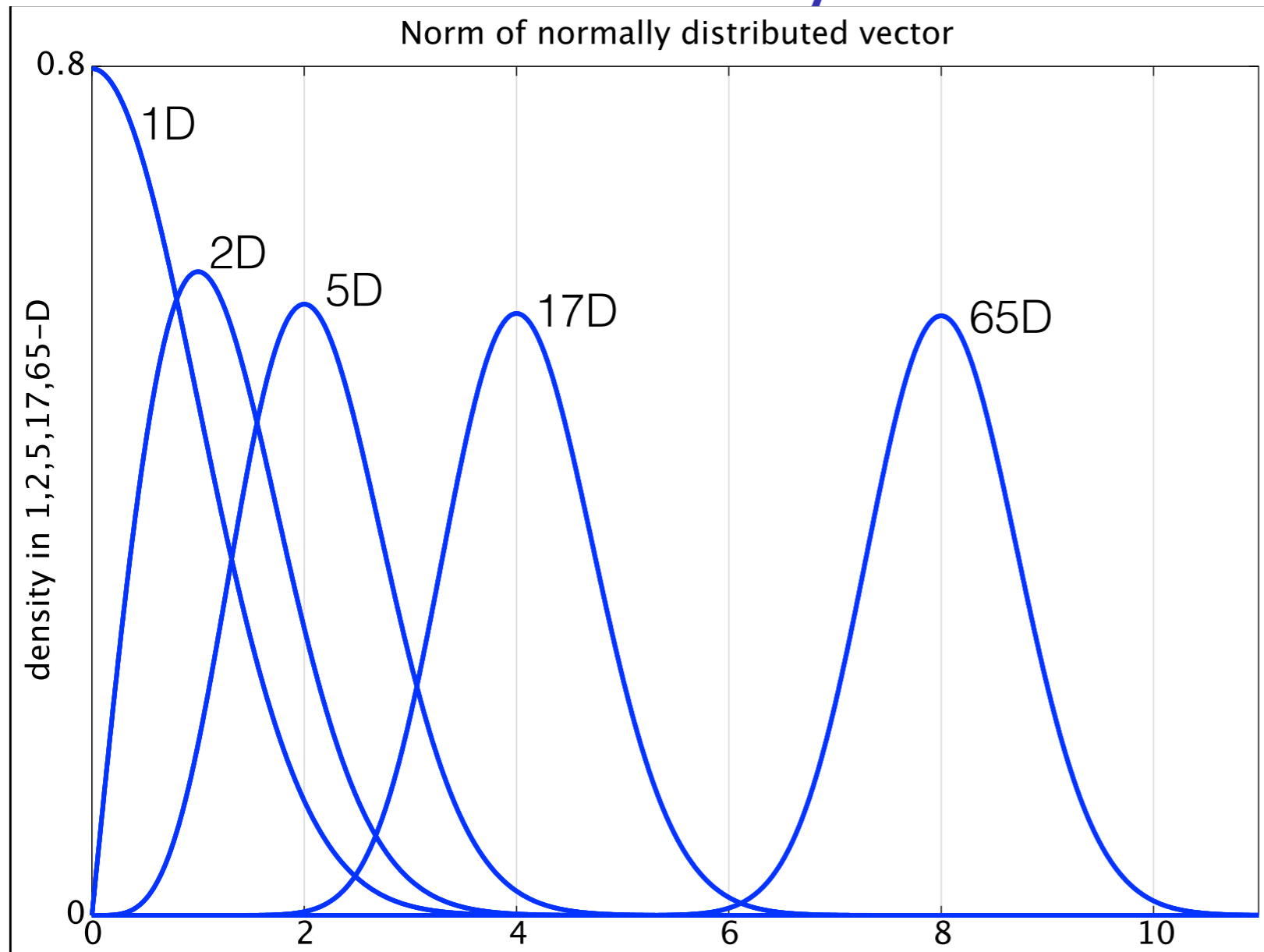
\mathbf{b}_i : eigenvector of \mathbf{C} , corresponding to d_i

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

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



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:

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

Stochastic Search

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

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

While not terminate

- 1 Sample distribution $P(\mathbf{x}|\theta) \rightarrow \mathbf{x}_1, \dots, \mathbf{x}_\lambda \in \mathbb{R}^n$
- 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_θ

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

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

where

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

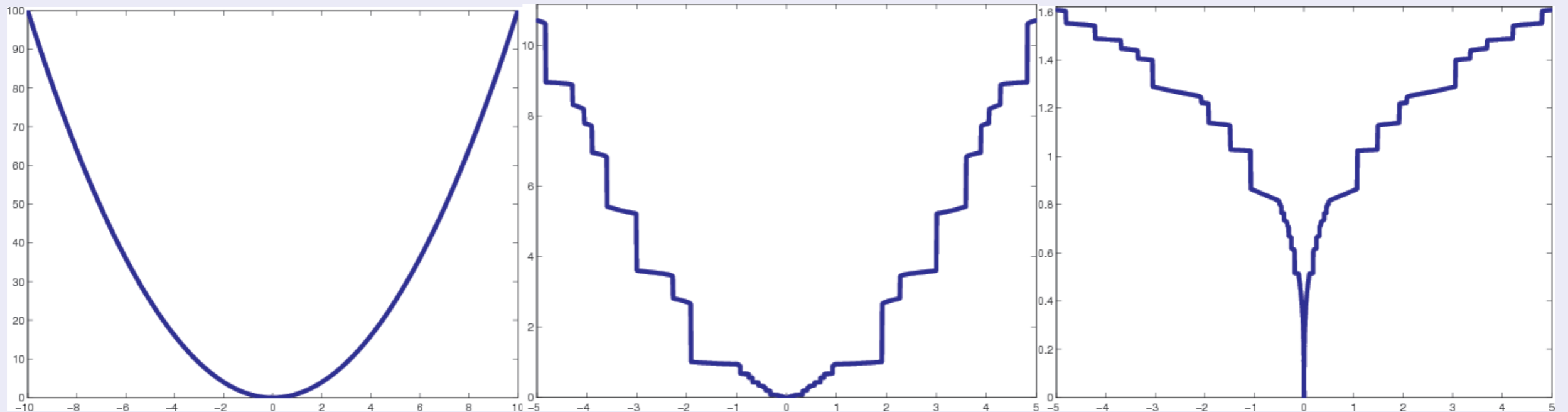
The best μ points are selected from the new solutions (non-elitistic) and weighted intermediate recombination is applied.

Invariance Under Monotonically Increasing Functions

Rank-based algorithms

Update of all parameters uses only the ranks

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



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

g is strictly monotonically increasing
 g preserves ranks

3

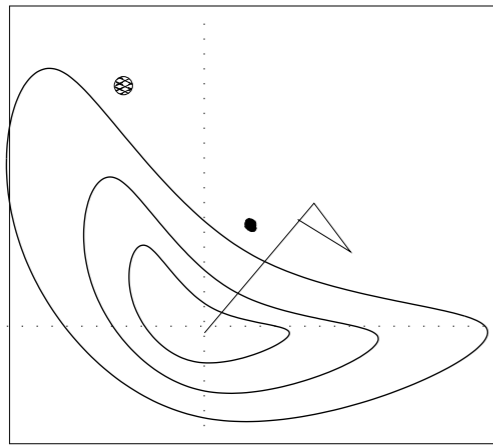
³ Whitley 1989. The GENITOR algorithm and selection pressure: Why rank-based allocation of reproductive trials is best,

ICGA

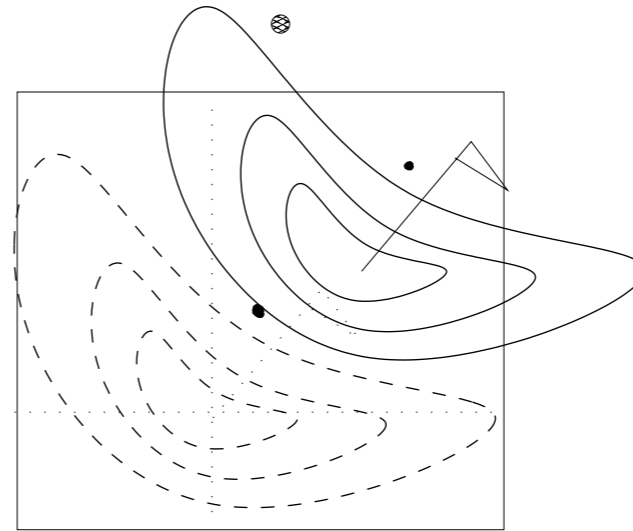
Basic Invariance in Search Space

- translation invariance

is true for most optimization algorithms



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

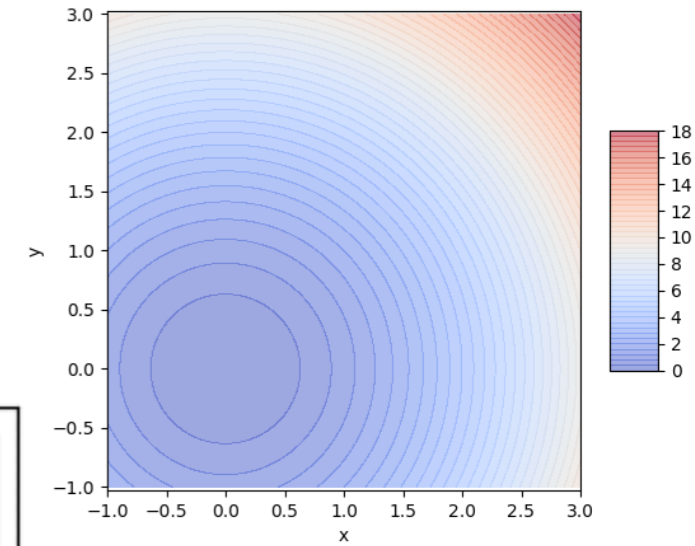
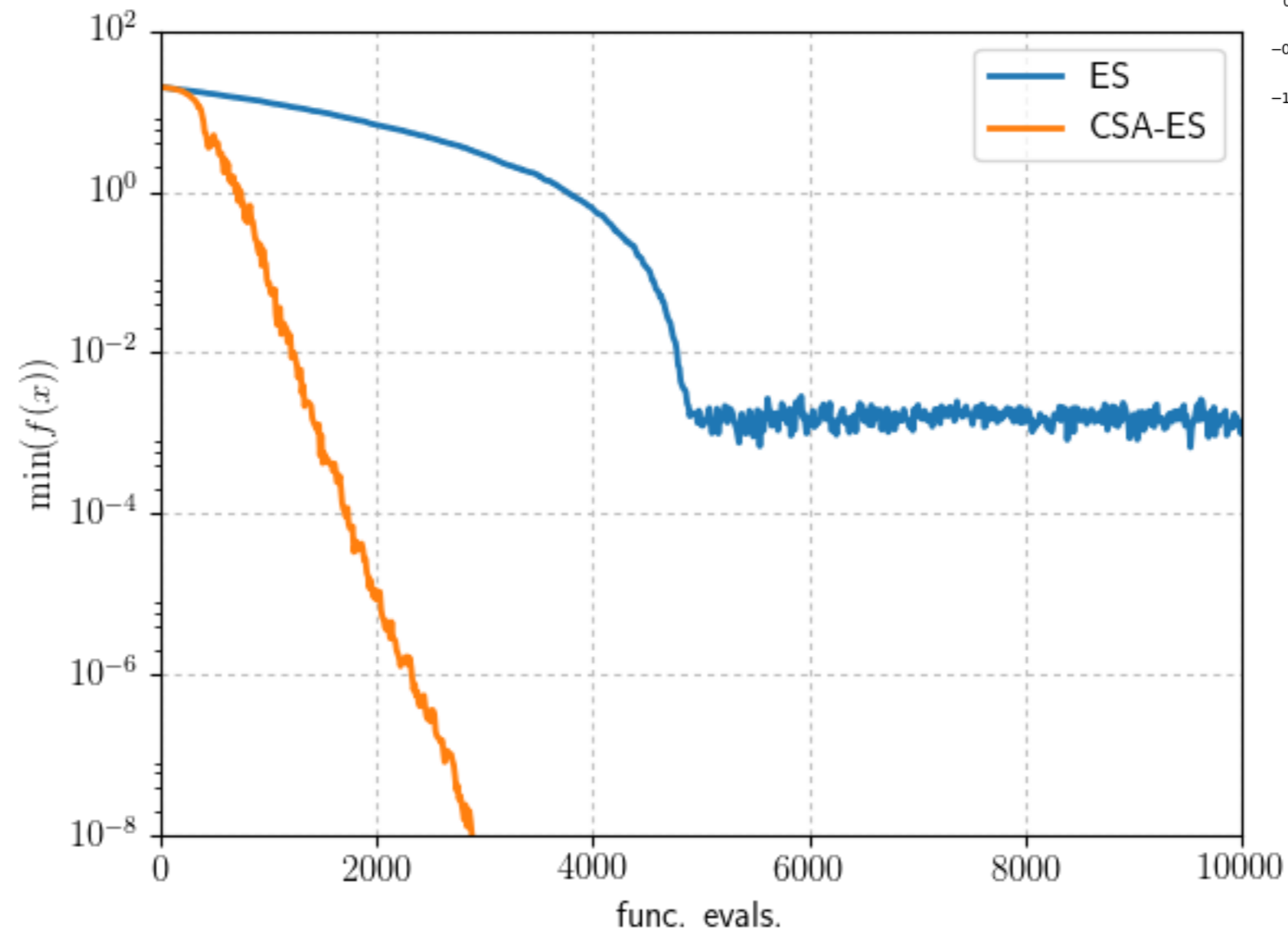


Identical behavior on f and f_a

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

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

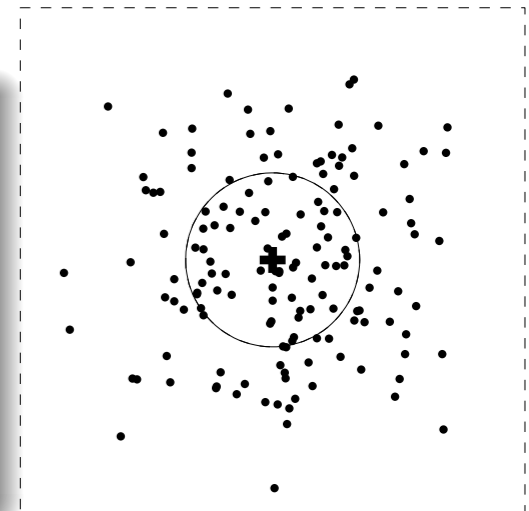
$$\mathbf{x}_i \sim \mathbf{m} + \sigma \mathcal{N}_i(\mathbf{0}, \mathbf{C}) \quad \text{for } i = 1, \dots, \lambda$$

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 σ and \mathbf{C} .



Methods for Step-Size Control

- **1/5-th success rule^{ab}**, often applied with “+”-selection
 - increase step-size if more than 20% of the new solutions are successful, decrease otherwise
- **σ -self-adaptation^c**, applied with “,”-selection
 - mutation is applied to the step-size and the better, according to the objective function value, is selected
 - simplified “global” self-adaptation
- **path length control^d** (Cumulative Step-size Adaptation, CSA)^e
 - self-adaptation derandomized and non-localized
- **two-point adaptation^f** (TPA)
 - akin to a rudimentary line search along the mean shift

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

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

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

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

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

^fHansen *et al* 2014, How to assess step-size adaptation mechanisms in a derandomised search, *PPSN IX*

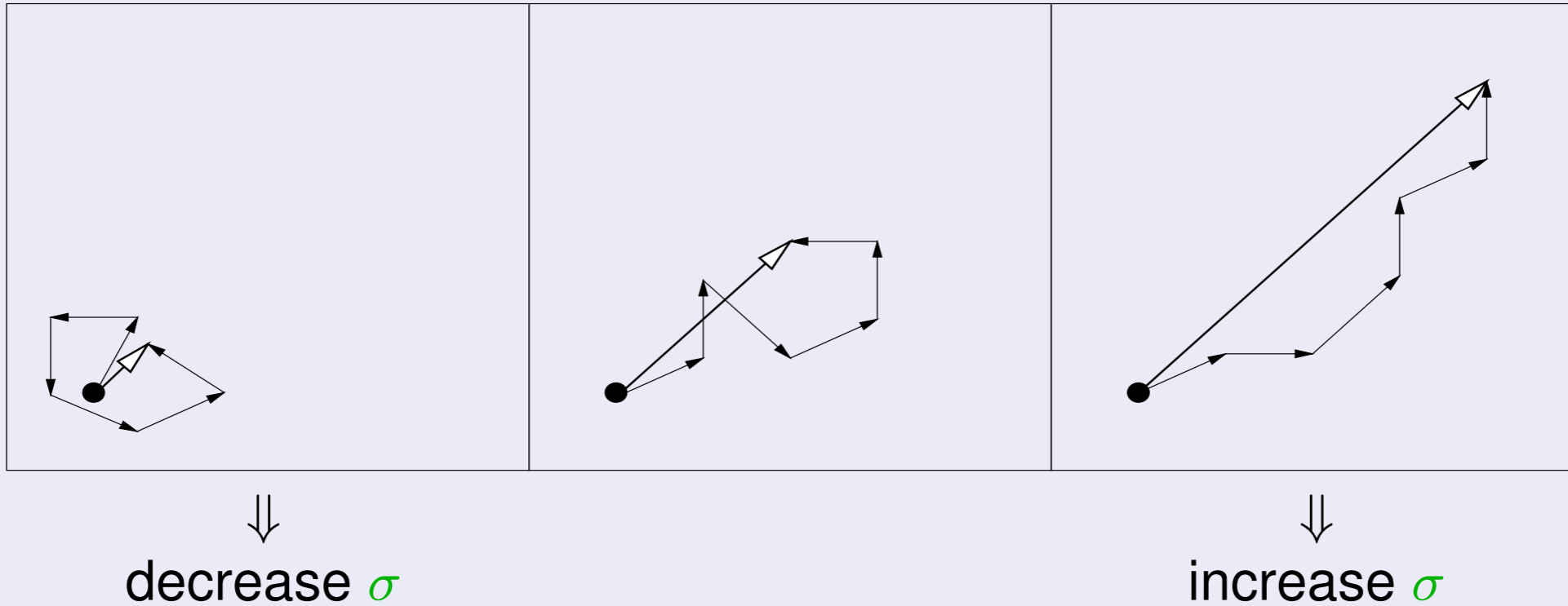
Path Length Control (CSA)

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 $c_\sigma \approx 4/n$, $d_\sigma \approx 1$.

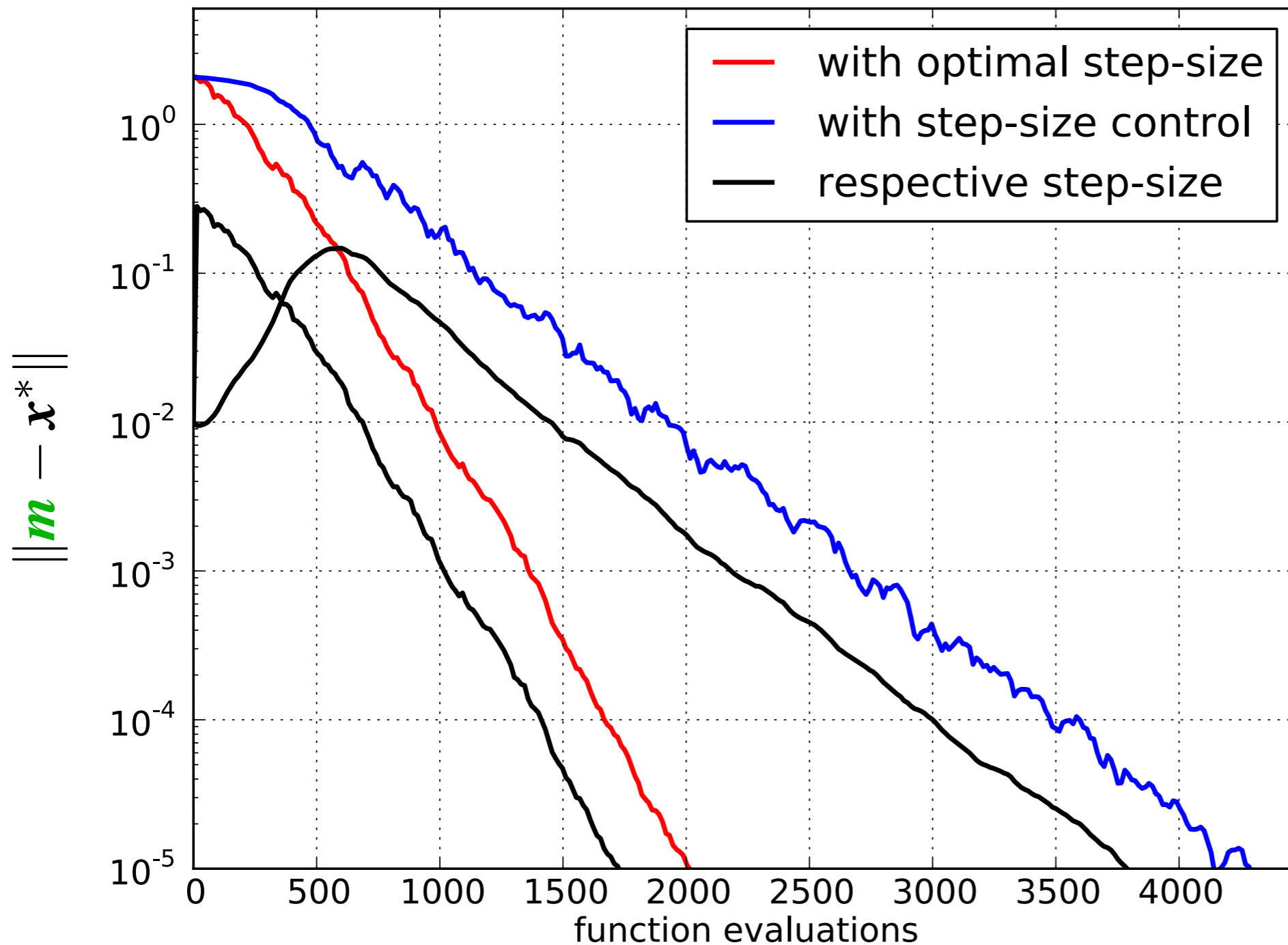
$$\mathbf{m} \leftarrow \mathbf{m} + \sigma \mathbf{y}_w \quad \text{where } \mathbf{y}_w = \sum_{i=1}^{\mu} w_i \mathbf{y}_{i:\lambda} \quad \text{update mean}$$

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

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

$>1 \iff \|\mathbf{p}_\sigma\|$ is greater than its expectation

(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

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

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

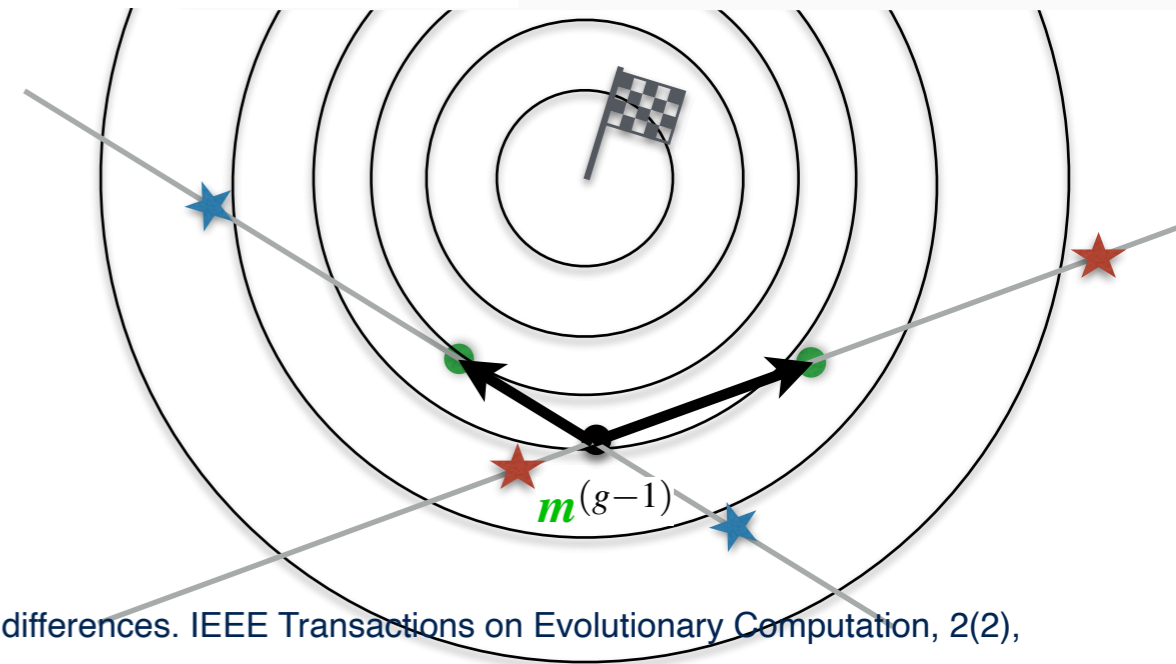
- Compare the ranking of \mathbf{x}_1 and \mathbf{x}_2 among λ current population.

