Foundations and Recent Advances on Natural Evolution Strategies

Tutorial @ CEC'23

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Tutorial Goals

We will explain Natural Evolution Strategies (NES)

- NES = BBO framework that uses the ***natural*** gradient to update distribution params.
- Natural gradient = gradient accounting for parameter space geometry

The goals of this tutorial are to enable the participants:

- to understand core ideas and promising variants of NES
- to know recent advances for practical challenges
- to use NES algorithms in research and/or industrial applications
- to recognize future challenges in this area

Tutorial Outline

Part 1: Introduction to NES

Part 2: Theoretical Foundations

Part 3: Recent Advances

Part 4: Practical Guide

Part 5: Conclusion

Part 1:
Introduction to NES

Black-Box Optimization on Continuous Domain

This tutorial: focus on continuous black-box optimization

Goal of black-box optimization (BBO):

$$x^* = \underset{x \in \mathcal{X}}{\operatorname{argmax}}\ f(x)$$

- X is continuous space

- Objective function is "**black-box**"
  - Not assume availability of gradient
  - We only use function evaluation value

Stochastic Relaxation for BBO [WSG+14]

- We want to optimize f(x), but the gradient wrt. x is not available
- Instead of directly finding x*, NES searches the distribution parameter θ*:

$$x^* = \underset{x \in \mathcal{X}}{\operatorname{argmax}}\ f(x)$$

Stochastic Relaxation

$$\theta^* = \underset{\theta \in \Theta}{\operatorname{argmax}}\ \mathbb{E}_{x \sim p(x;\theta)}[f(x)] =: J(\theta)$$

Gradient for Distribution Parameter [WSG+14]

- Suppose we can find $\nabla_\theta \log p(x;\theta)$
- By using the so-called 'log-likelihood trick'*:

$$\begin{aligned}\nabla_\theta J(\theta) &= \nabla_\theta \int f(x)p(x;\theta)dx \\ &= \int f(x)\nabla p(x;\theta)dx \\ &= \int f(x)\nabla \log p(x;\theta)p(x;\theta)dx \\ &= \mathbb{E}_{x\sim p(x;\theta)}[f(x)\nabla_\theta \log p(x;\theta)]\end{aligned}$$

* Interchangeability of integration and differentiation is assumed

Gradient for Distribution Parameter [WSG+14]

- Suppose we can find $\nabla_\theta \log p(x;\theta)$
- By using the so-called 'log-likelihood trick'*:

$$\nabla_\theta J(\theta) = \nabla_\theta \int f(x)p(x;\theta)dx$$

Exchange of integration and differentiation

$$= \int f(x)\nabla p(x;\theta)dx$$

$$= \int f(x)\nabla \log p(x;\theta)p(x;\theta)dx$$

$$= \mathbb{E}_{x\sim p(x;\theta)}[f(x)\nabla_\theta \log p(x;\theta)]$$

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$$= \int f(x)\nabla p(x;\theta)dx$$

$$= \int f(x)\nabla \log p(x;\theta)p(x;\theta)dx$$

$$\nabla \log p(x;\theta) = \frac{\nabla p(x;\theta)}{p(x;\theta)}$$

$$= \mathbb{E}_{x\sim p(x;\theta)}[f(x)\nabla_\theta \log p(x;\theta)]$$

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$$= \mathbb{E}_{x\sim p(x;\theta)}[f(x)\nabla_\theta \log p(x;\theta)]$$

cannot calculate analytically
⇒ appriximation

* Interchangeability of integration and differentiation is assumed

Stochastic Relaxation for BBO: Basic Algorithm

For i = 1, ...,λ: (λ is population size)

- generate solution x_i from the distribution p(x_i; θ)
- evaluate x_i on objective function f
- calculate derivative of log-likelihood on x_i

Approximate the gradient: $$\nabla_\theta J(\theta) \approx \frac{1}{\lambda} \sum_{i=1}^{\lambda} f(x_i) \nabla_\theta \log p(x_i; \theta)$$

Update the distribution parameter: $$\theta \leftarrow \theta + \eta \cdot \nabla_\theta J(\theta)$$

Multivariate Gaussian Distribution

- One can use any distribution whose derivative of log-likelihood is obtained
- Most widely used one: multivariate Gaussian distribution (MGD)
- Distribution parameters:
  - Mean vector : $m \in \mathbb{R}^d$
  - Covariance matrix: $\Sigma \in \mathbb{R}^{d \times d}$
- Density of the distribution:

$$p(x;\theta) = \frac{1}{\sqrt{(2\pi)^d \det(\Sigma)}} \cdot \exp\left(-\frac{1}{2}(x-m)^\top \Sigma^{-1}(x-m)\right)$$

Vanilla gradient for Multivariate Gaussian Distribution

- We first calculate the log-likelihood for estimating gradient:

$$\log p(x;\theta) = -\frac{d}{2}\log(2\pi) - \frac{1}{2}\log\det(\Sigma) - \frac{1}{2}(x-m)^\top \Sigma^{-1}(x-m)$$

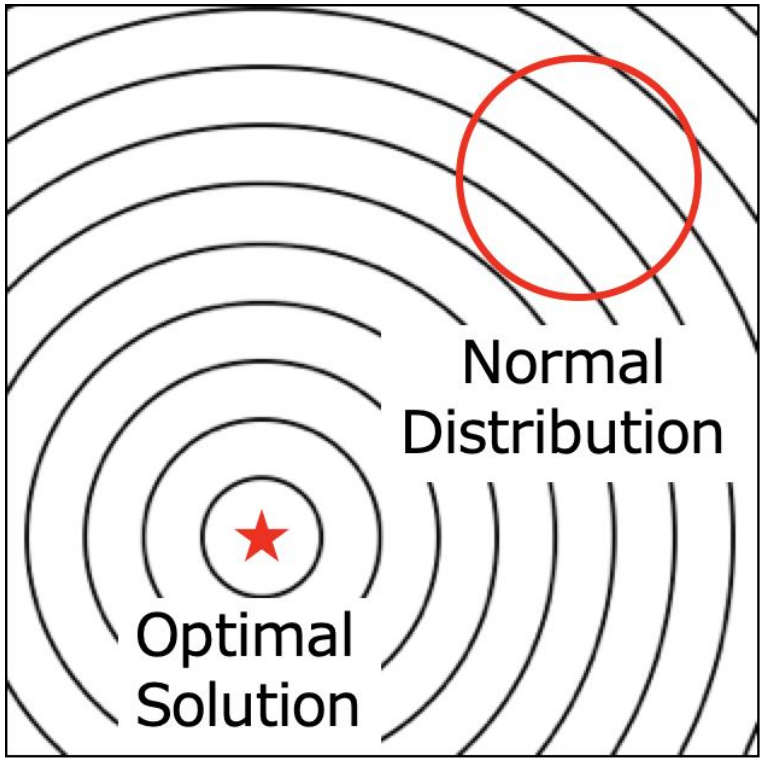
- (Vanilla) gradient for the log-likelihood:

$$\nabla_m \log p(x;\theta) = \Sigma^{-1}(x-m)$$

$$\nabla_\Sigma \log p(x;\theta) = \frac{1}{2}\Sigma^{-1}(x-m)(x-m)^\top - \frac{1}{2}\Sigma^{-1}$$

Illustrative Behavior with Multivariate Gaussian (MGD)

1. Generates solutions from the MGD
2. Evaluates solutions and estimates gradient
3. Updates the parameters
4. Repeats until the criterion is met