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

> 0 if forward direction ranks better

- Update the step-size

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



[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.

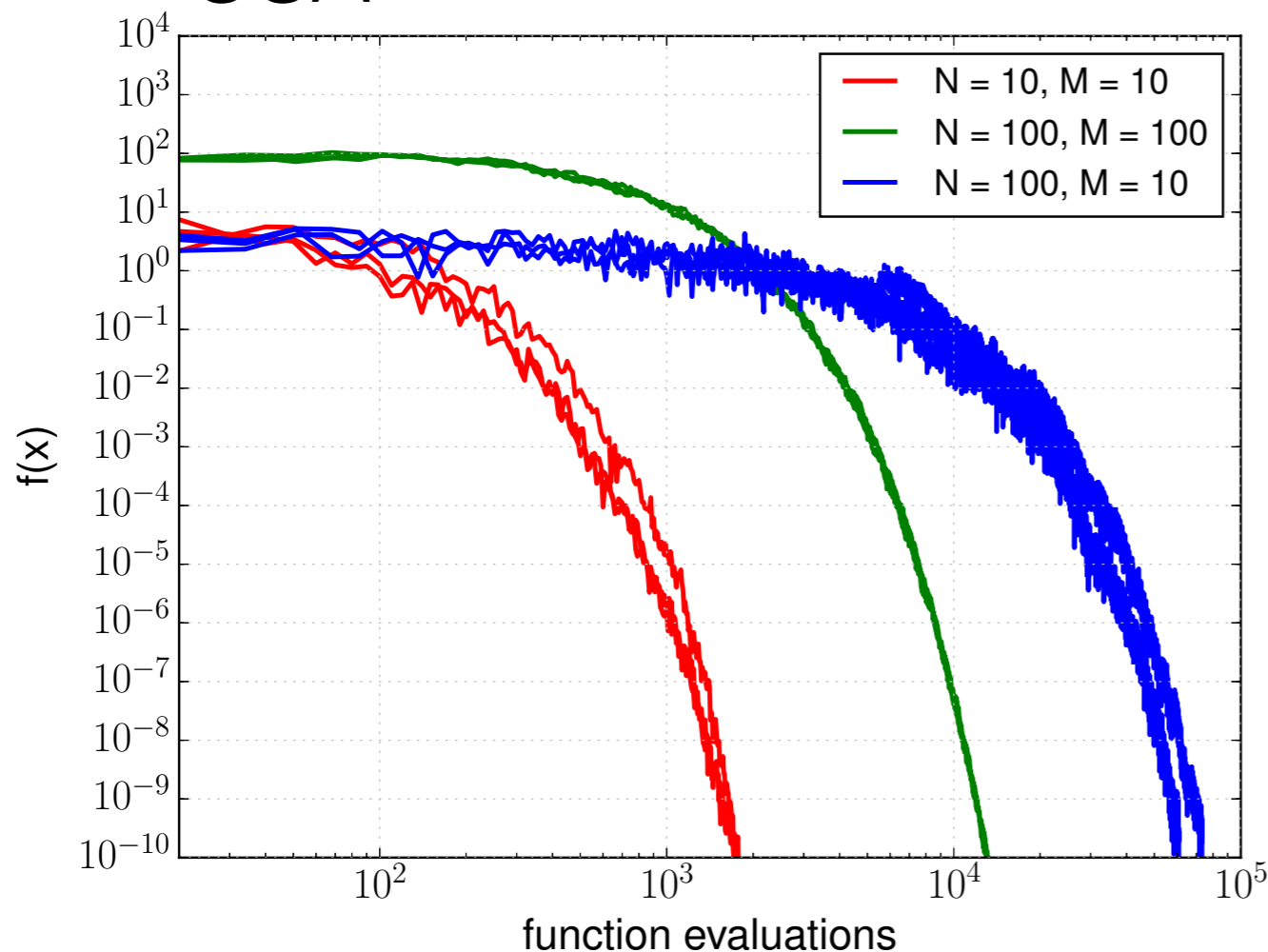
[Akimoto and Hansen, 2020] Akimoto, Y. and Hansen, N. (2020). Diagonal acceleration for covariance matrix adaptation evolution strategies. *Evolutionary computation*, 28(3), pages 405–435.

On Sphere with Low Effective Dimension

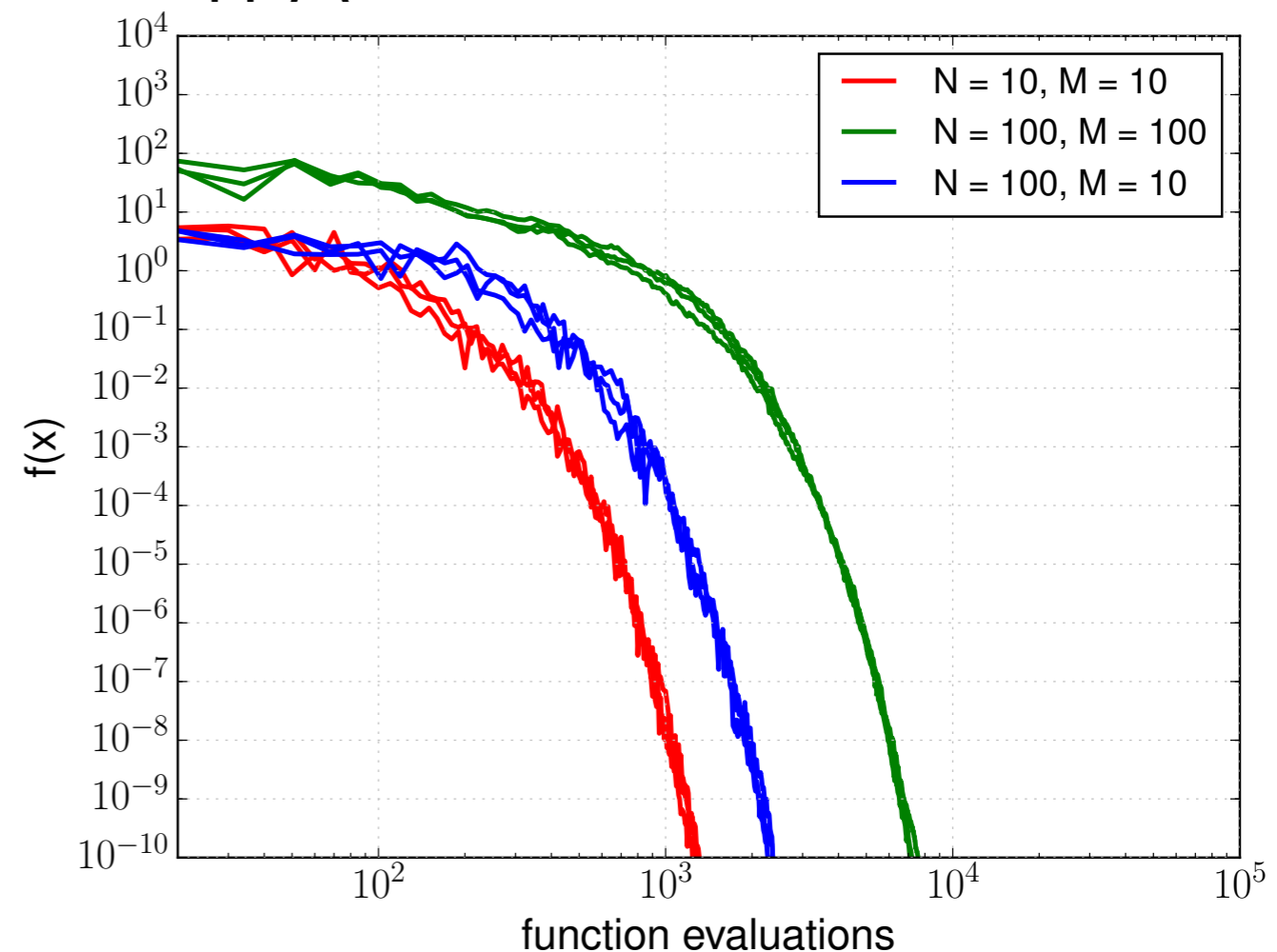
On a function with low effective dimension

- $f(\mathbf{x}) = \sum_{i=1}^M [\mathbf{x}]_i^2$, $\mathbf{x} \in \mathbb{R}^N$, $M \leq N$.
- $N - M$ 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*

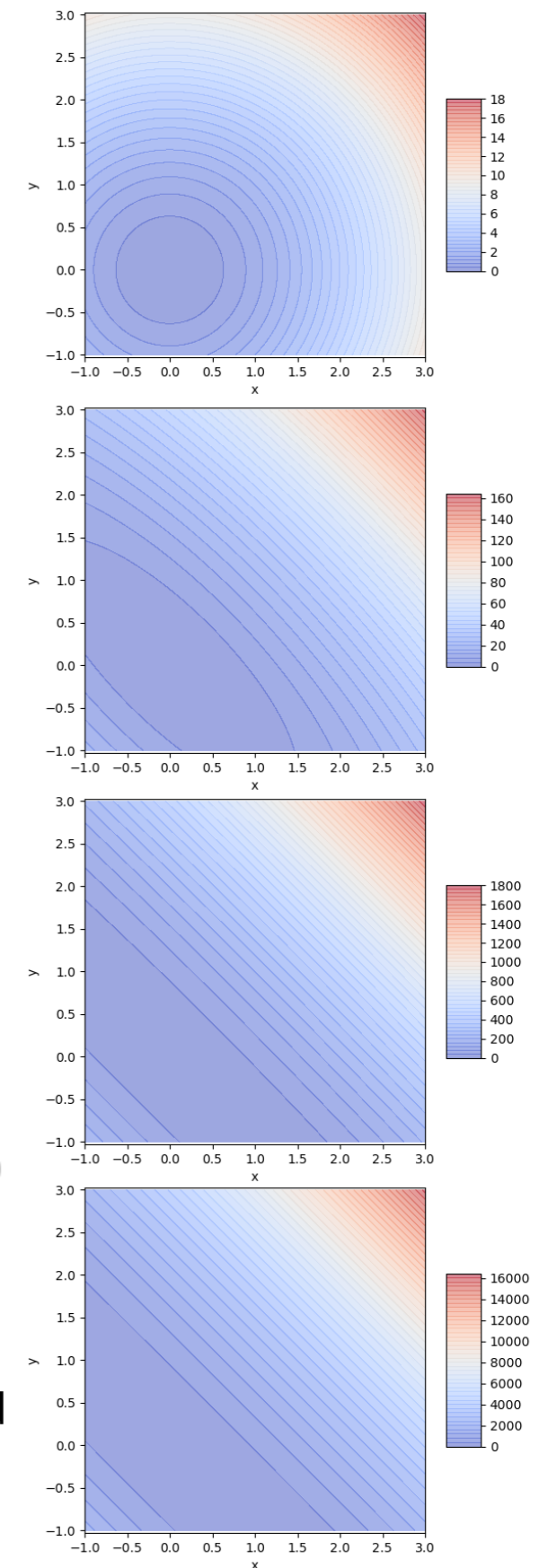
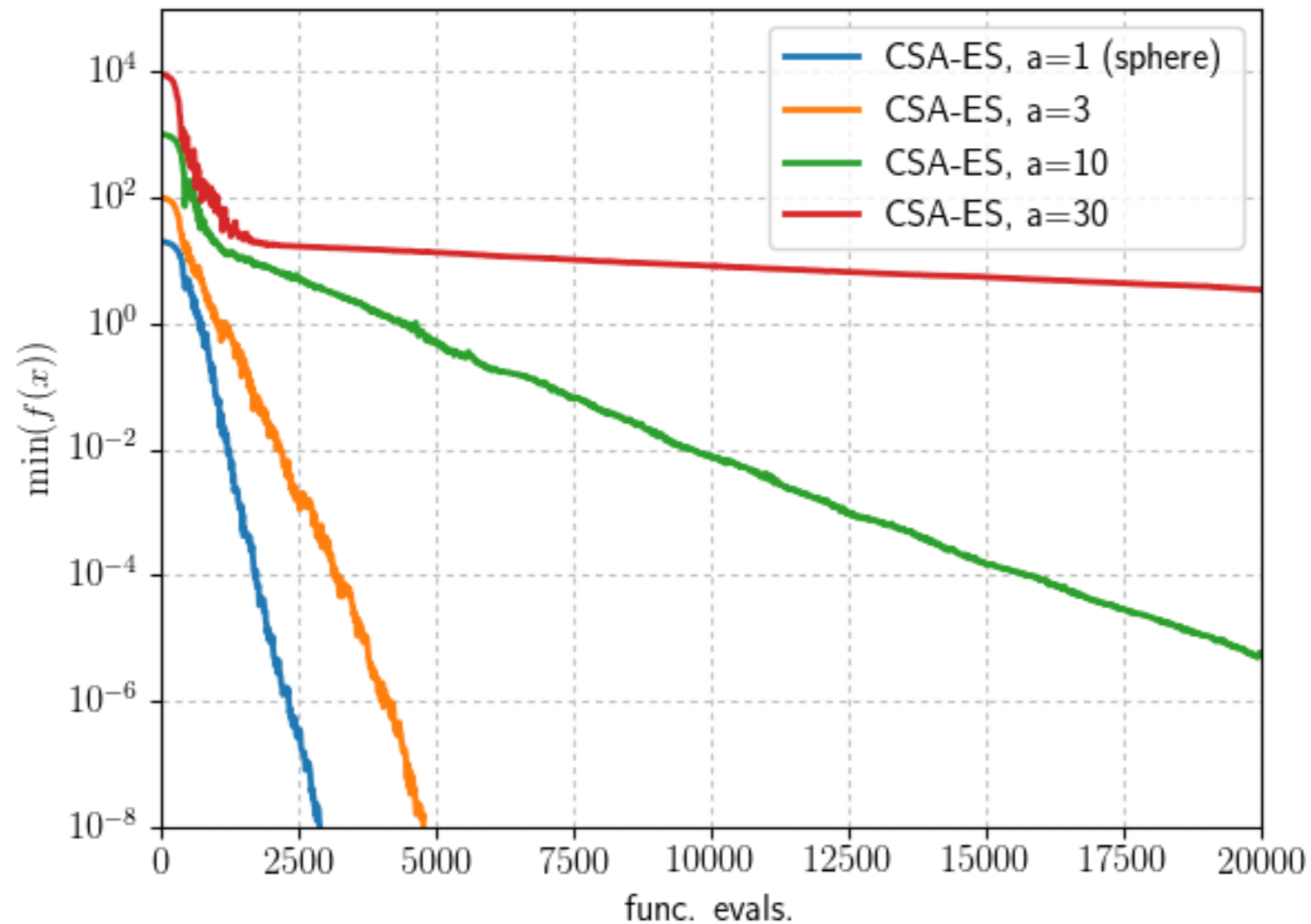
An advantage over CSA and TPA: Cheap Computation

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

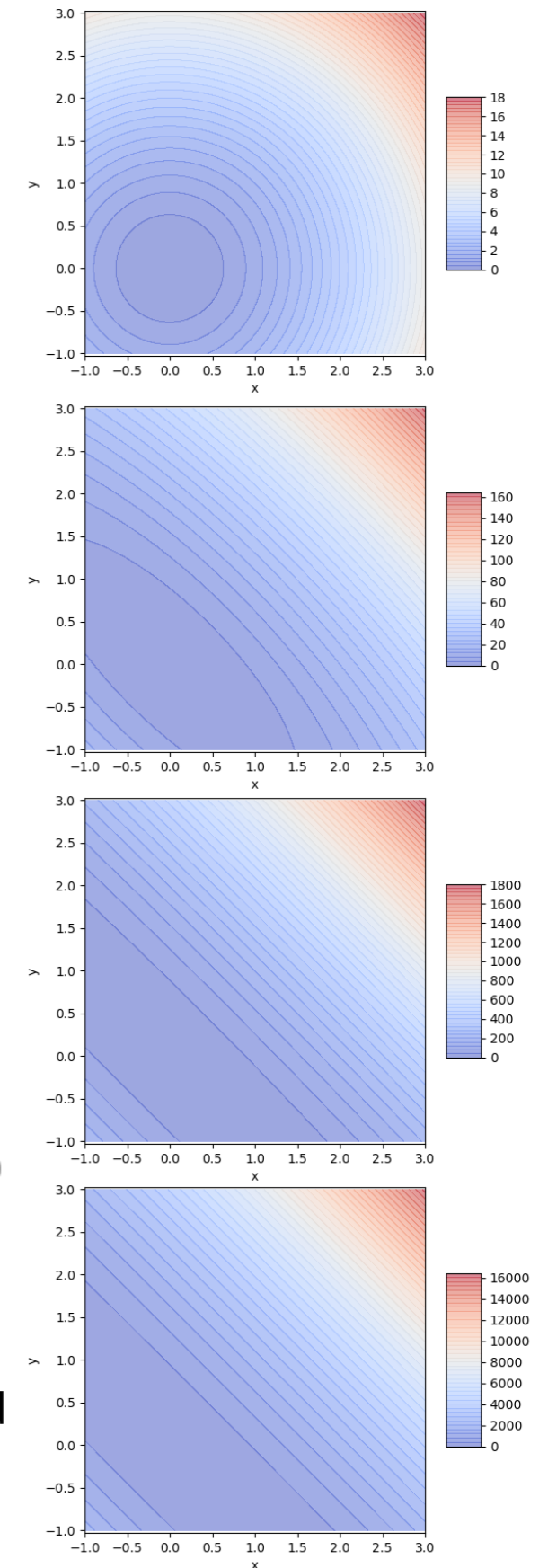
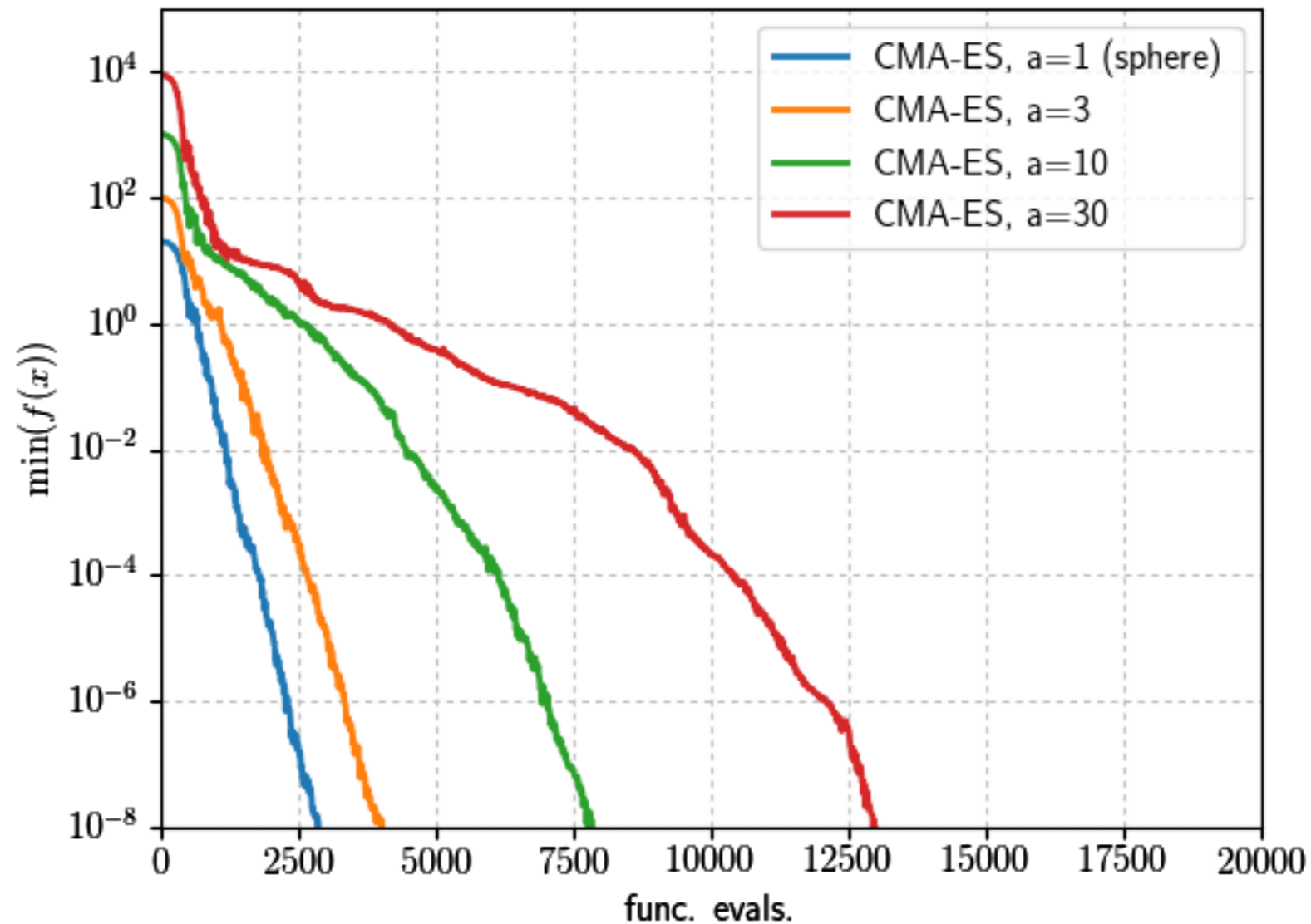
Step-Size Control Is Not Enough



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**

Step-Size Control Is Not Enough



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Evolution Strategies

Recalling

New search points are sampled normally distributed

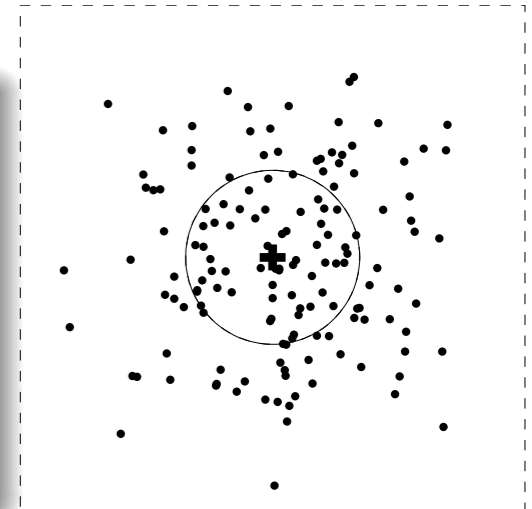
$$\mathbf{x}_i \sim \mathbf{m} + \sigma \mathcal{N}_i(\mathbf{0}, \mathbf{C}) \quad \text{for } i = 1, \dots, \lambda$$

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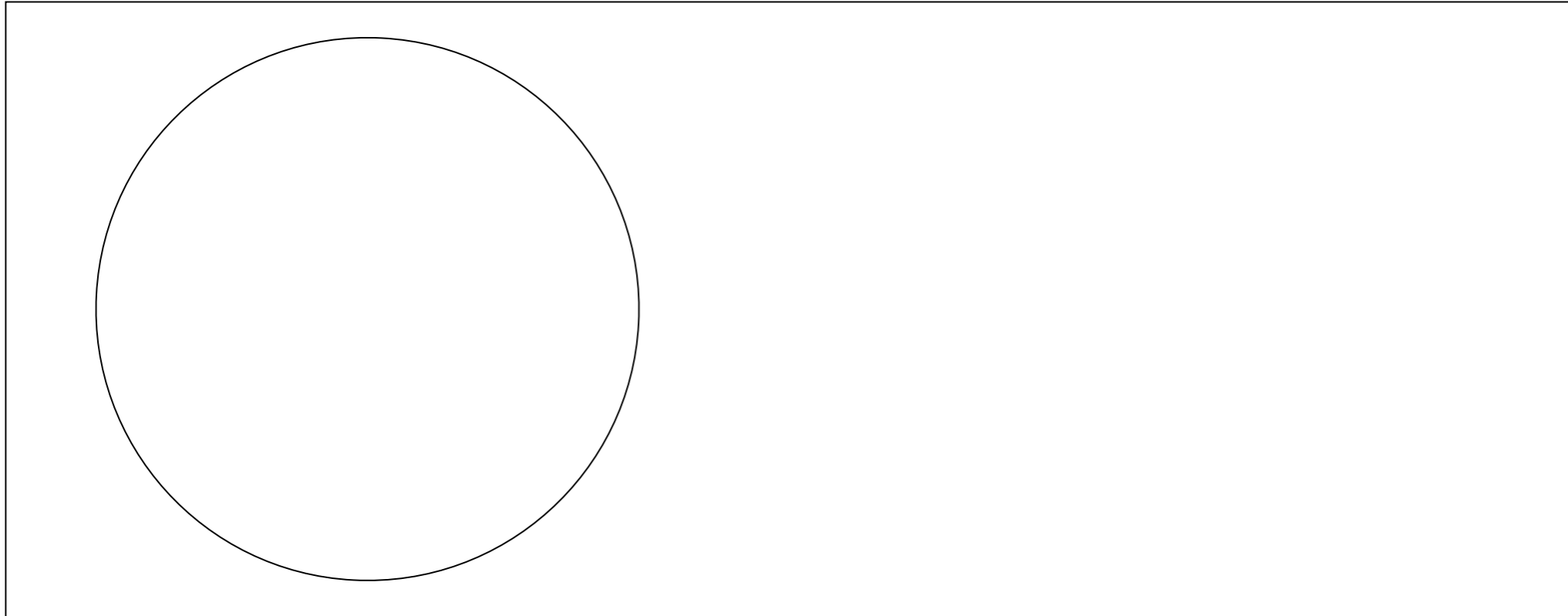
The remaining question is how to update \mathbf{C} .



Covariance Matrix Adaptation

Rank-One Update

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



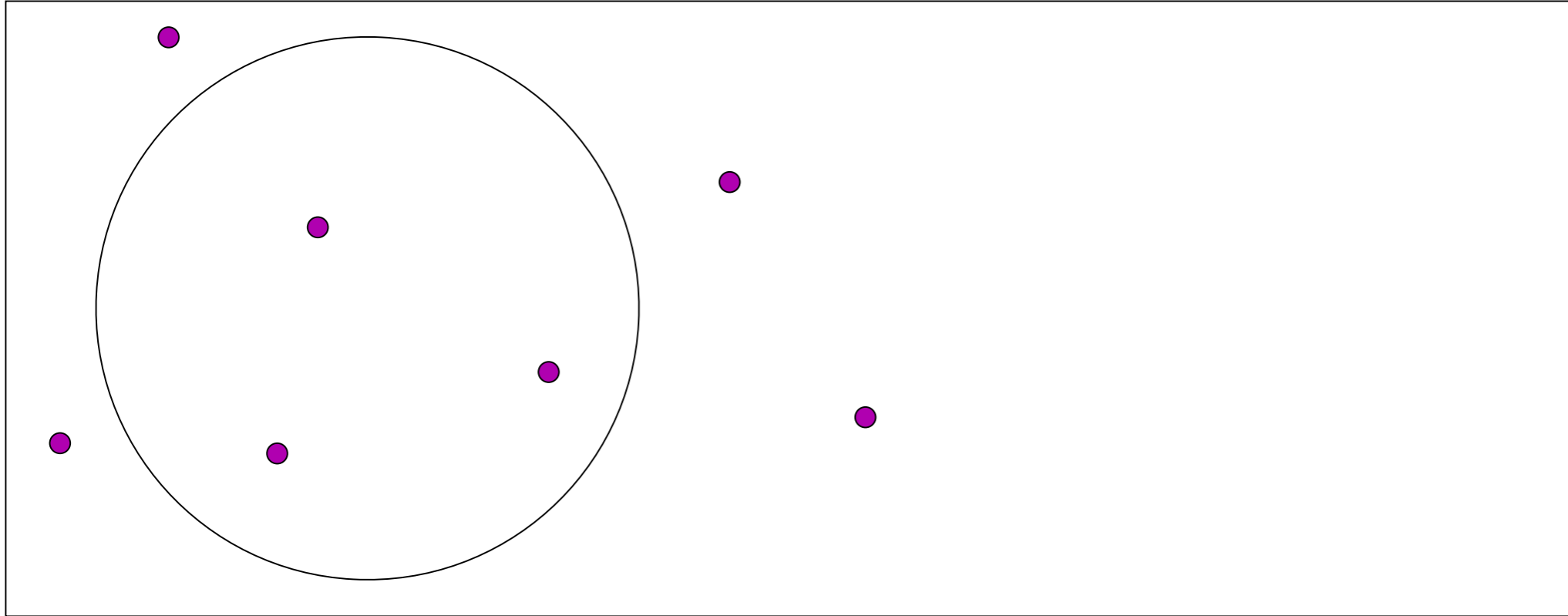
initial distribution, $\mathbf{C} = \mathbf{I}$

...equations

Covariance Matrix Adaptation

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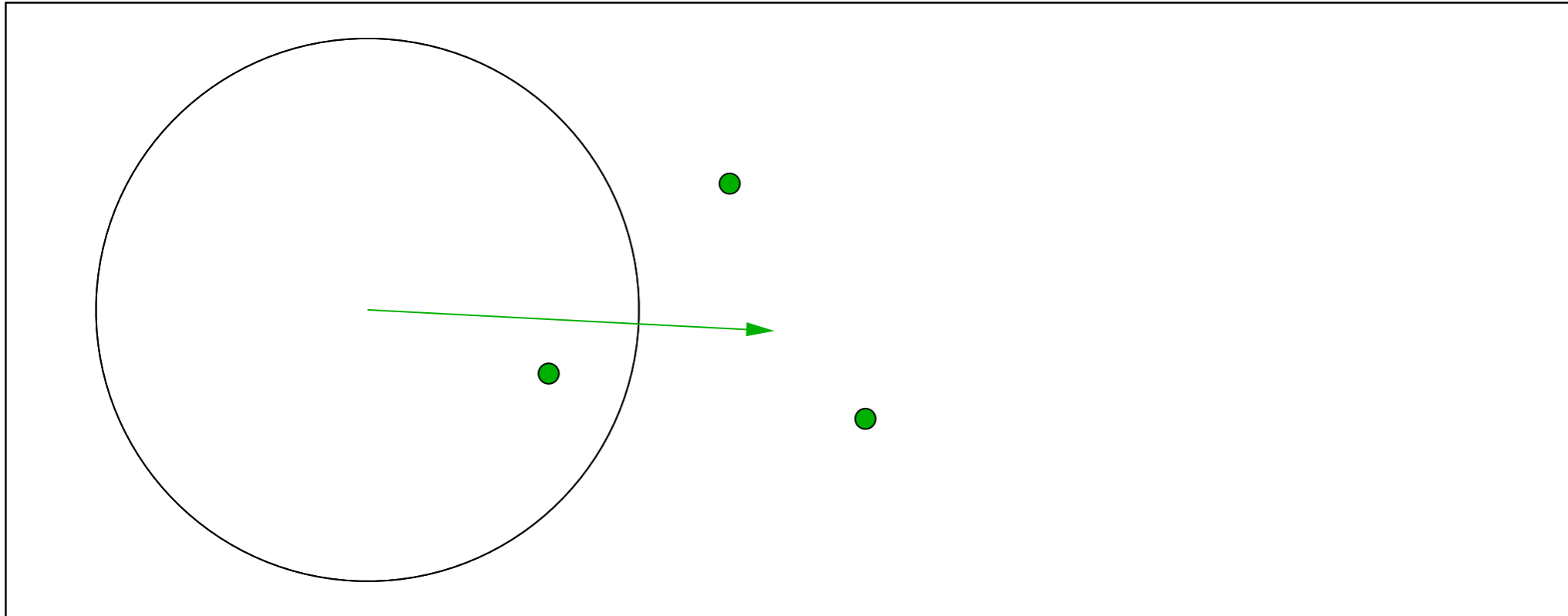
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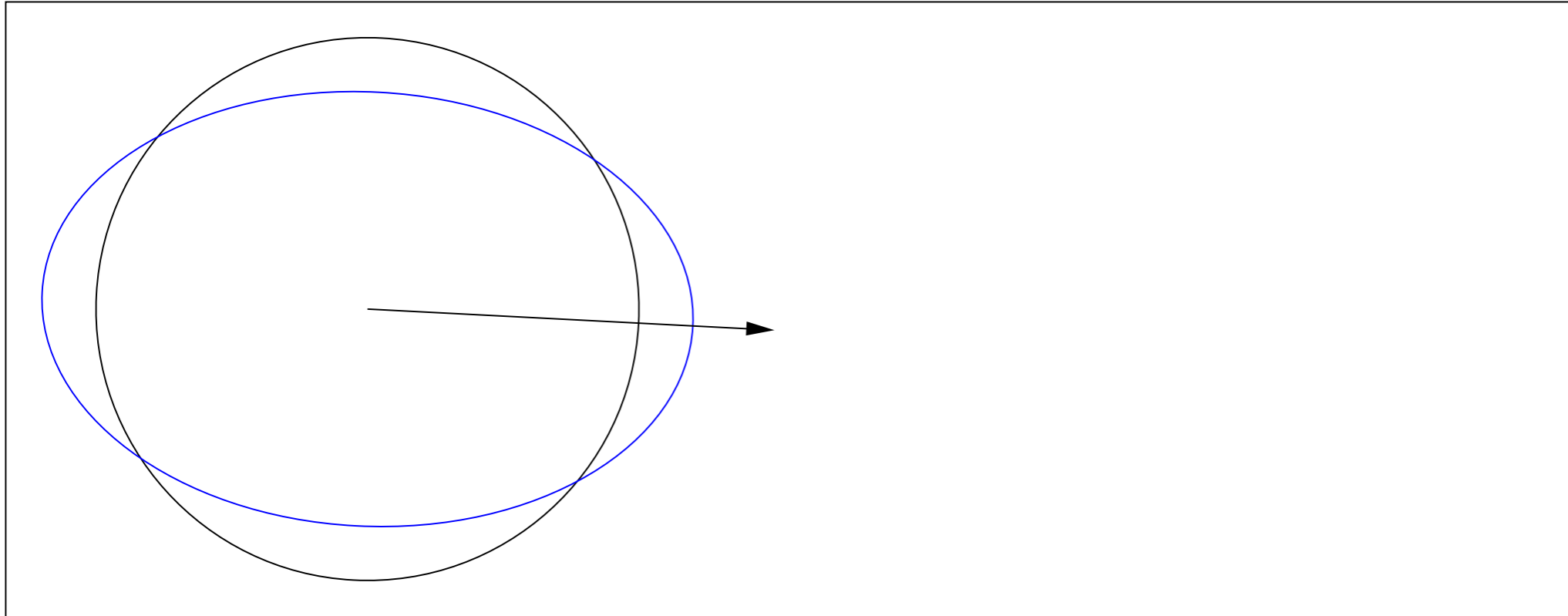
\mathbf{y}_w , movement of the population mean \mathbf{m} (disregarding σ)

... equations

Covariance Matrix Adaptation

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

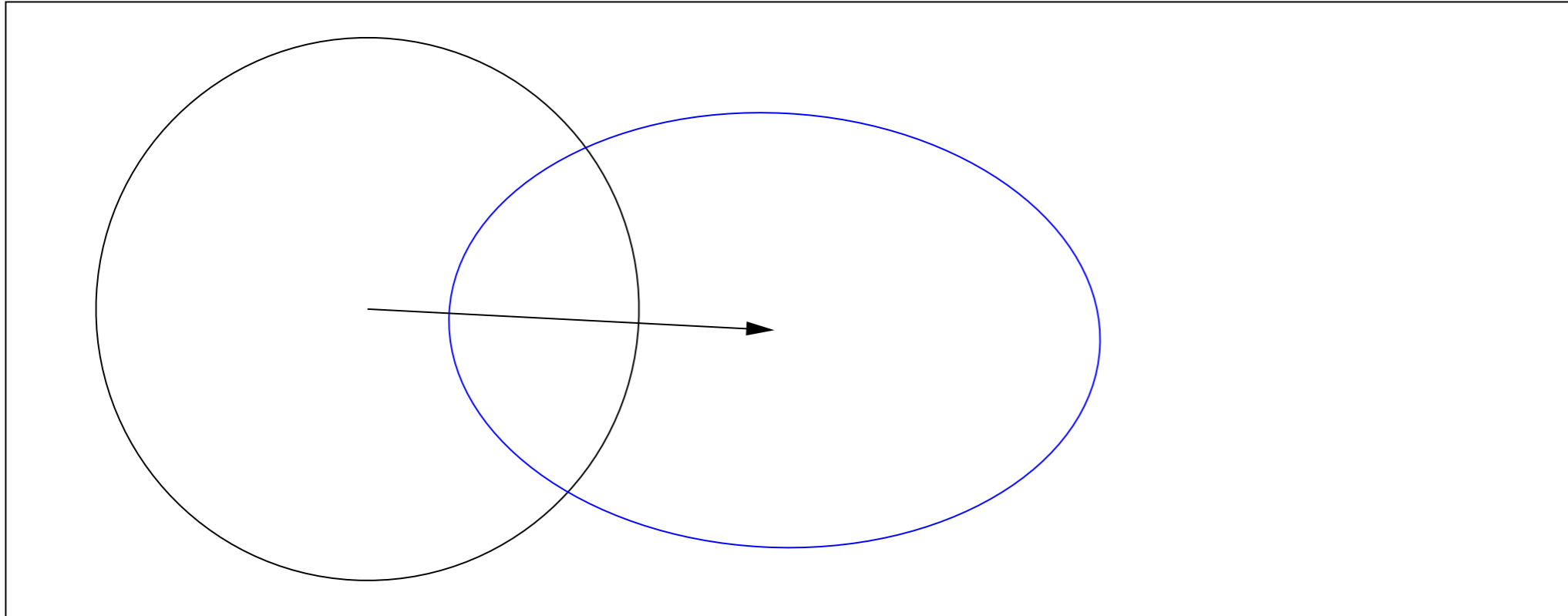
$$\mathbf{C} \leftarrow 0.8 \times \mathbf{C} + 0.2 \times \mathbf{y}_w \mathbf{y}_w^T$$

... equations

Covariance Matrix Adaptation

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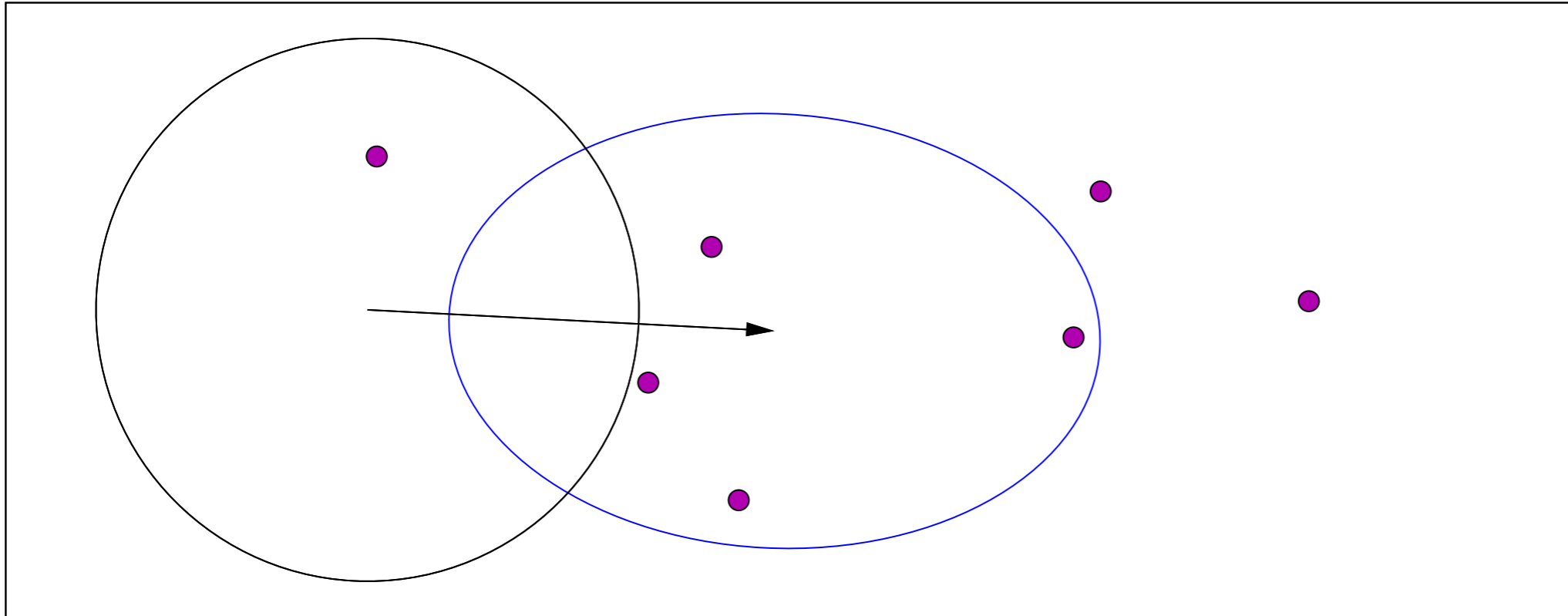
new distribution (disregarding σ)