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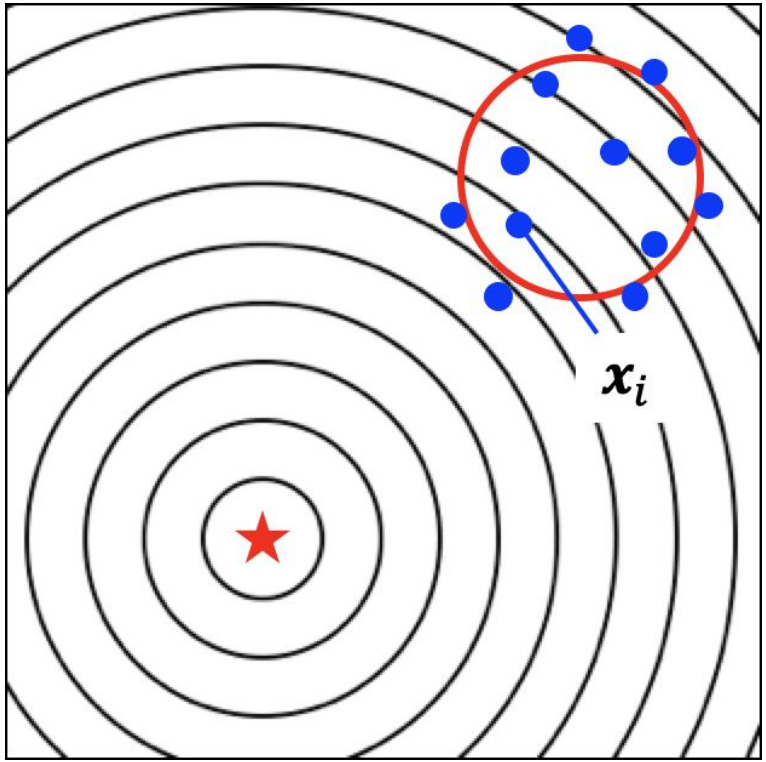

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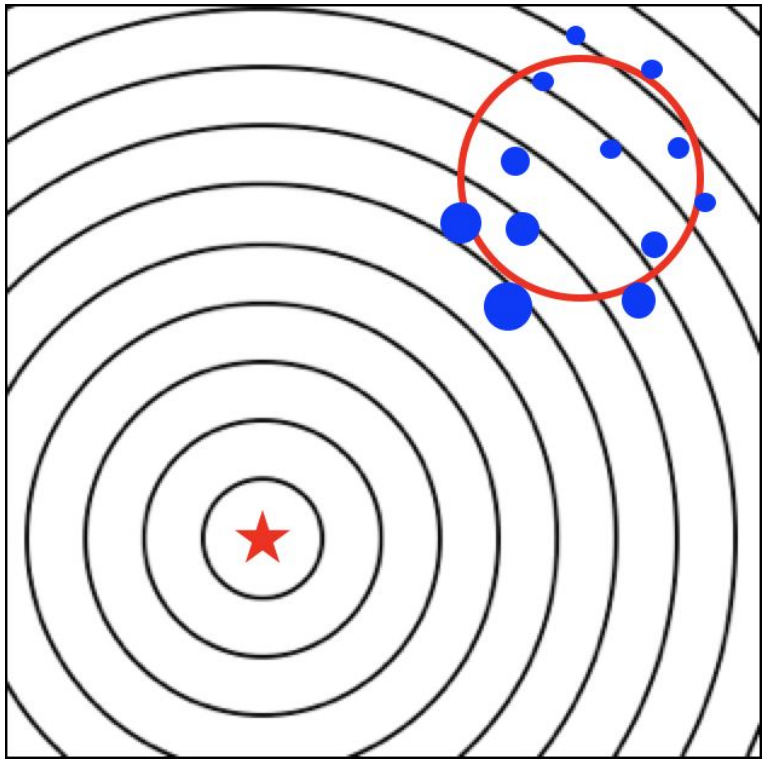