... equations

Covariance Matrix Adaptation

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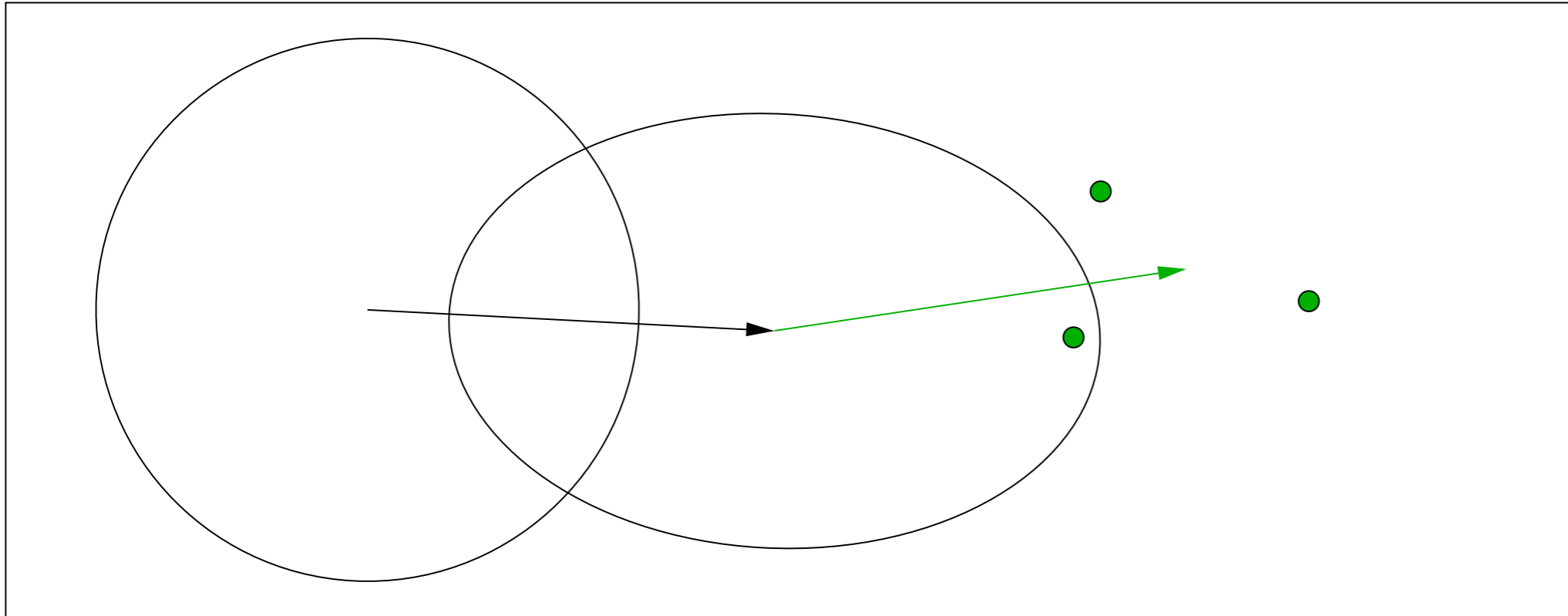
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... equations

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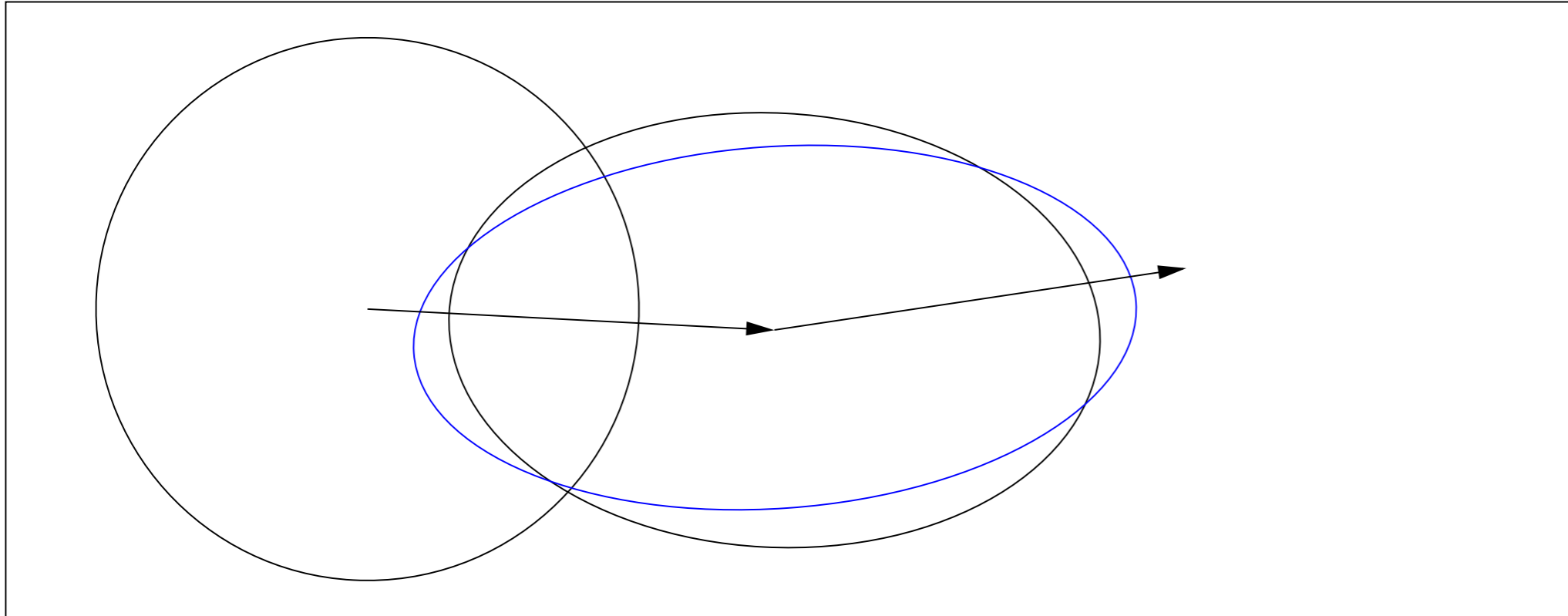
movement of the population mean \mathbf{m}

... equations

Covariance Matrix Adaptation

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

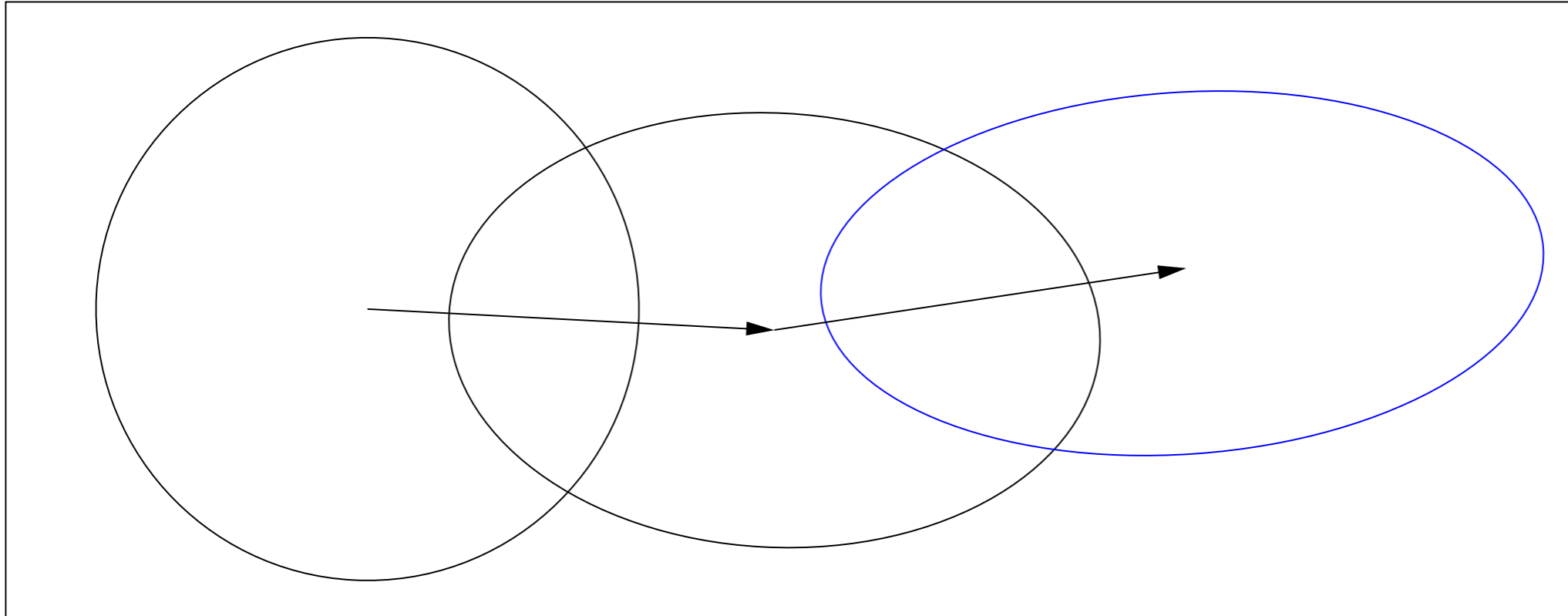
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... equations

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

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

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

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

The rank-one update has been found independently in several domains^{6 7 8 9}

⁶ Kjellström&Taxén 1981. Stochastic Optimization in System Design, IEEE TCS

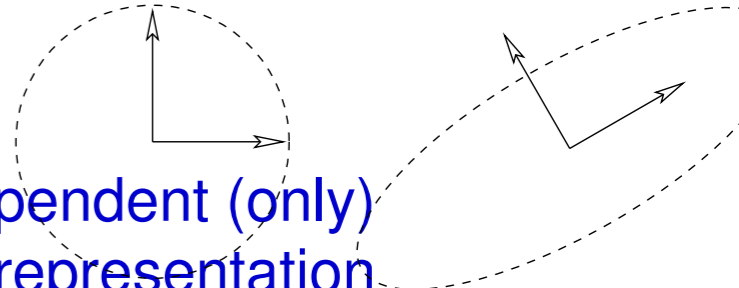
⁷ Hansen&Ostermeier 1996. Adapting arbitrary normal mutation distributions in evolution strategies: The covariance matrix adaptation, ICEC

⁸ Ljung 1999. System Identification: Theory for the User

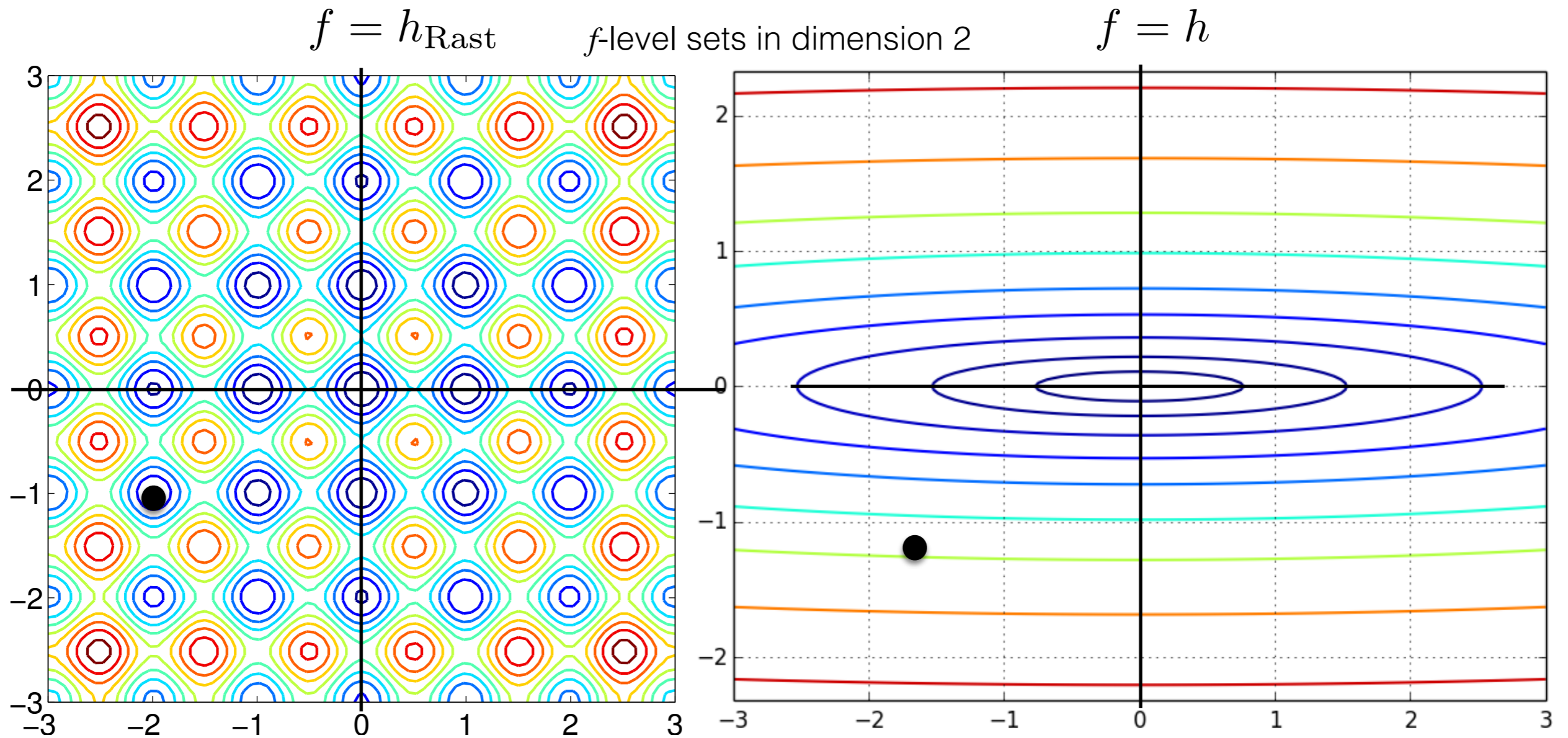
⁹ Haario et al 2001. An adaptive Metropolis algorithm, JSTOR

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

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



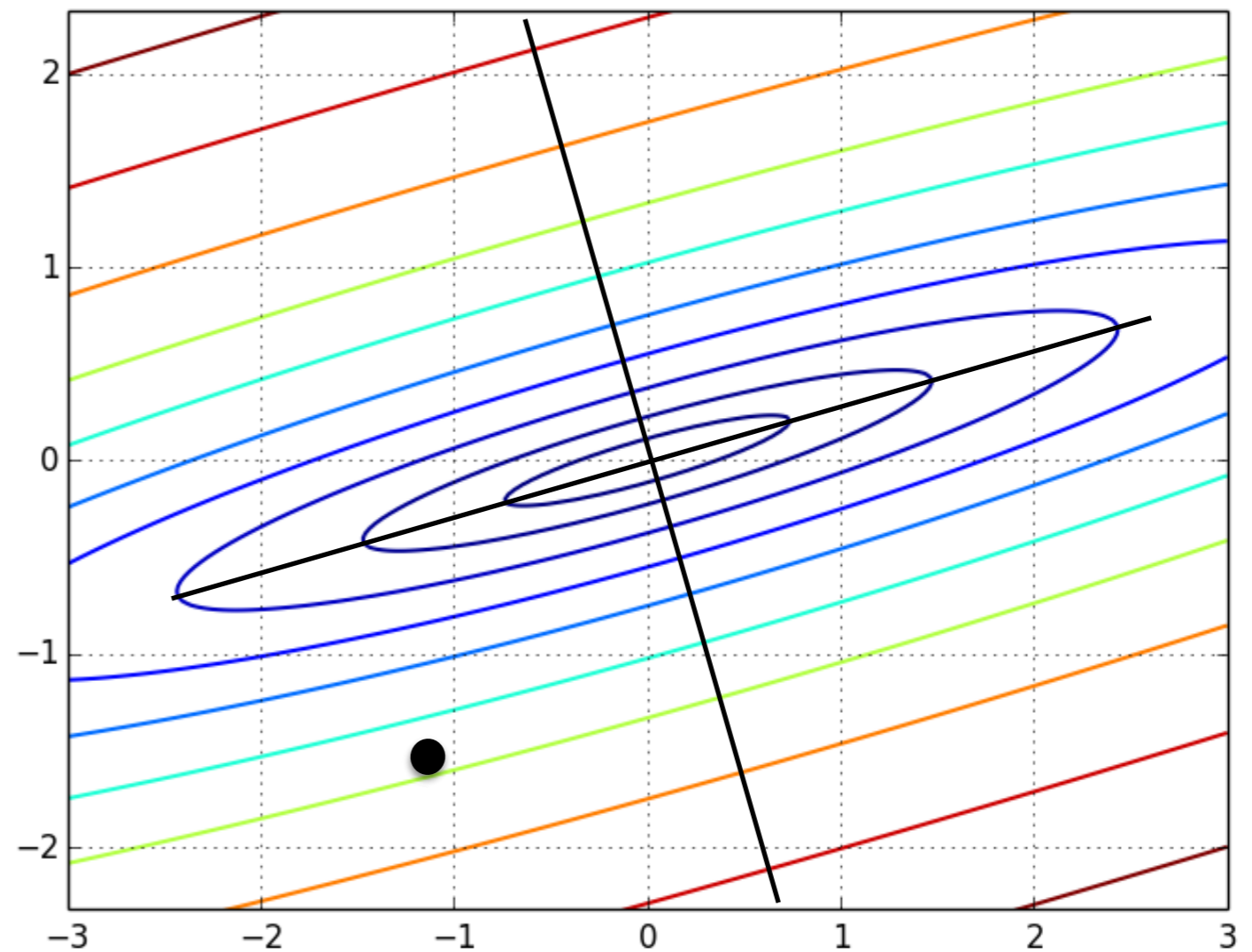
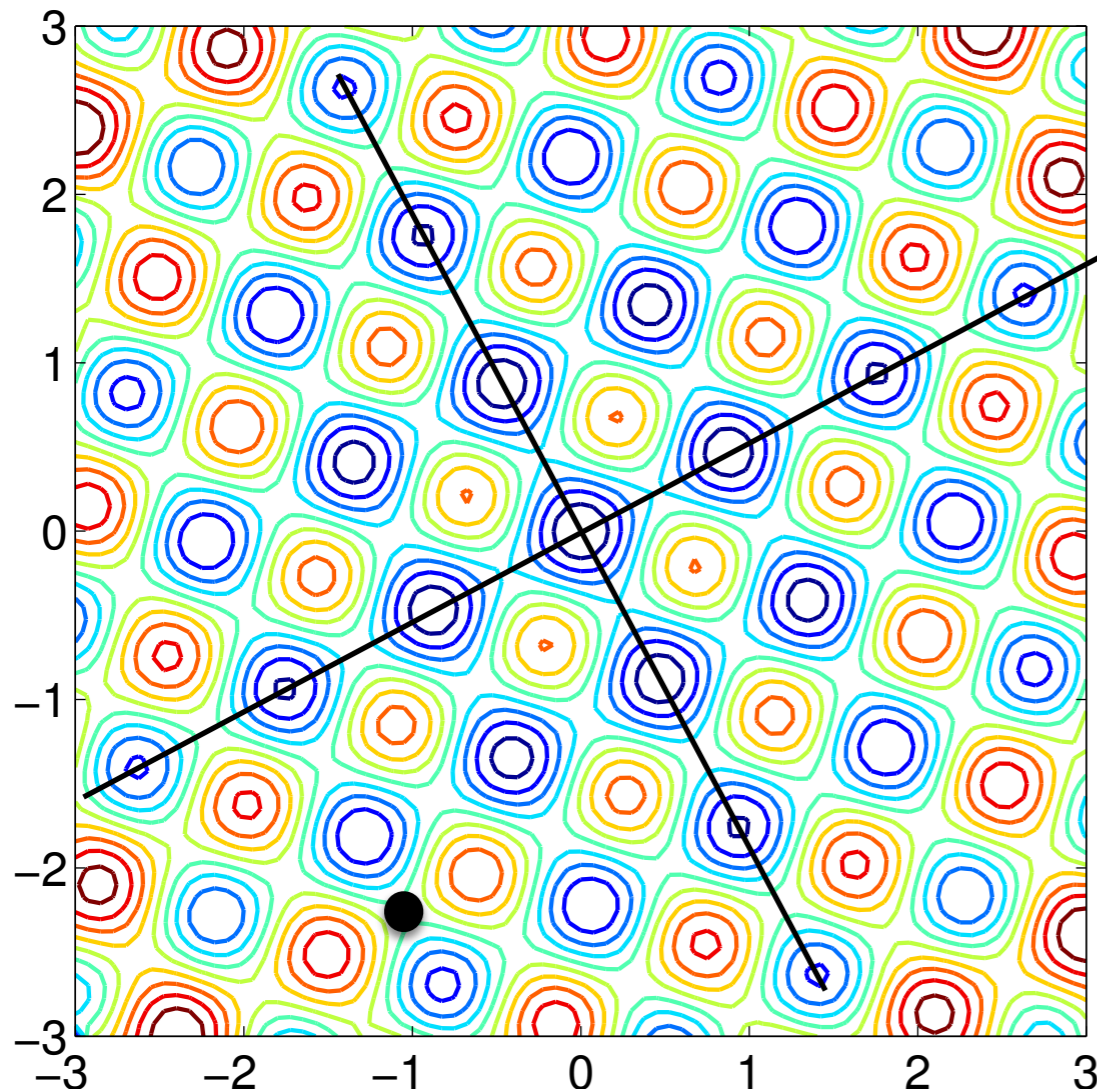
for example, invariance under search space rotation
 (separable \Leftrightarrow non-separable)

Invariance Under Rigid Search Space Transformation

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

f -level sets in dimension 2

$$f = h \circ R$$



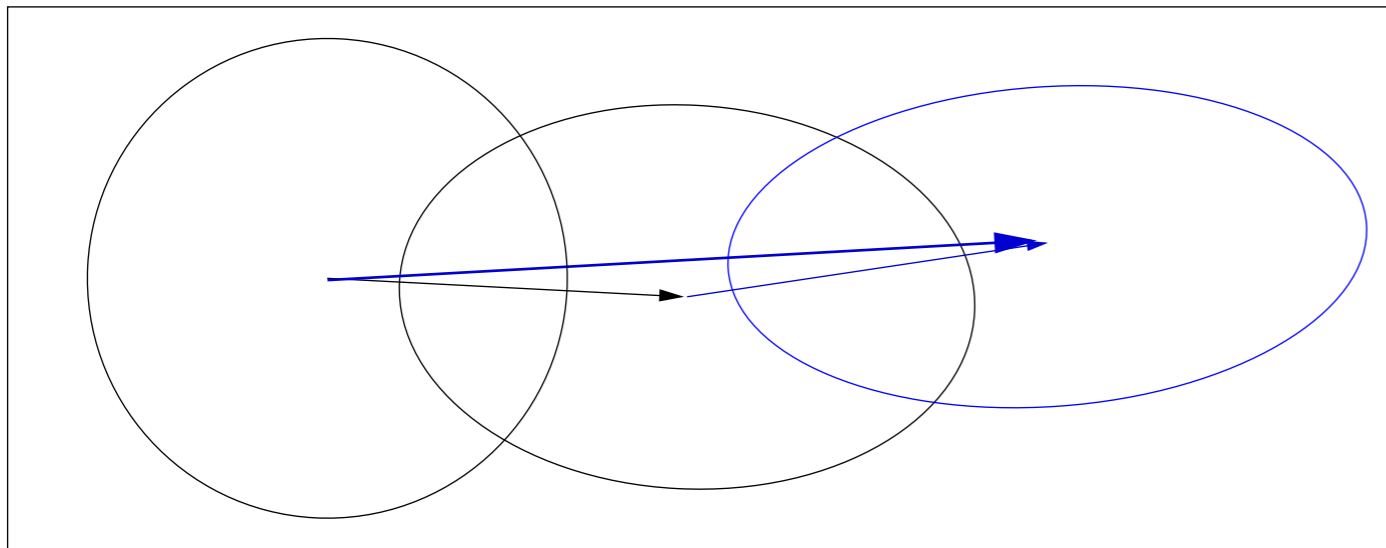
for example, invariance under search space rotation
(separable \Leftrightarrow **non-separable**)

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):

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

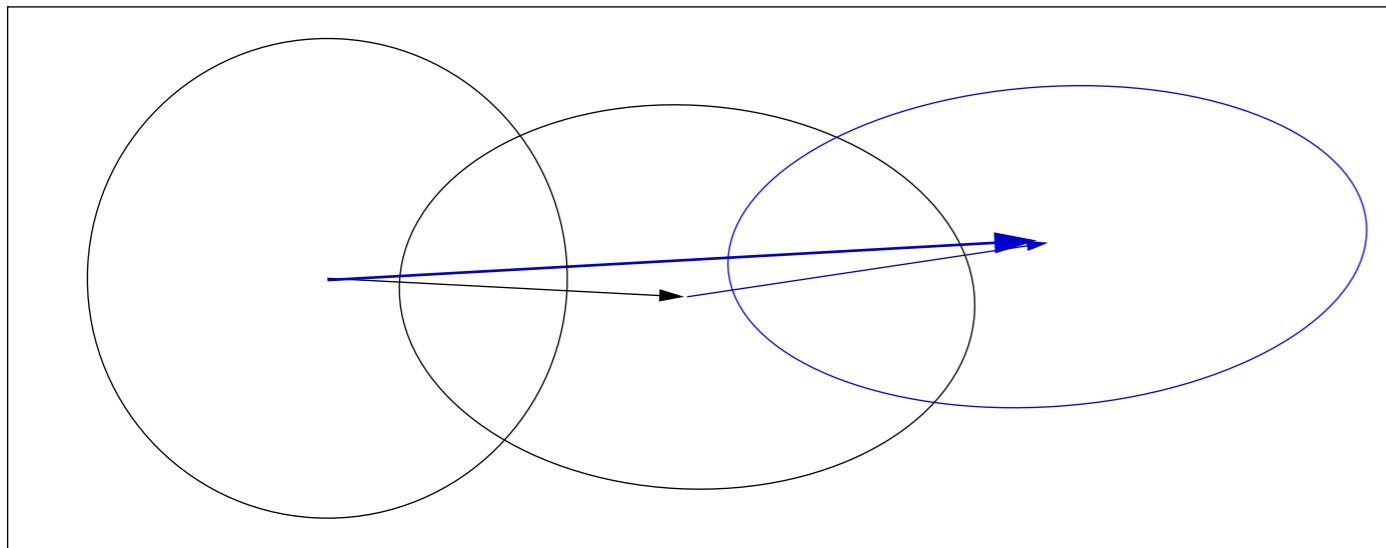
where $\mu_w = \frac{1}{\sum w_i^2}$, $c_c \ll 1$. **History information** is accumulated in the evolution path.

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“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...

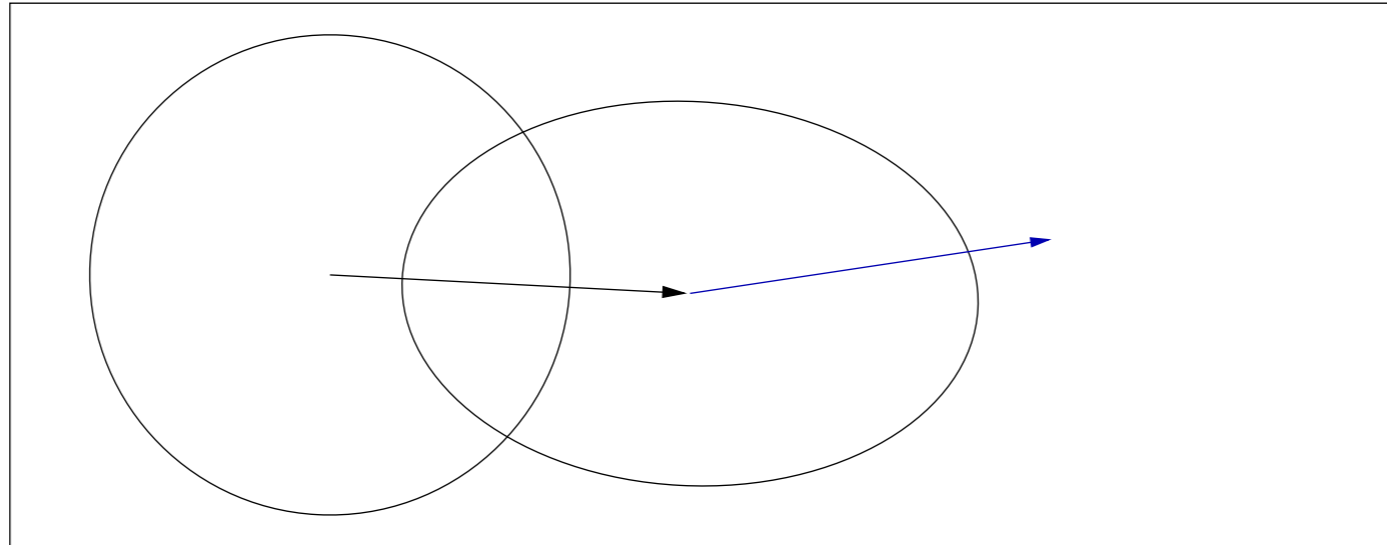
...why?

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*.

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

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

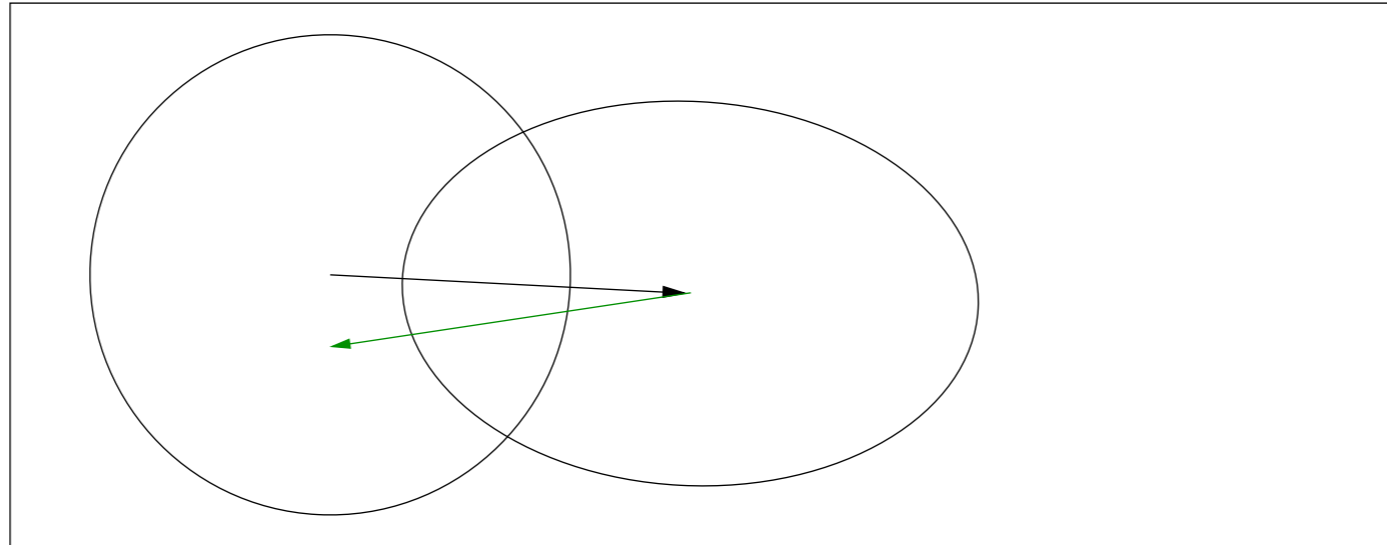
where $\mu_w = \frac{1}{\sum w_i^2}$, $c_{\text{cov}} \ll c_c \ll 1$ such that $1/c_c$ is the “backward time horizon”.

Cumulation

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

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

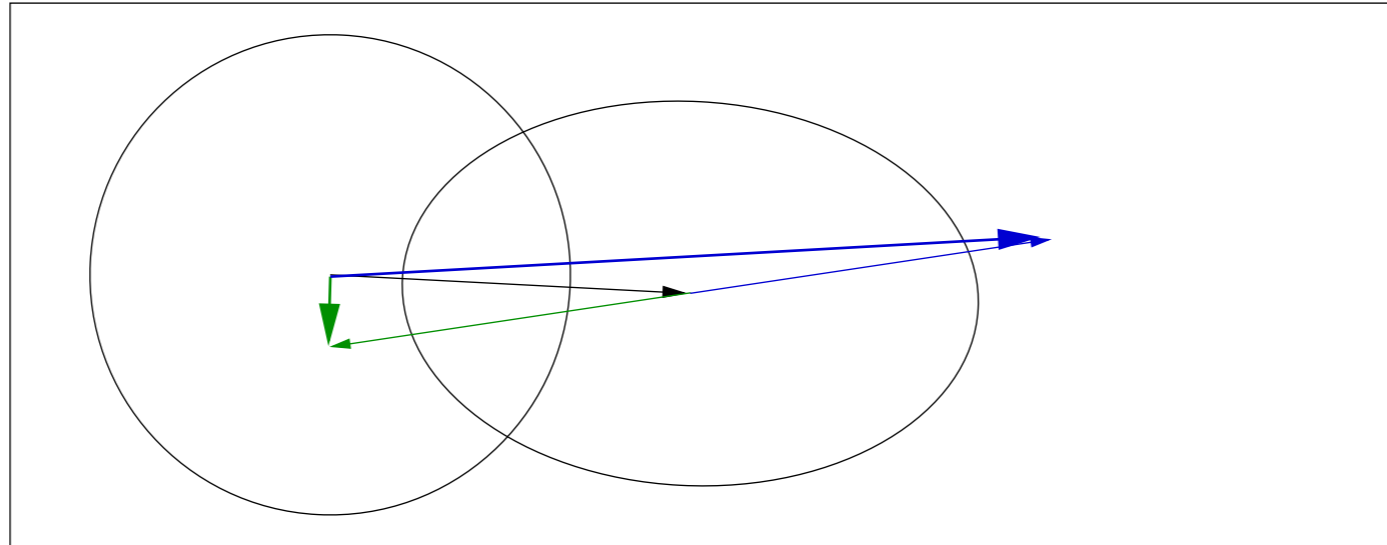
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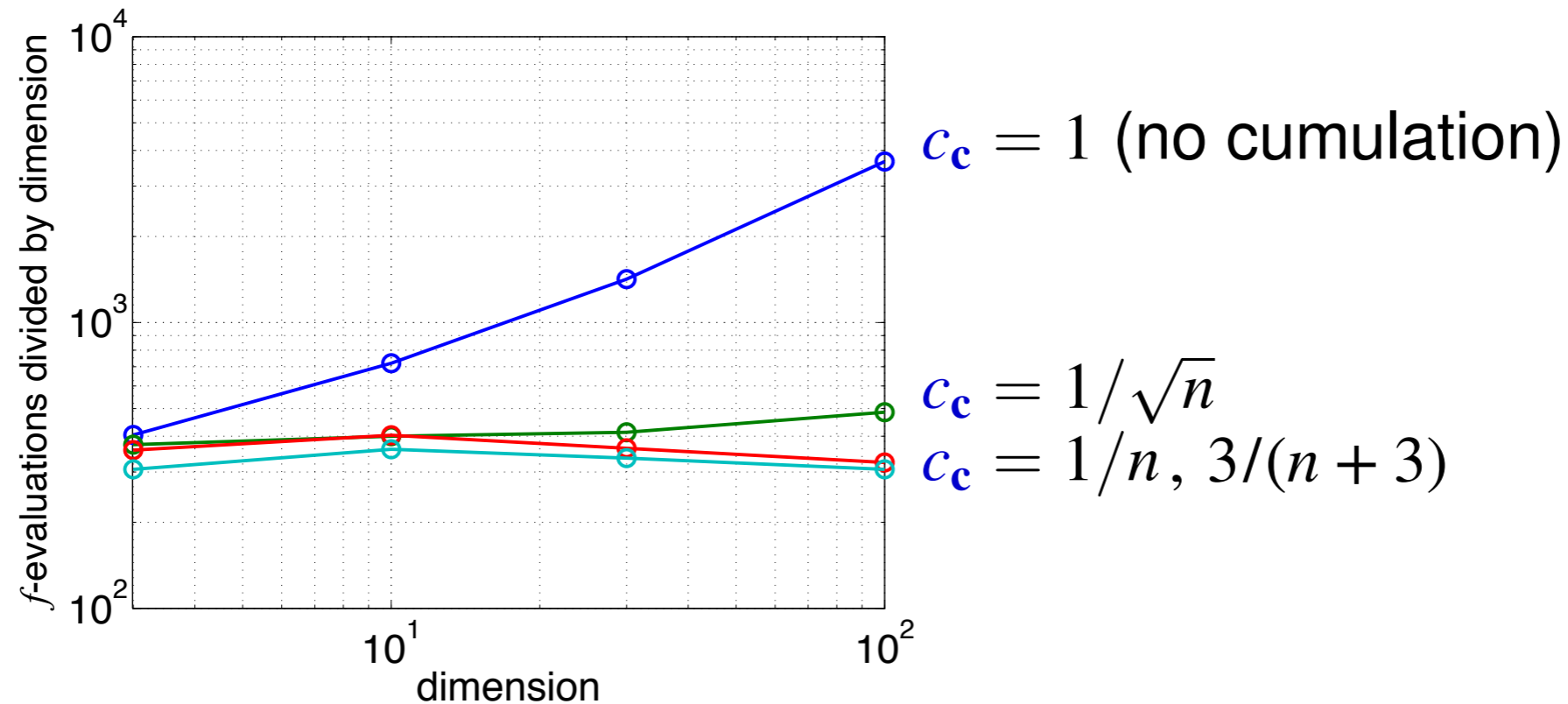
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Using an **evolution path** for the **rank-one update** of the covariance matrix reduces the number of function evaluations to adapt to a straight ridge **from about $\mathcal{O}(n^2)$ to $\mathcal{O}(n)$** .^(a)

^aHansen & 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- μ Update

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

The rank- μ update extends the update rule for **large population sizes** λ using $\mu > 1$ vectors to update \mathbf{C} at each generation step.

The 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 μ steps and has rank $\min(\mu, n)$ with probability one.

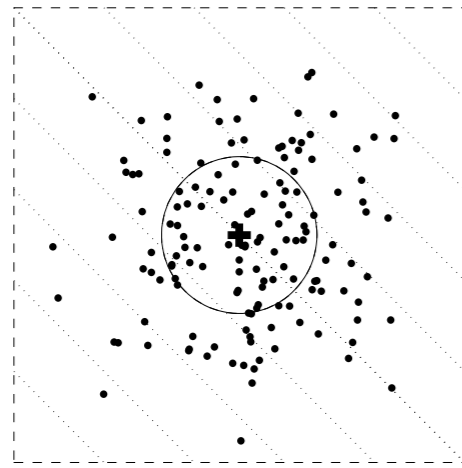
with $\mu = \lambda$ weights can be negative ¹⁰

The rank- μ update then reads

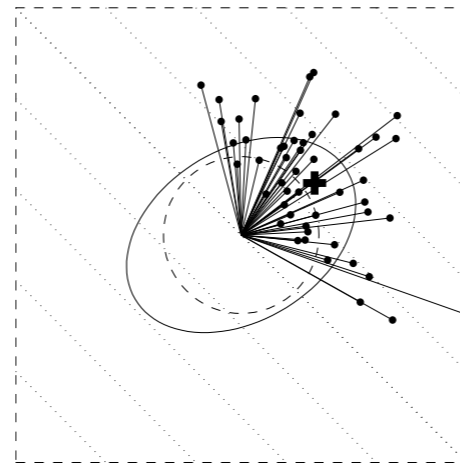
$$\mathbf{C} \leftarrow (1 - c_{\text{cov}}) \mathbf{C} + c_{\text{cov}} \mathbf{C}_\mu$$

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

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

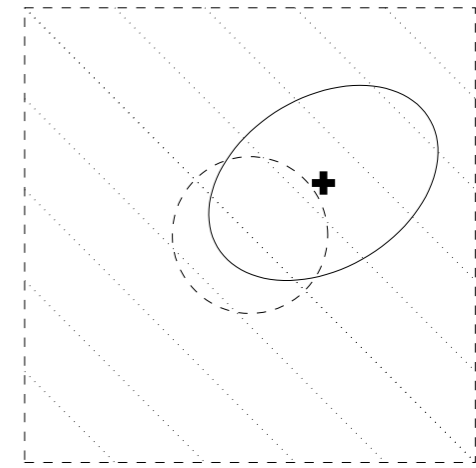


$$x_i = m + \sigma y_i, \quad y_i \sim \mathcal{N}(\mathbf{0}, \mathbf{C})$$



$$\mathbf{C}_\mu = \frac{1}{\mu} \sum y_{i:\lambda} y_{i:\lambda}^\top$$

$$\mathbf{C} \leftarrow (1 - 1) \times \mathbf{C} + 1 \times \mathbf{C}_\mu$$

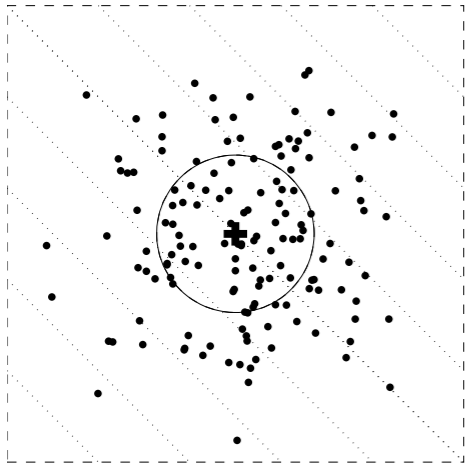


$$m_{\text{new}} \leftarrow m + \frac{1}{\mu} \sum y_{i:\lambda}$$

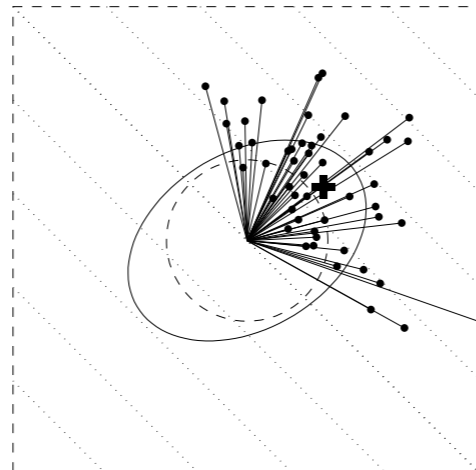
new distribution

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

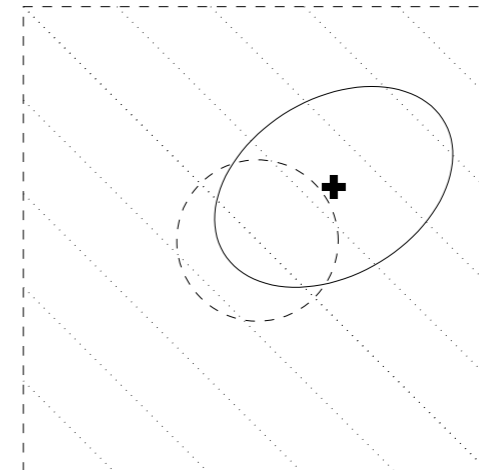
calculating \mathbf{C} where
 $\mu = 50$,
 $w_1 = \dots = w_\mu = \frac{1}{\mu}$,
and $c_{\text{cov}} = 1$

Rank- μ CMA versus Estimation of Multivariate Normal Algorithm EMNA_{global}¹¹

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

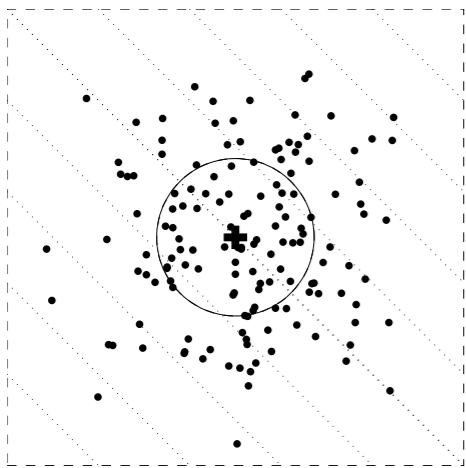


$$\mathbf{C} \leftarrow \frac{1}{\mu} \sum (x_{i:\lambda} - m_{\text{old}})(x_{i:\lambda} - m_{\text{old}})^T$$

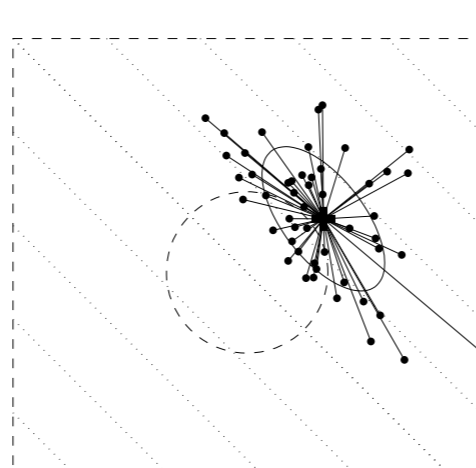


$$m_{\text{new}} = m_{\text{old}} + \frac{1}{\mu} \sum y_{i:\lambda}$$

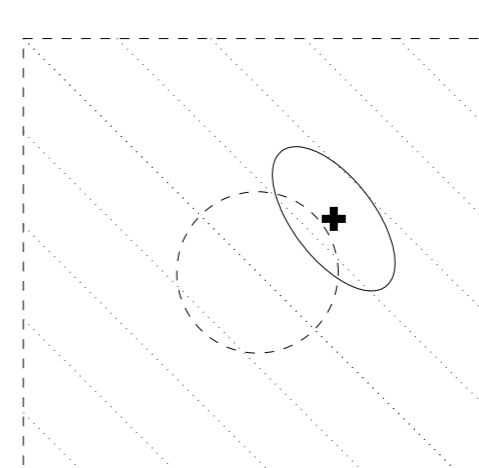
rank- μ CMA
conducts a
PCA of
steps



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



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



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

EMNA_{global}
conducts a
PCA of
points

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

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

new distribution

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

¹¹ 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- μ update

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

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

say $\lambda \geq 3n + 10$

The rank-one update

- uses the evolution path and reduces the number of necessary **function evaluations** to learn straight ridges from $\mathcal{O}(n^2)$ to $\mathcal{O}(n)$.