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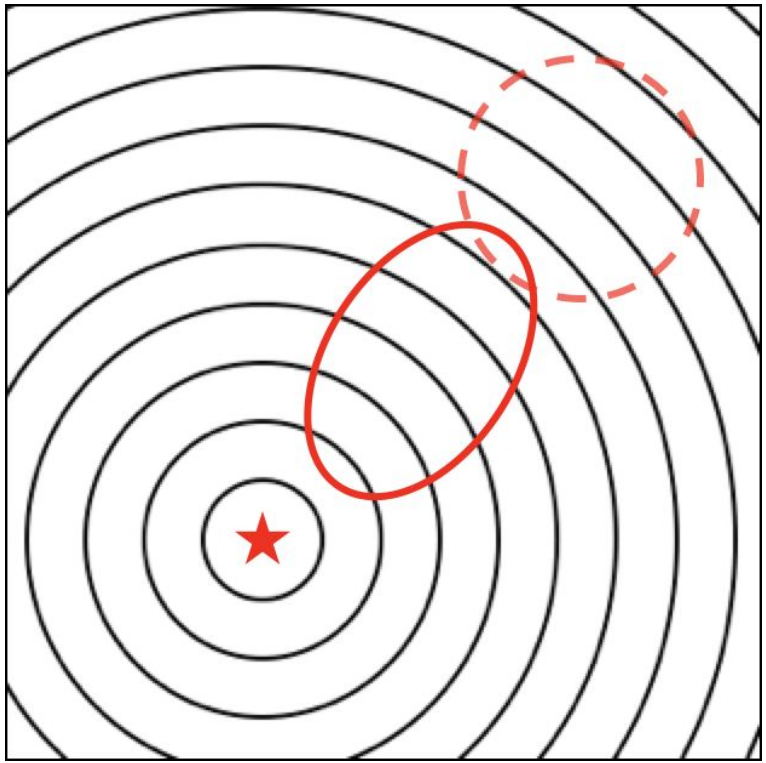

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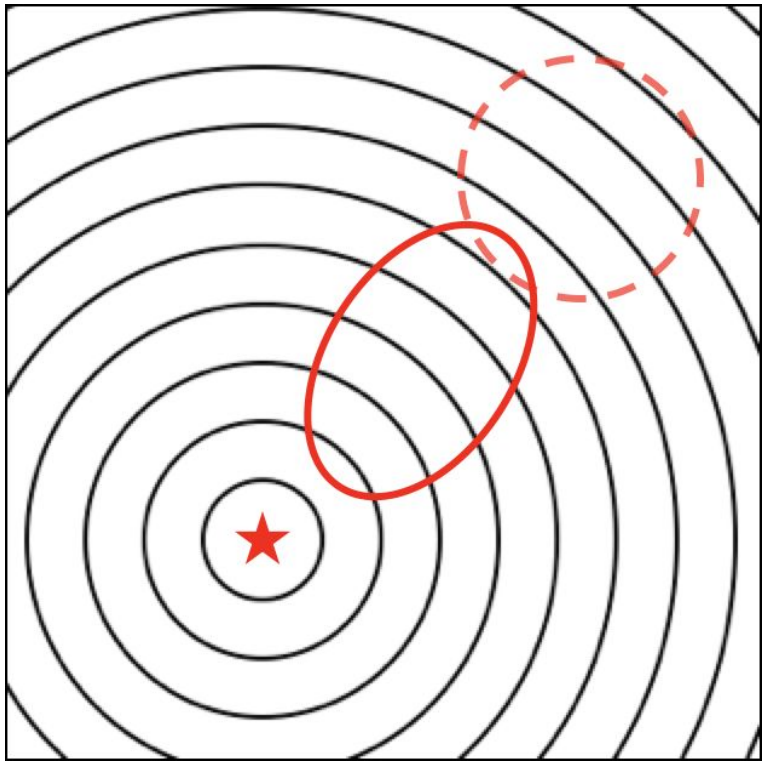


Critical Issue of Vanilla Gradient

- Rethinking vanilla gradient:
  - The vanilla gradient can be characterized as the steepest ascent within the small **Euclidean distance** in the parameter space

$$\Delta_\theta^* = \lim_{\epsilon \to 0} \underset{\|\Delta_\theta\| = \epsilon}{\operatorname{argmax}} J(\theta + \Delta_\theta)$$

  - The update depends on the choice of parameterization
- Actually, the vanilla gradient can show unstable and unsatisfying performance*

More natural distance (divergence) in probability distribution space is needed

* this depends on the choice of parameterization.
In some cases, vanilla gradient and natural gradient coincides (*local coordinate*)

Natural Gradient: Motivation

- Natural gradient [AD98,Ama98]:
  - considering parameter geometry in probability space
- Natural gradient can be formalized as the solution of constrained optimization:

$$\max_{\Delta_\theta} J(\theta + \Delta_\theta) \approx J(\theta) + \nabla_\theta J(\theta)^\top \Delta_\theta,$$
$$\text{s.t.} \quad D_{\mathrm{KL}}(p_{\theta+\Delta_\theta} || p_\theta) = \epsilon$$