Rank-one update and rank- μ update can be combined

... all equations

¹²Hansen, 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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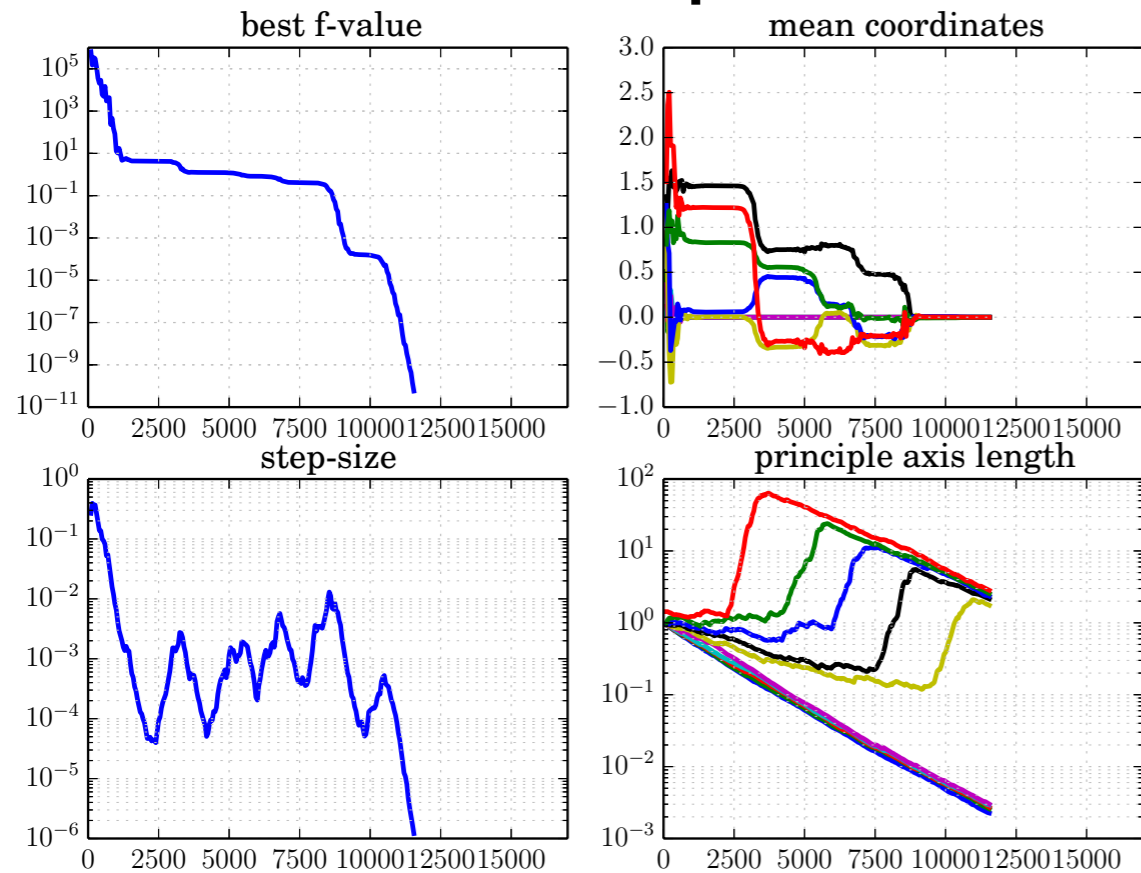
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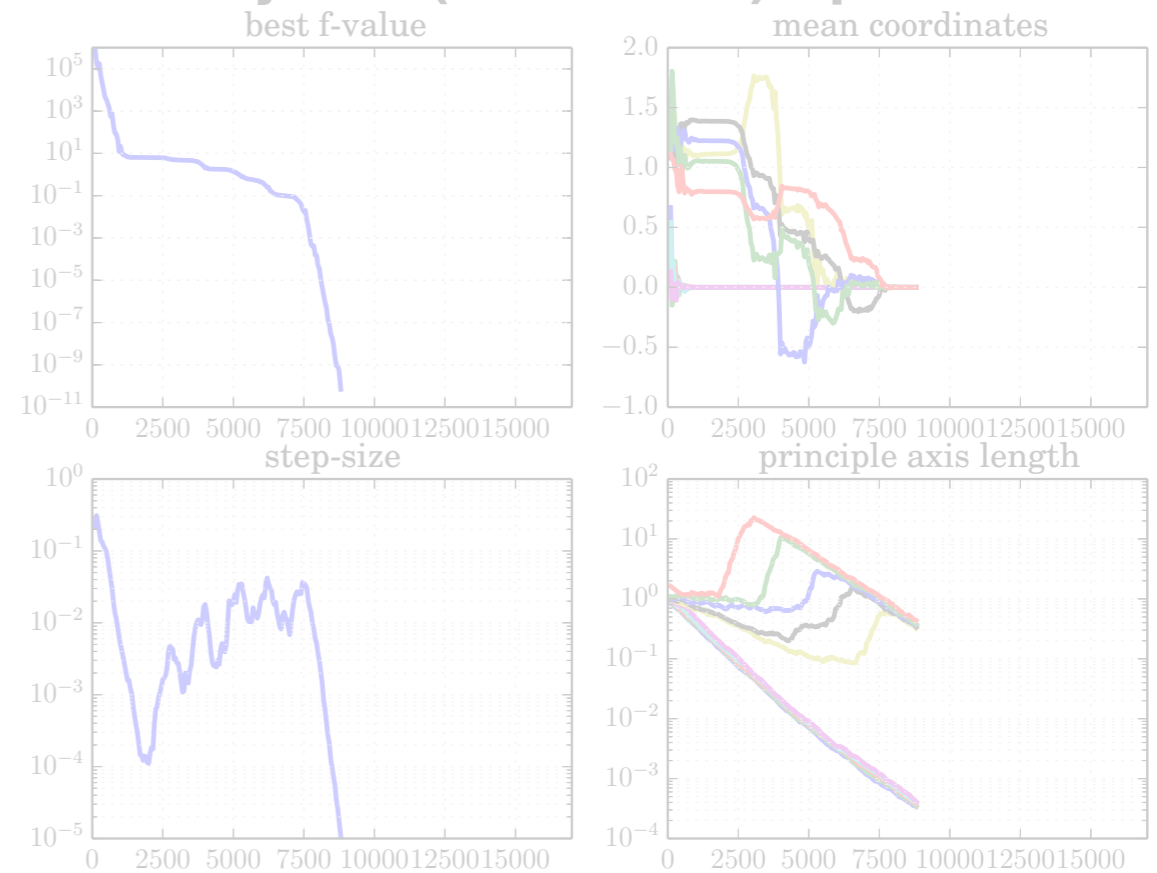
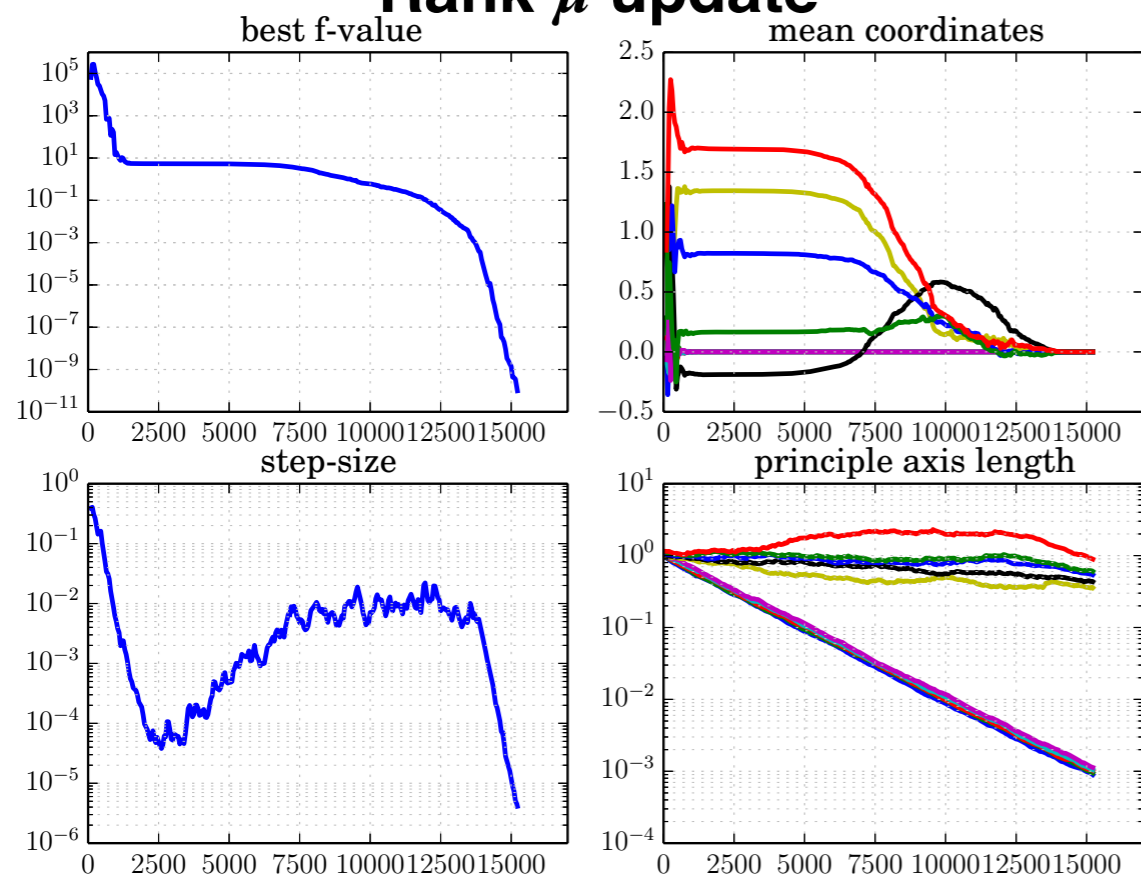
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Rank-one update



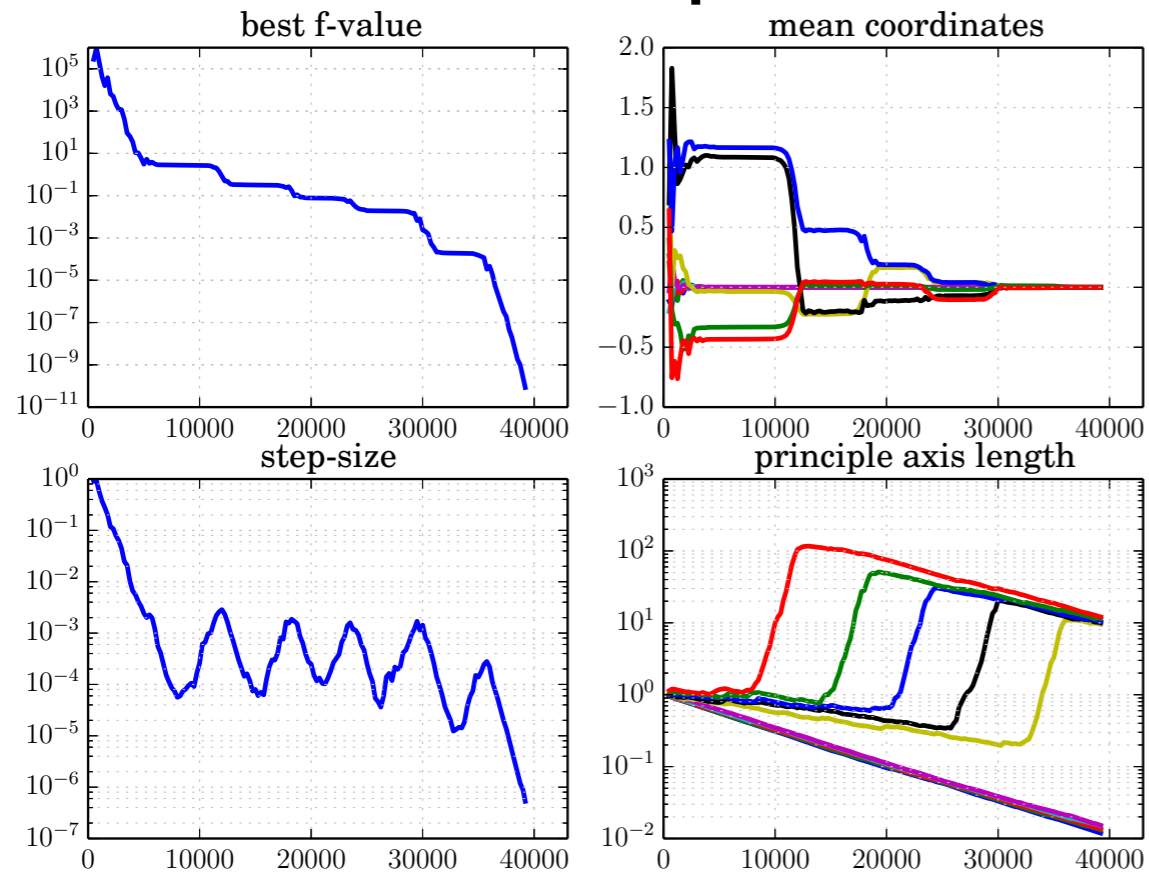
Hybrid (combined) update

Rank- μ update

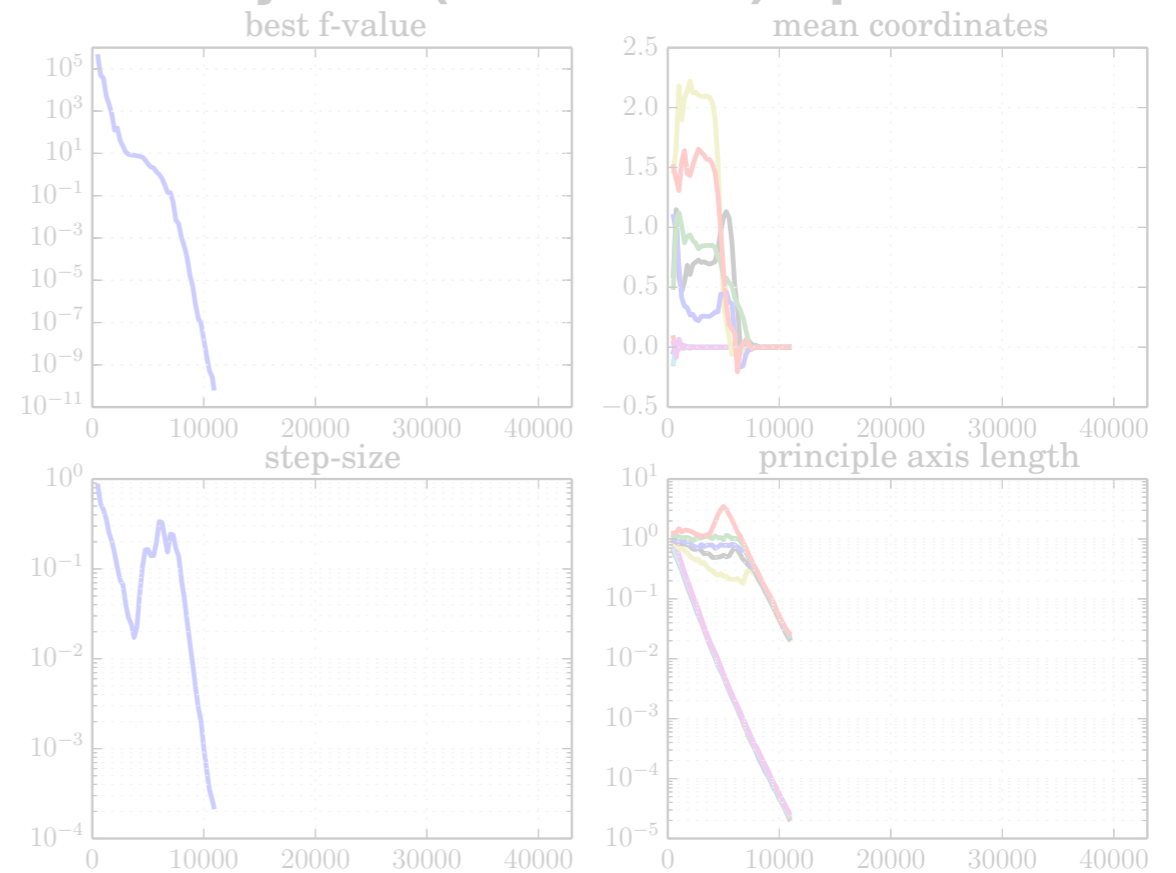
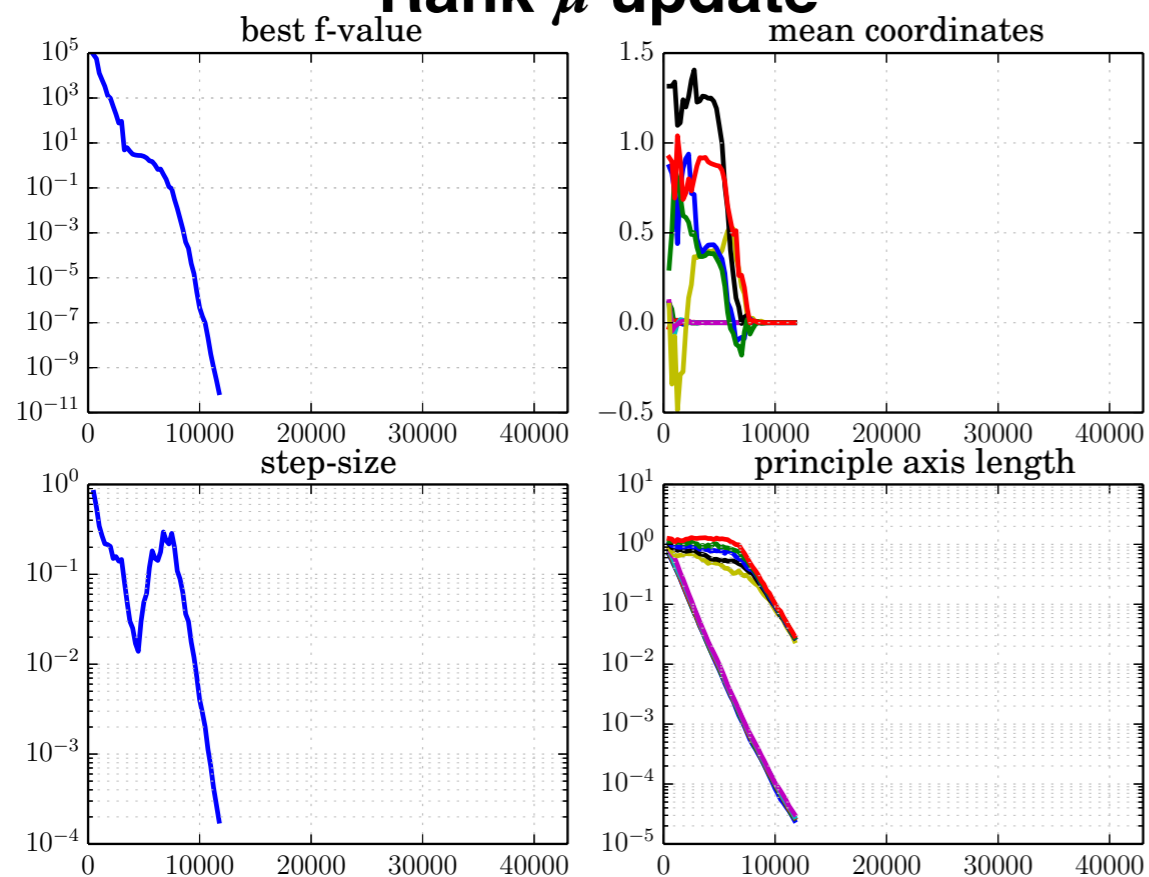
$$f_{\text{TwoAxes}}(x) = \sum_{i=1}^5 x_i^2 + 10^6 \sum_{i=6}^{10} x_i^2$$

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

Rank-one update



Hybrid (combined) update

Rank- μ update

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

$$\lambda = 50$$

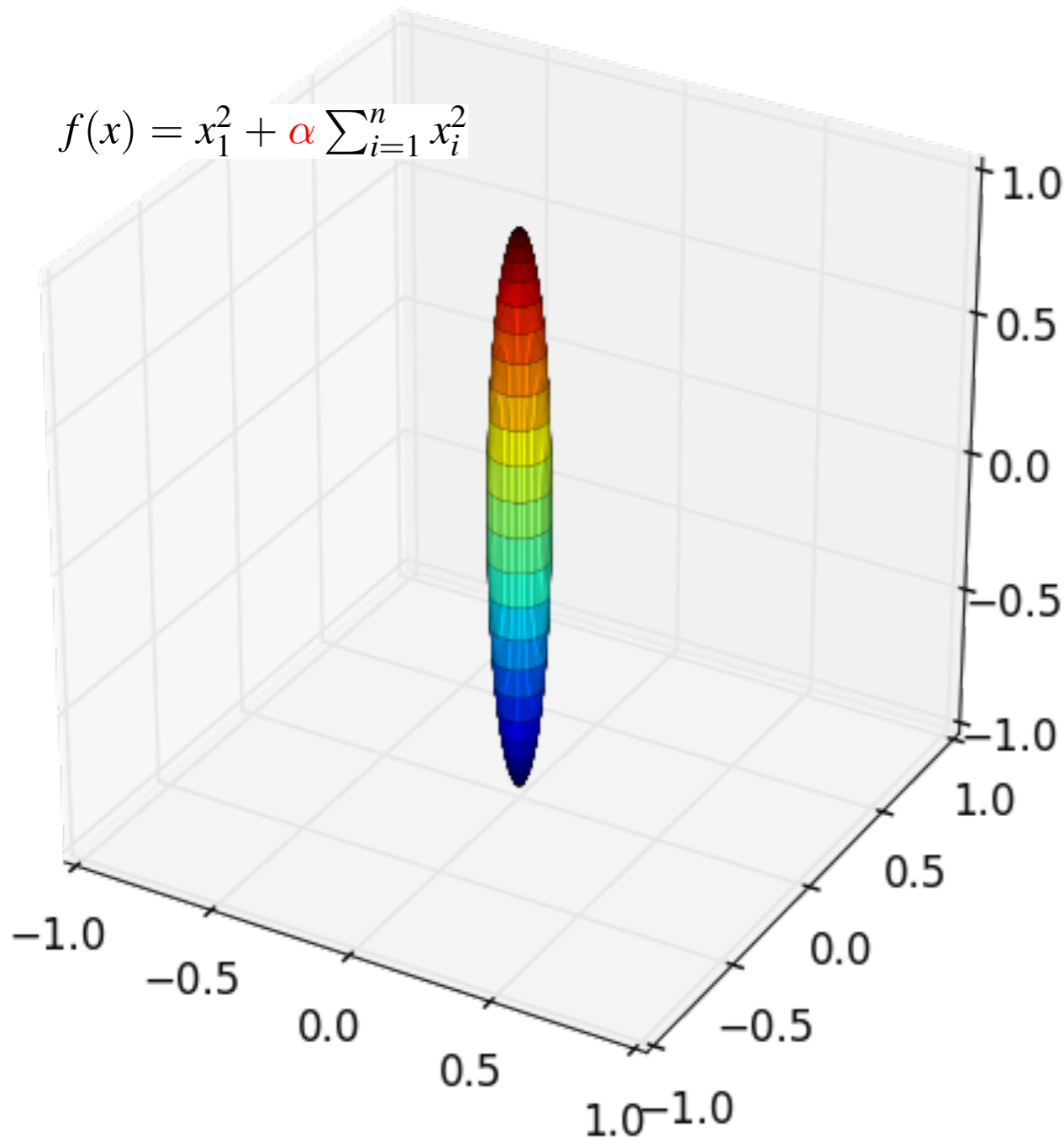
Different Types of Ill-Conditioning

(α : Axes Ratio = 10)

Cigar Type:

1 long axis = n-1 short axes

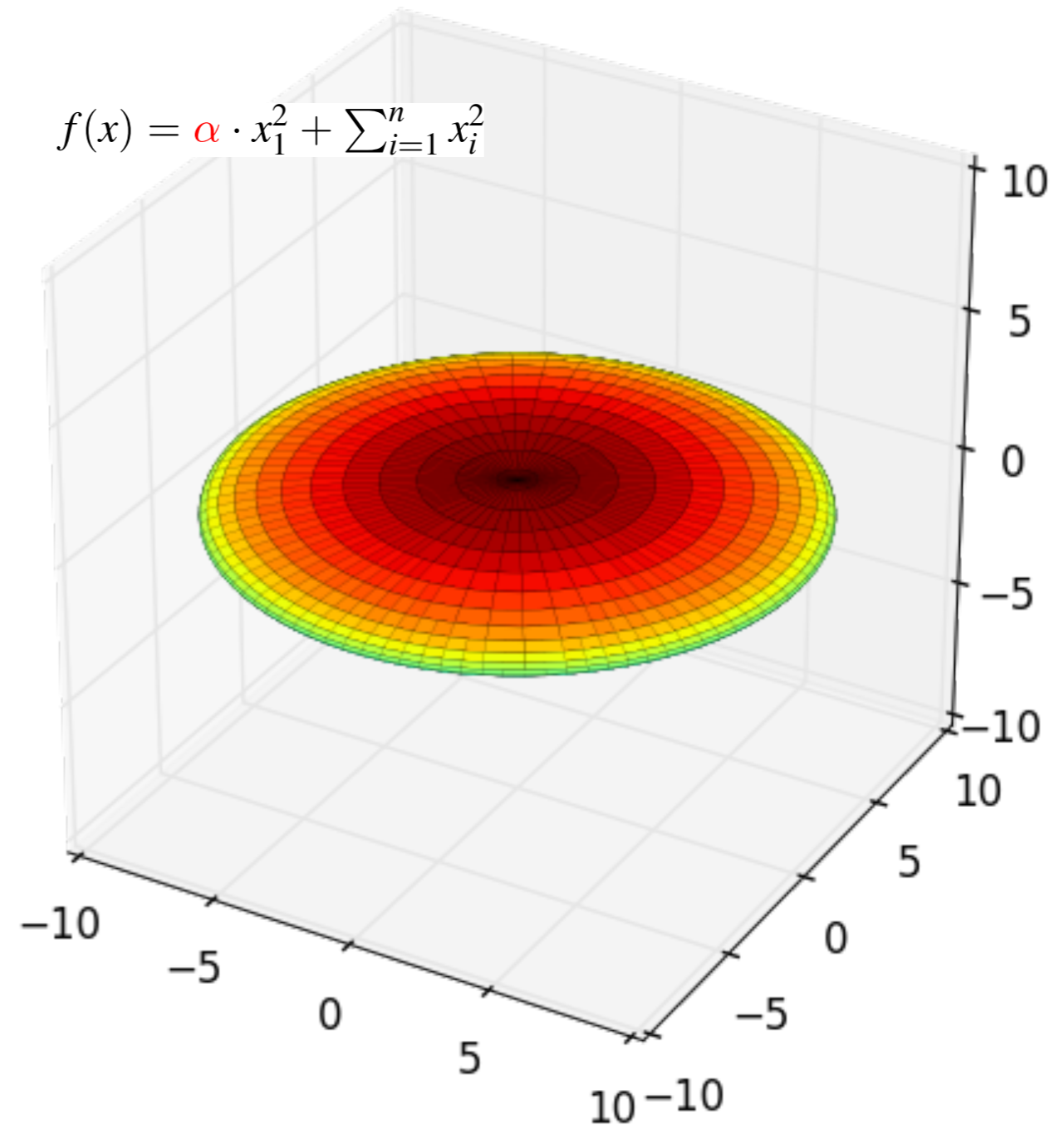
$$f(x) = x_1^2 + \alpha \sum_{i=1}^n x_i^2$$



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)

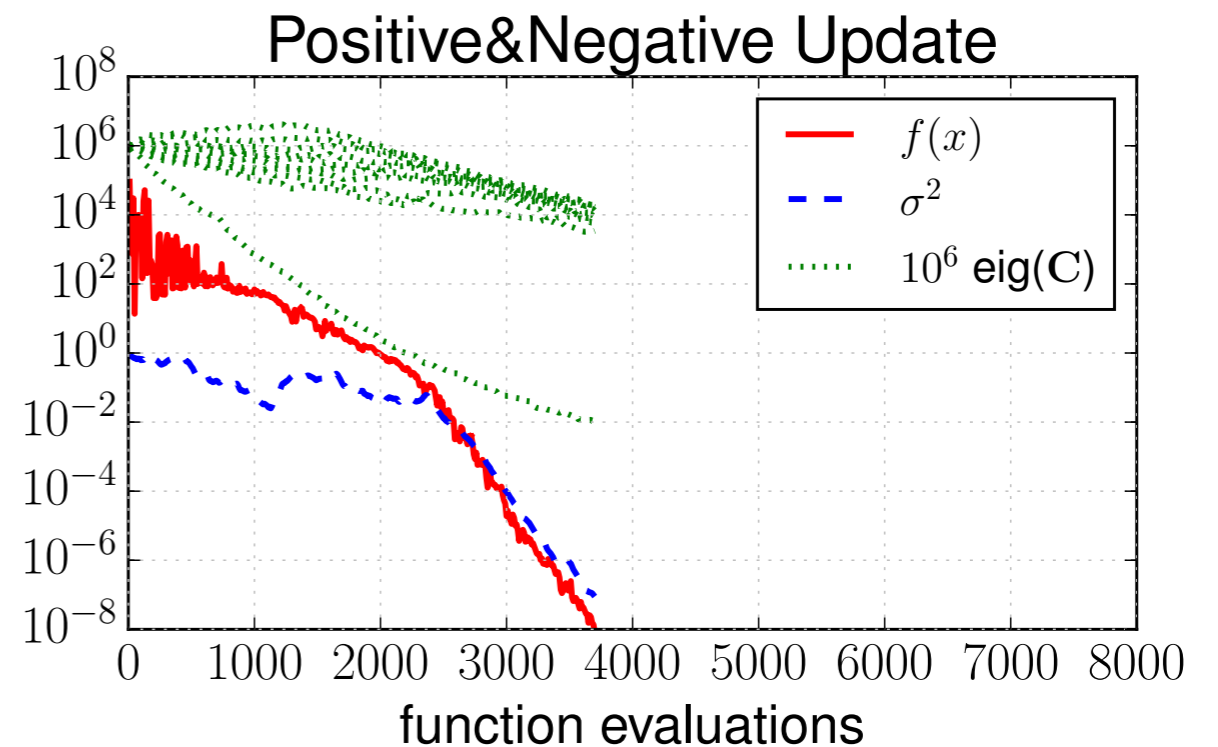
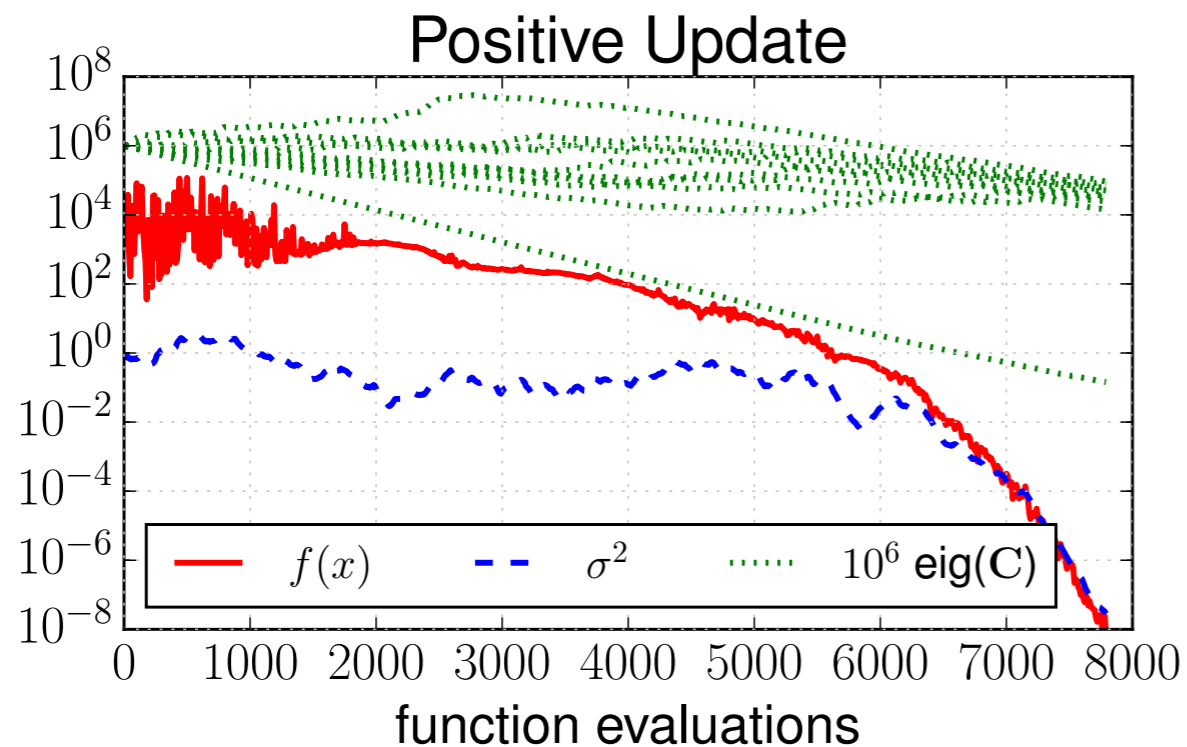
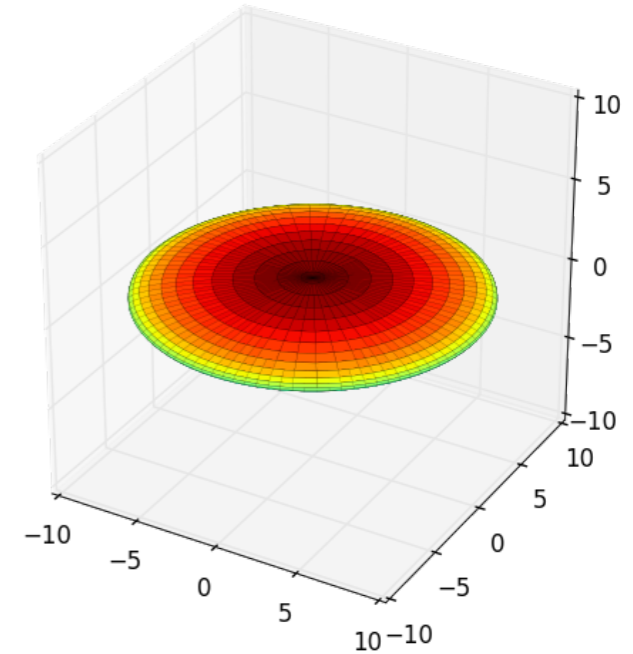
$$\mathbf{C} \leftarrow \mathbf{C} + \underbrace{c_1 \mathbf{p}_c \mathbf{p}_c^T + c_\mu \sum_{i=1}^{\lfloor \lambda/2 \rfloor} w_i \mathbf{y}_{i:\lambda} \mathbf{y}_{i:\lambda}^T}_{\text{increasing the variances in promising directions}} - \underbrace{c_\mu \sum_{i=\lambda - \lfloor \lambda/2 \rfloor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

- 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 $i \geq \lambda - \mu$): 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 compensate each other

- cumulation: excels to learn a long axis, but inefficient for a large λ
- rank- μ update: efficient for a large λ
- 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_μ^- 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 $\mathbf{y}_w = \sum_{i=1}^{\mu} w_i \mathbf{y}_{\text{rk}^{-1}(i)}$ 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 σ

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

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

Not covered: termination, restarts, useful output, search boundaries and encoding, corrections for: positive definiteness guaranty, \mathbf{p}_c variance loss, c_σ and d_σ for large λ