  - point: Kullback-Leibler (KL) divergence rather than Euclidean distance
    - KL div. is commonly used to measure the diff. of distributions

Relation between KL divergence and FIM

- Fisher information matrix (FIM) is the curvature of the KL divergence:

$$D_{\mathrm{KL}}(p_{\theta+\Delta_\theta}||p_\theta) = \frac{1}{2}\Delta_\theta^\top F \Delta_\theta + \mathcal{O}(\|\Delta_\theta\|^3) \ (\Delta_\theta \to 0)$$

where *F* is the FIM given θ:

$$F = \mathbb{E}_{x\sim p(x;\theta)}[\nabla_\theta \log p(x;\theta) \nabla_\theta \log p(x;\theta)^\top]$$

- Now, we rewrite the constrained optimization problem using FIM

Form of Natural Gradient [WSG+14]

- We want to solve the following constrained optimization problem:

$$\max_{\Delta_\theta} J(\theta) + \nabla_\theta J(\theta)^\top \Delta_\theta \quad \text{s.t.} \quad \frac{1}{2}\Delta_\theta^\top F \Delta_\theta = \epsilon$$

- Using Lagrangian multiplier,

$$\mathcal{L}(\theta, \Delta_\theta, c) = J(\theta) + \nabla_\theta J(\theta)^\top \Delta_\theta - c\left(\frac{1}{2}\Delta_\theta^\top F \Delta_\theta - \epsilon\right)$$

$$\nabla_{\Delta_\theta}\mathcal{L}(\theta, \Delta_\theta, c) = \nabla_\theta J(\theta) - cF\Delta_\theta$$

$$\therefore F\Delta_\theta^* = c^{-1}\nabla_\theta J(\theta)$$

- If F is invertible, the natural gradient $\tilde{\nabla}_\theta J(\theta)$ is given by Δ_θ^*; thus, (ingnoring const.,)

$$\tilde{\nabla}_\theta J(\theta) = F^{-1}\nabla_\theta J(\theta)$$

Fitness Shaping [GSY+10]

- Fitness shaping: replace function values with *weights* $(w_1 \geq \cdots \geq w_\lambda)$

$$F^{-1}\nabla_\theta J(\theta) \approx \frac{1}{\lambda}\sum_{i=1}^{\lambda} f(x_i) F^{-1}\nabla_\theta \log p(x_i;\theta)$$

Fitness Shaping

$$\sum_{i=1}^{\lambda} w_i F^{-1}\nabla_\theta \log p(x_{i:\lambda};\theta)$$

$x_{i:\lambda}$: *i*-th best solution

NES uses only ranking rather than function value itself

- It makes NES invariant under monotonically increasing transformation of *f*
- Moreover, effect of speeding up is theoretically suggested [Bey14]

FIM for Multivariate Gaussian Distribution

In natural gradient method, calculating the FIM inverse is needed

For MGD, FIM (inverse) can be calculated as follows [ANOK10]:

$$F = \begin{bmatrix} \Sigma^{-1} & O \\ O & \frac{1}{2}\Sigma^{-1} \otimes \Sigma^{-1} \end{bmatrix} \text{ and } F^{-1} = \begin{bmatrix} \Sigma & O \\ O & 2\Sigma \otimes \Sigma \end{bmatrix}$$

$\otimes$: Kronecker product

By combining FIM inverse and the vanilla gradient (and fitness shaping),

$$m^{(t+1)} = m^{(t)} + \eta_m \sum_{i=1}^{\lambda} w_i (x_{i:\lambda} - m^{(t)})$$

$$\Sigma^{(t+1)} = \Sigma^{(t)} + \eta_\Sigma \sum_{i=1}^{\lambda} w_i ((x_{i:\lambda} - m^{(t)})(x_{i:\lambda} - m^{(t)})^\top - \Sigma^{(t)})$$

Another: choose a coordinate system such that the FIM becomes Identity matrix *I*

'local' coordinate system

Exponential Parameterization [GSY+10]

- Caution: need to ensure that cov. remains positive definite
  - However, the updated cov. may not be positive definite matrix