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
 - λ : offspring number, new solutions sampled, population size
 - μ : 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_μ : learning rate for rank- μ update of \mathbf{C}
- related to σ -update
 - $1 - c_\sigma$: decay rate of the evolution path
 - d_σ : damping for σ -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 ...]
```

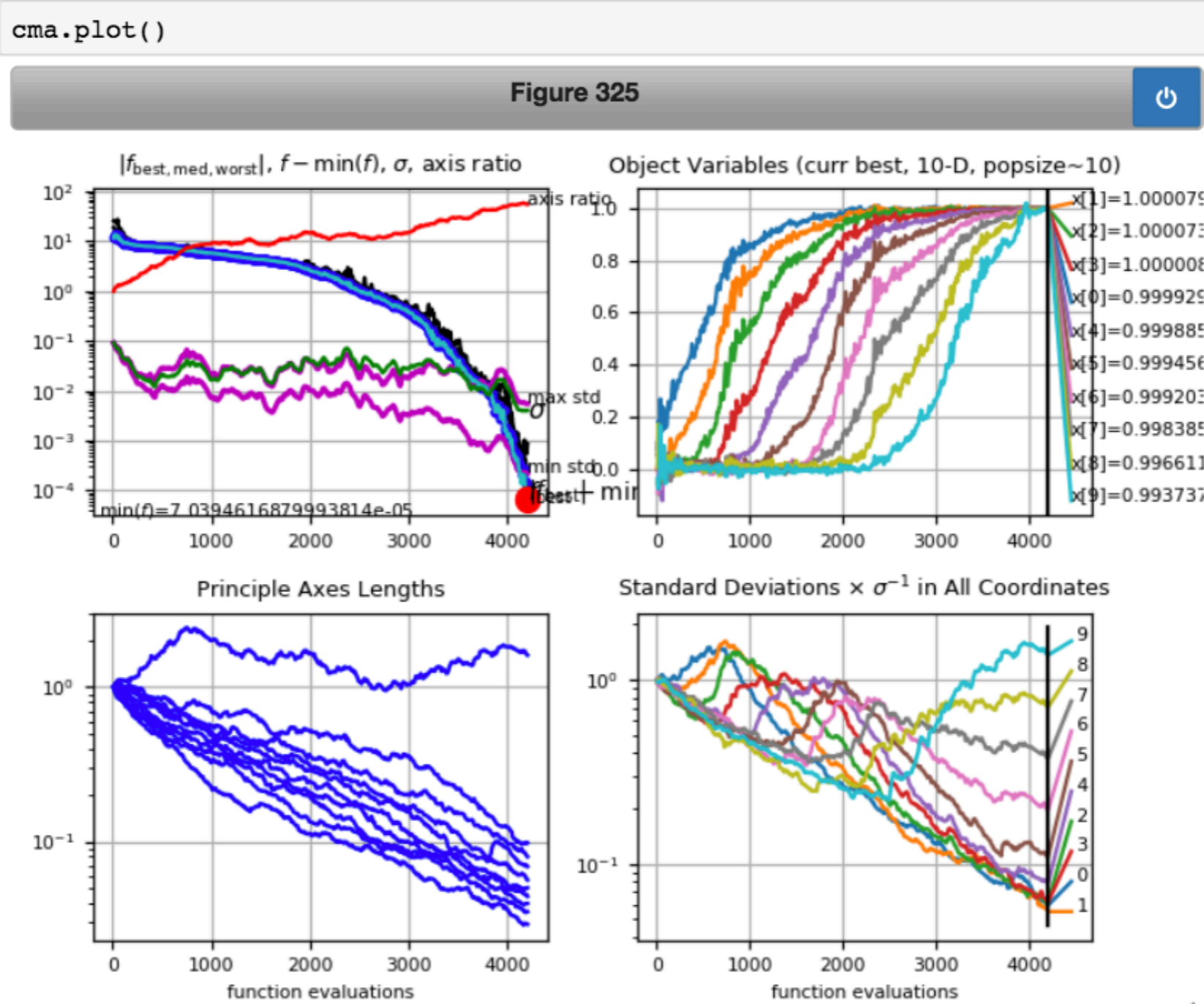
```
std deviations: [ 0.00023937  0.00022203  0.00024836  0.00024782  0.00031258  0.00043481
```

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

Python CMA-ES Demo

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

Optimizing 10D Rosenbrock Function



Multimodality

Two approaches for multimodal functions: Try again with

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

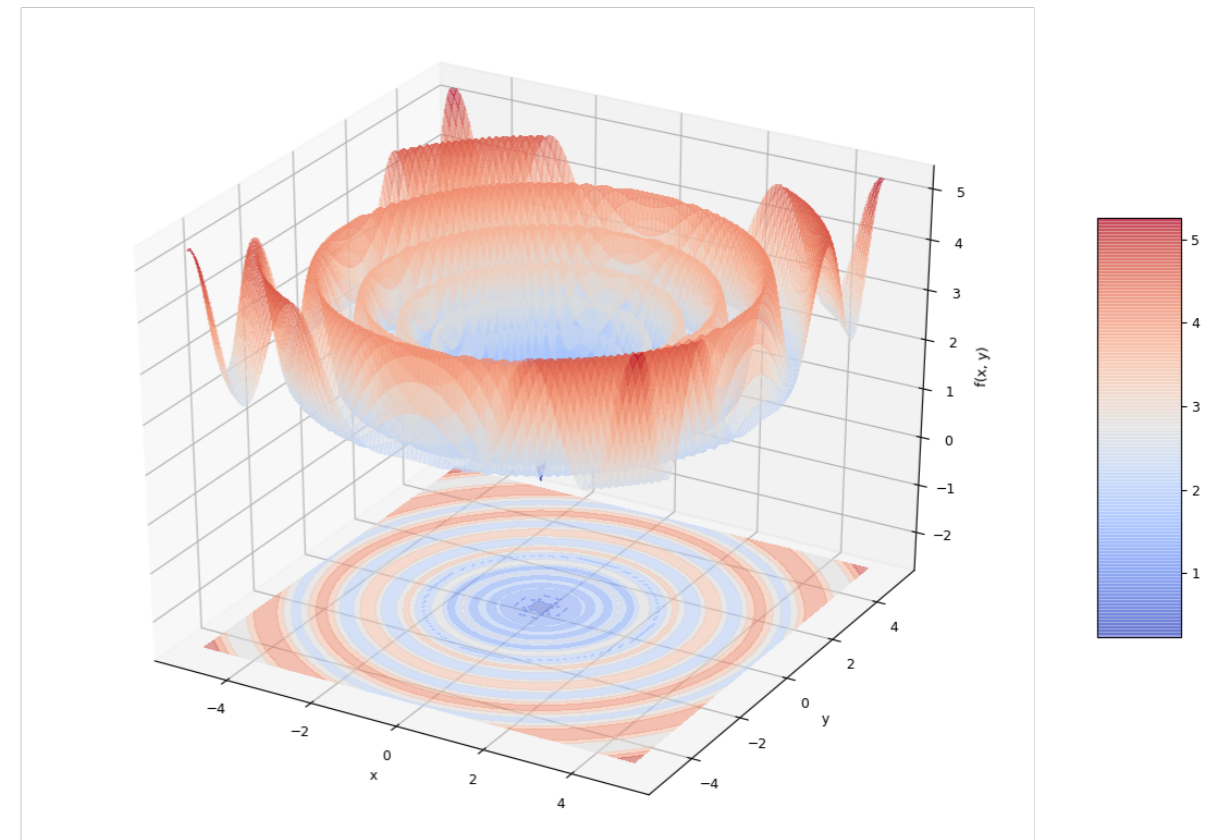
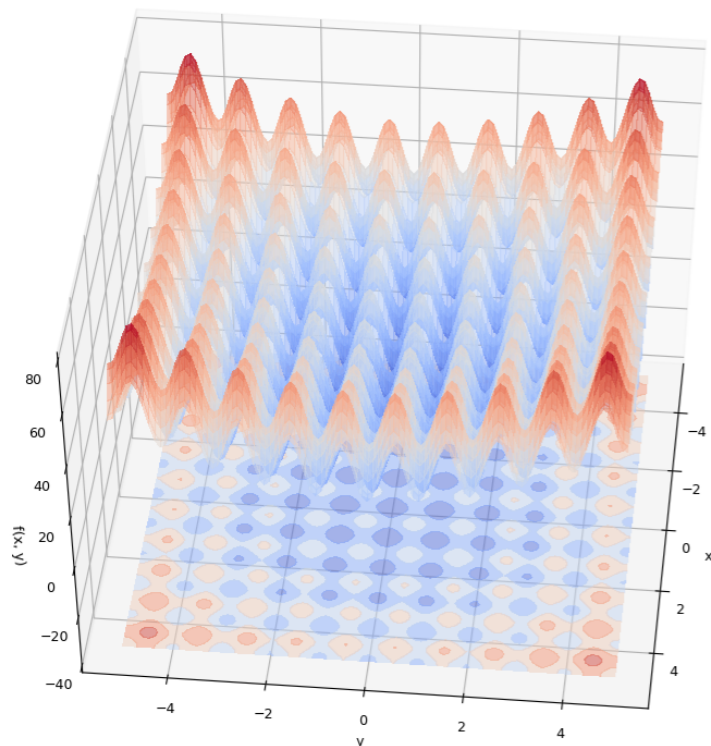
Multimodality

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.

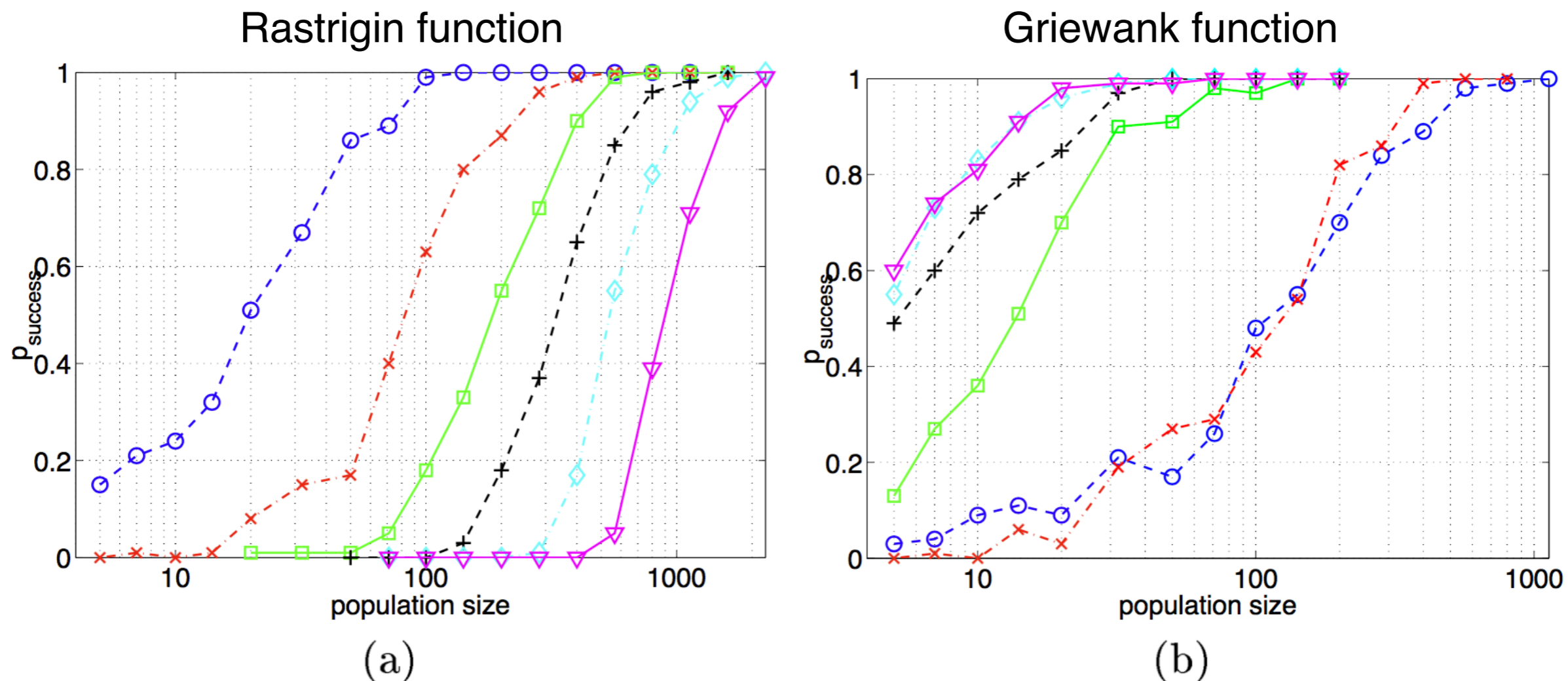


Fig. 1. Success rate to reach $f_{\text{stop}} = 10^{-10}$ versus population size for (a) Rastrigin function (b) Griewank function for dimensions $n = 2$ ('---○---'), $n = 5$ ('-·-×-·-'), $n = 10$ ('—□—'), $n = 20$ ('- - + - -'), $n = 40$ ('-·-◇-·-'), and $n = 80$ ('—▽—').

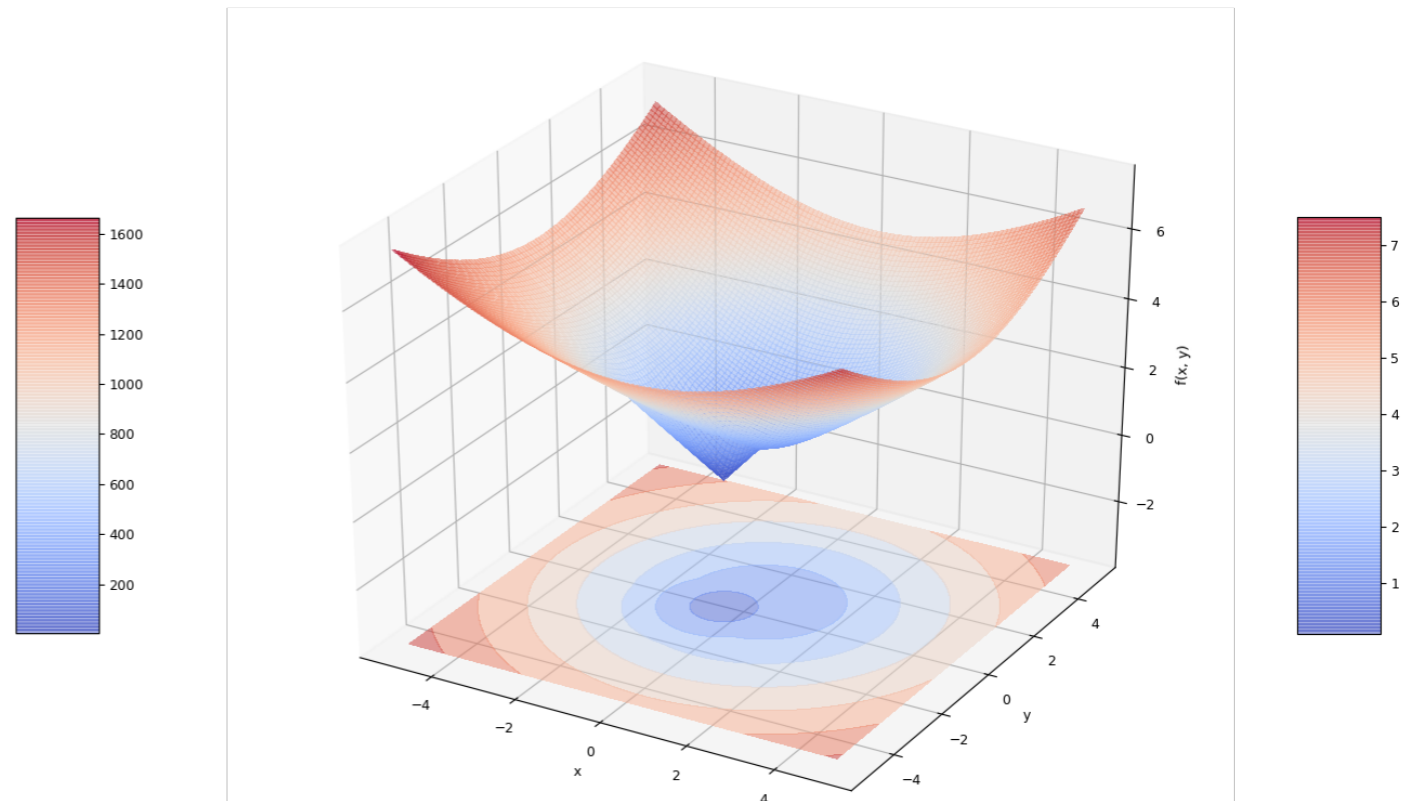
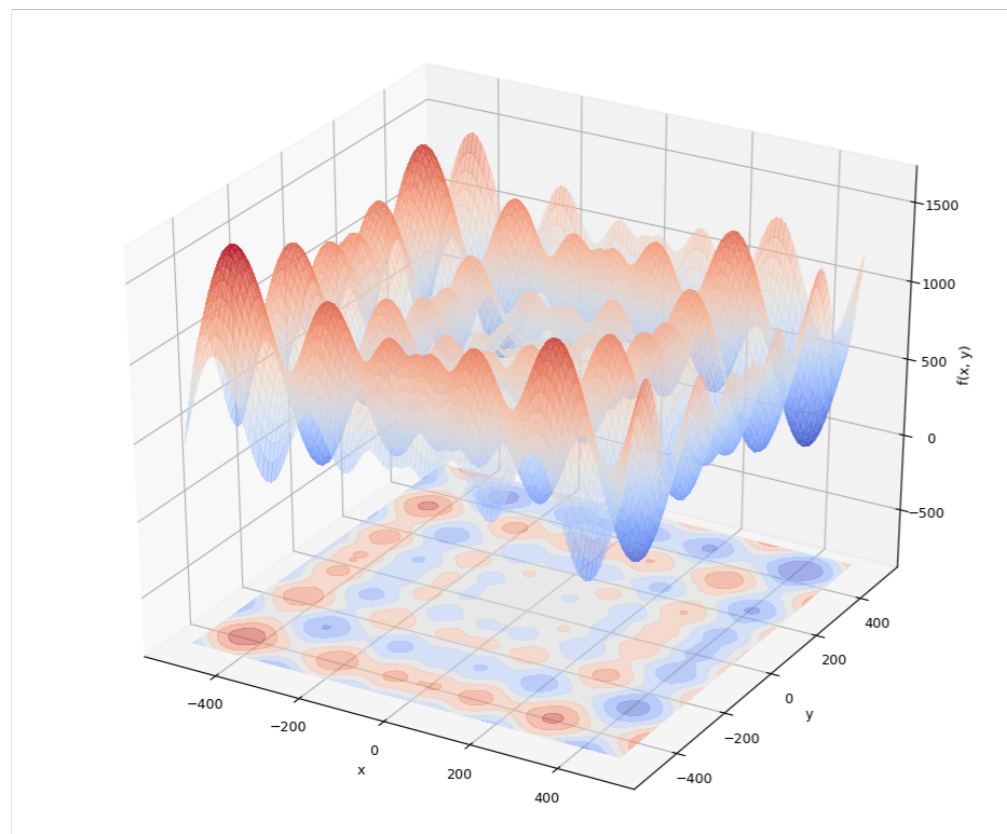
Multimodality

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 can have 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]
 - ▶ $\mathbf{C} = \mathbf{D}(\mathbf{I} + \sum_{i=1}^k \mathbf{v}_i\mathbf{v}_i^T)\mathbf{D}$. $\mathbf{v}_i \in \mathbb{R}^N$.

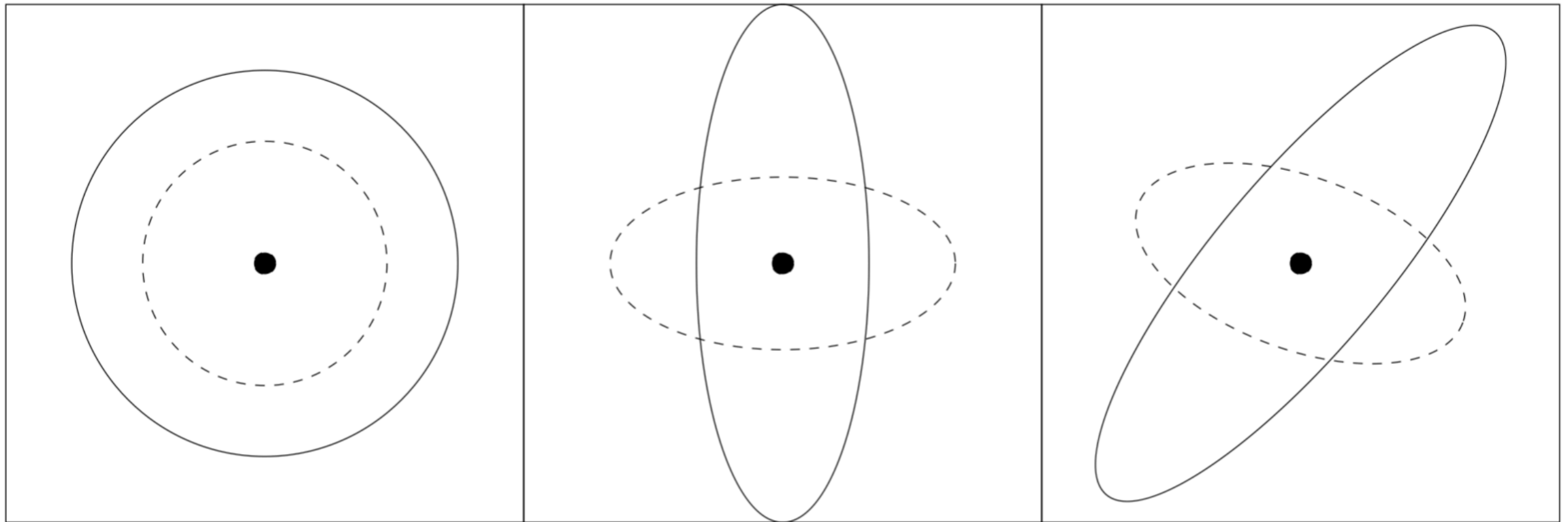
[Ros and Hansen, 2008] Ros, R. and Hansen, N. (2008). A simple modification in CMA-ES achieving linear time and space complexity. In Parallel Problem Solving from Nature - PPSN X, pages 296–305. Springer.

[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 σ

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

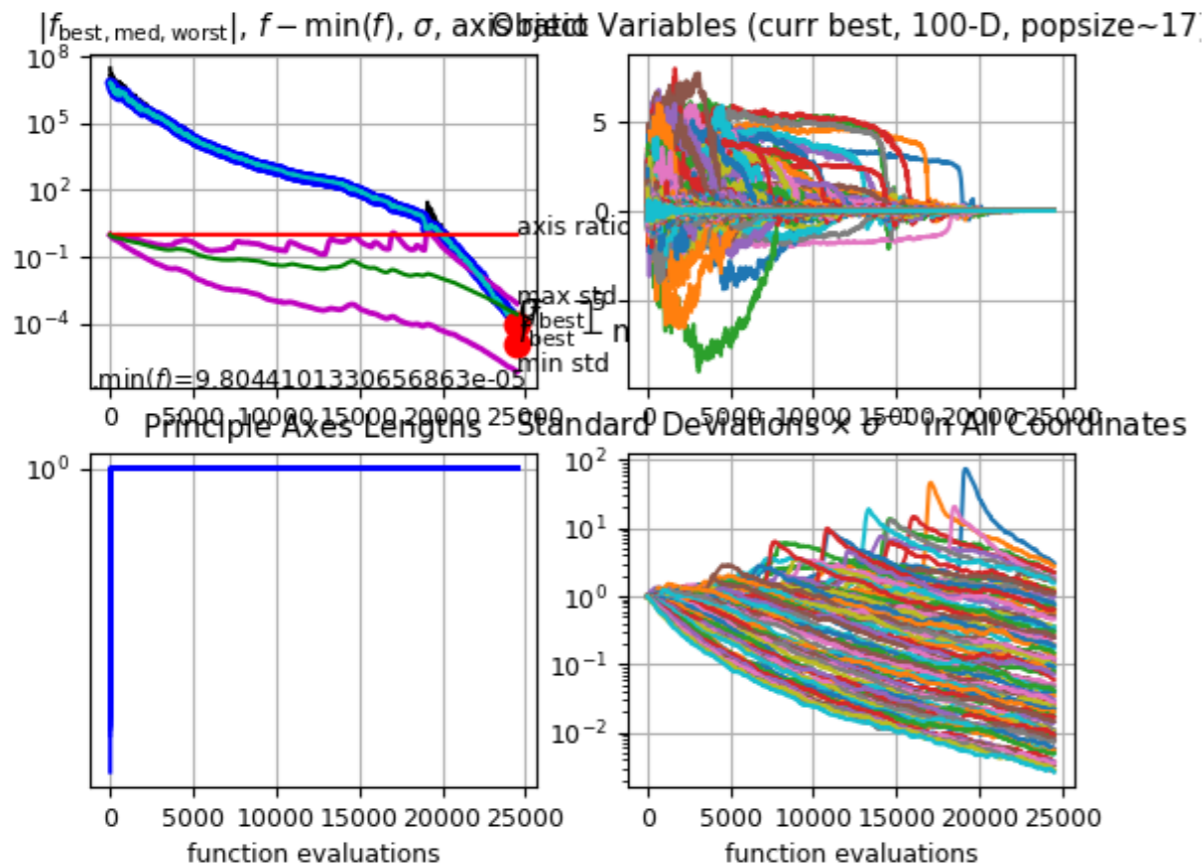
$\mathcal{N}(\mathbf{m}, \mathbf{C}) \sim \mathbf{m} + \mathbf{C}^{\frac{1}{2}} \mathcal{N}(\mathbf{0}, \mathbf{I})$
 $(n^2 + n)/2$ degrees of freedom

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

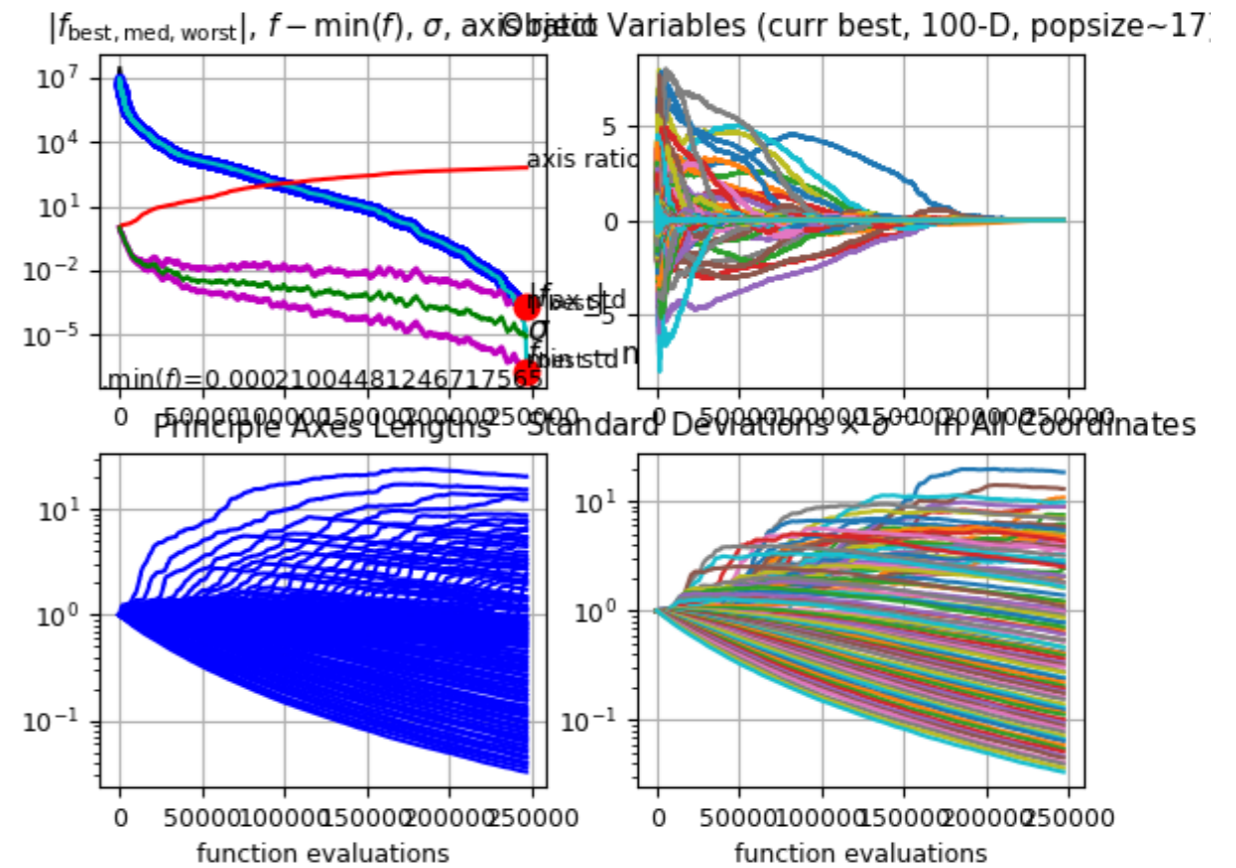
SEP
$$[\mathbf{C}_{\text{sep}}^{(t+1)}]_{k,k} = [\mathbf{C}^{(t)}]_{k,k} + c_1 \left([p_c]_k^2 - [\mathbf{C}^{(t)}]_{k,k} \right) + c_\mu \sum_{i=1}^{\mu} w_i \left([\mathbf{x}_i - \mathbf{m}^{(t)}]_k^2 - [\mathbf{C}^{(t)}]_{k,k} \right)$$

→ $(N + 2)/3$ 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

The Continuous Search Problem

Difficulties of a non-linear optimization problem are

- dimensionality and non-separability

demands to exploit problem structure, e.g. neighborhood
cave: 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/>