- Elegant fix: using exponential map under (natural) *local coordinates*

Let $\Sigma = AA^\top$

$$A^{(t+1)} = A^{(t)} \cdot \exp\left(\frac{\eta_\Sigma}{2} \sum_{i=1}^{\lambda} w_i (z_{i:\lambda} z_{i:\lambda}^\top - I)\right)$$

where $z_{i:\lambda} = A^{(t)^{-1}}(x_{i:\lambda} - m^{(t)})$

We can always obtain a feasible covariance matrix

Decomposing Covariance into Step-Size and Shape

- We decompose the A as $A = \sigma B$
  - step-size: $\sigma \in \mathbb{R}_+$
  - normalization transformation matrix: $B \in \mathbb{R}^{d \times d}$
- We can update each parameter separately:

$$\sigma^{(t+1)} = \sigma^{(t)} \cdot \exp\left(\frac{\eta_\sigma}{2} \cdot \mathrm{Tr}(G_M)/d\right)$$

$$B^{(t+1)} = B^{(t)} \cdot \exp\left(\frac{\eta_B}{2} \cdot \left(G_M - \frac{\mathrm{Tr}(G_M)}{d} I\right)\right)$$

where $G_M = \sum_{i=1}^{\lambda} w_i (z_{i:\lambda} z_{i:\lambda} - I)$

- $\det(B) = 1$ ⇒ We can have a clear interpretation:
  - σ controls volume (step-size), B controls shape

xNES (Exponential NES) [GSY+10]

Step 1: Sampling and Evaluation (i=1,...,λ)

$$z_i \sim \mathcal{N}(0, I), \quad x_i = m^{(t)} + \sigma^{(t)} B^{(t)} z_i$$

Step 2: Estimating Natural Gradient with Fitness Shaping

$$G_\delta = \sum_{i=1}^{\lambda} w_i z_{i:\lambda}, \quad G_M = \sum_{i=1}^{\lambda} w_i (z_{i:\lambda} z_{i:\lambda} - I)$$

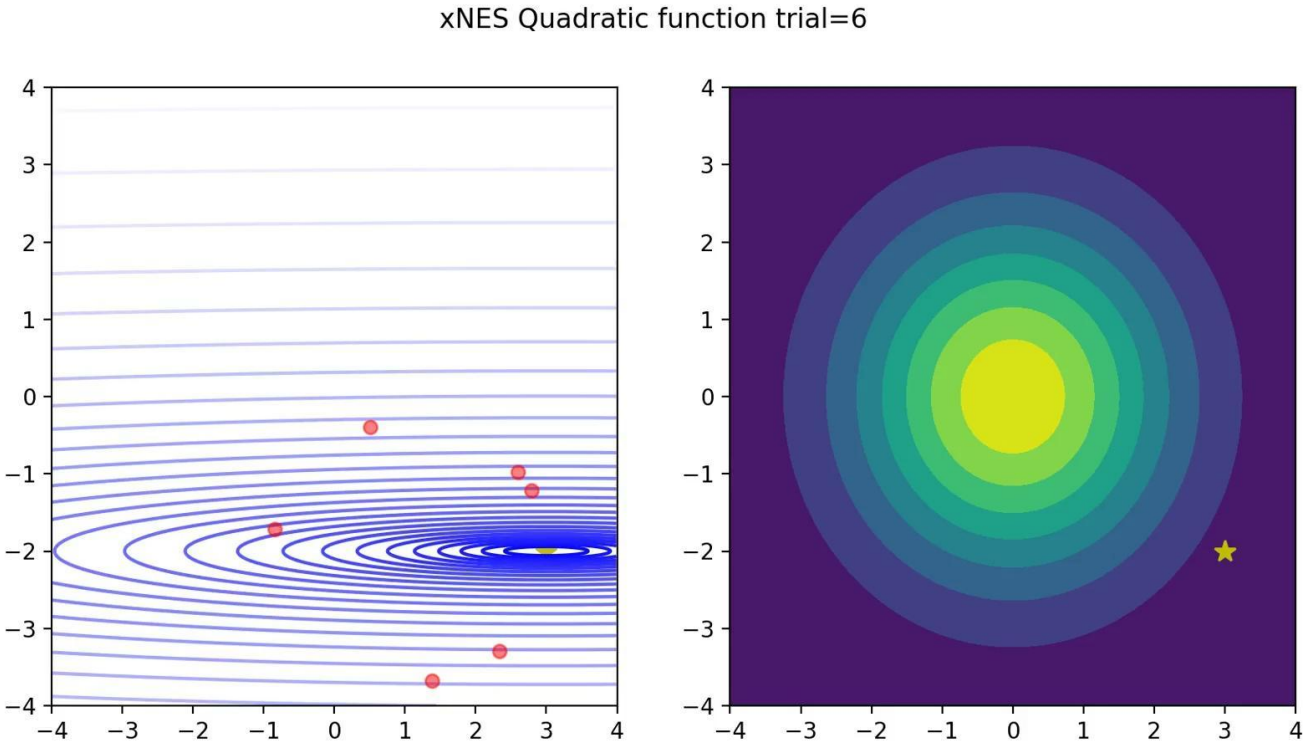
$$G_\sigma = \mathrm{Tr}(G_M)/d, \quad G_B = G_M - G_\sigma \cdot I$$

Step 3: Updating of Distribution Parameters

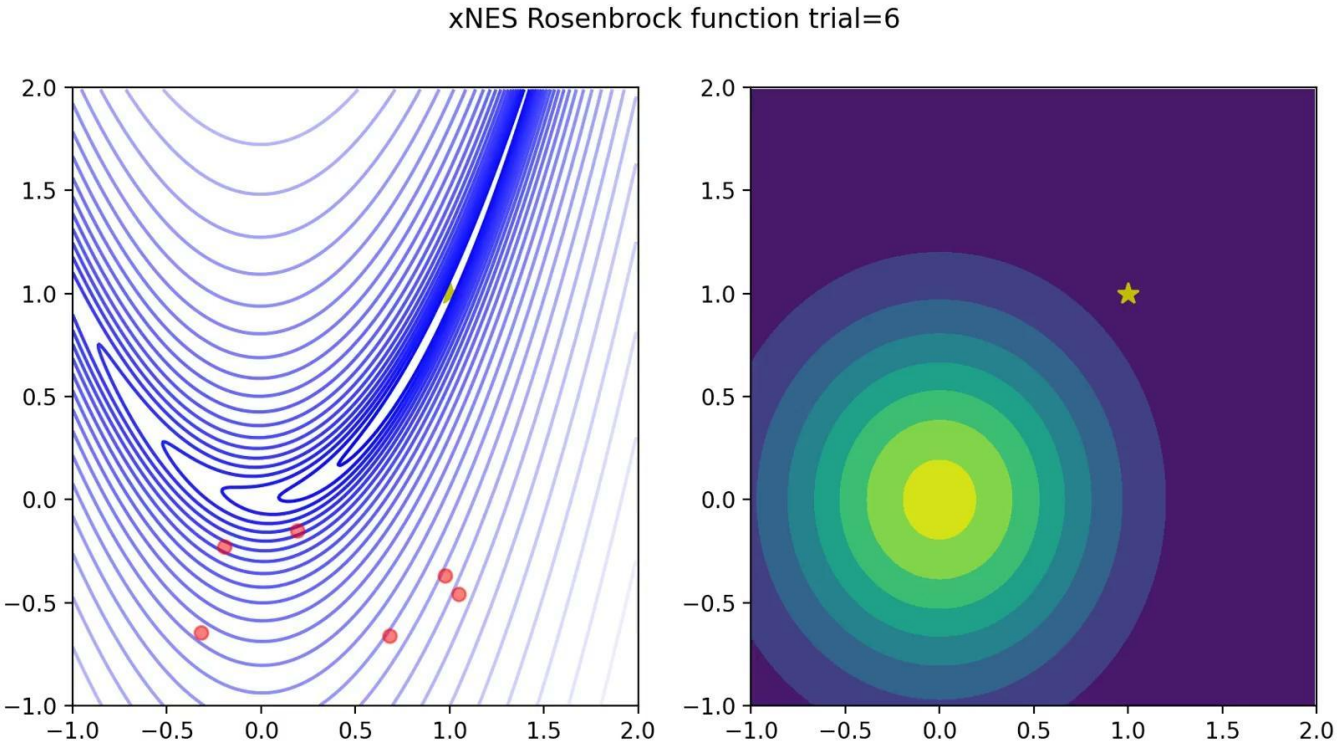
$$m^{(t+1)} = m^{(t)} + \eta_m \sigma^{(t)} B^{(t)} G_\delta, \quad \sigma^{(t+1)} = \sigma^{(t)} \cdot \exp(\eta_\delta / 2 \cdot G_\delta),$$

$$B^{(t+1)} = B^{(t)} \cdot \exp(\eta_B / 2 \cdot G_B)$$

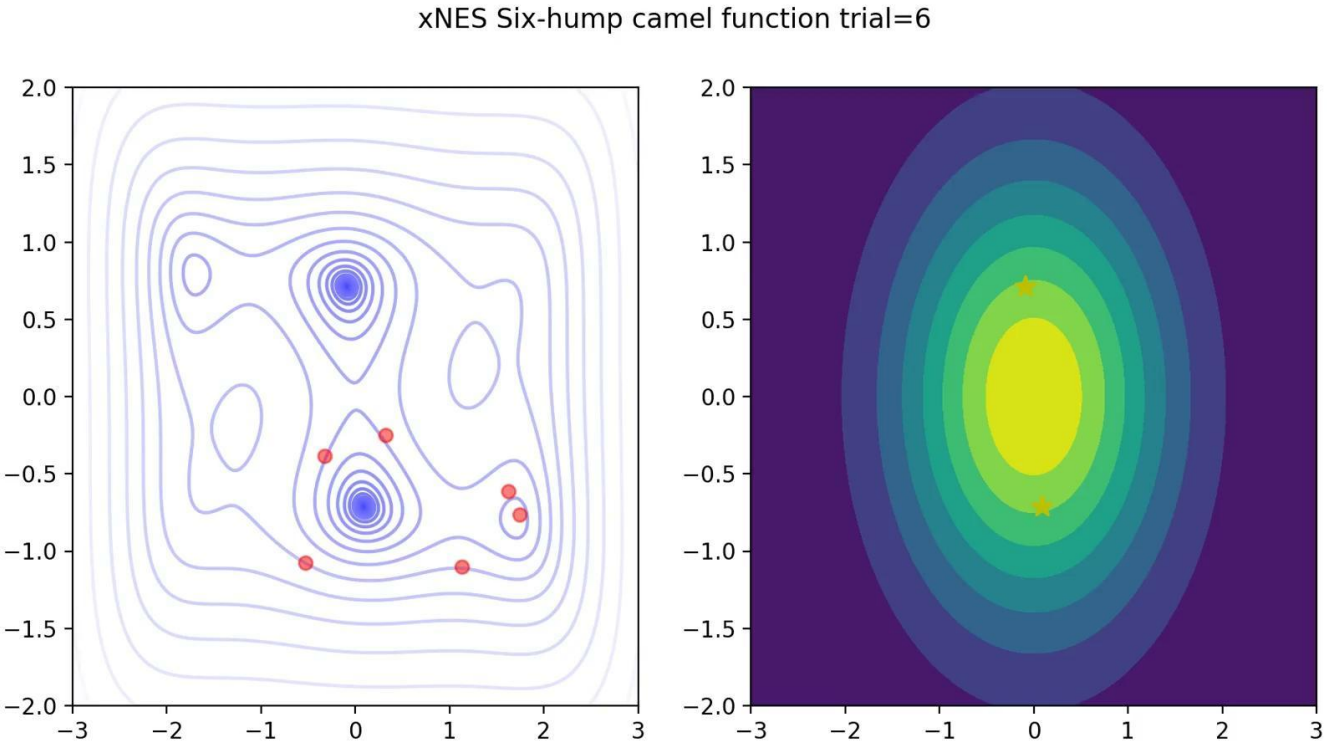
xNES Behavior: Quadratic function



xNES Behavior: Rosenbrock function



xNES Behavior: Six-hamp camel function



Comparison to Estimation of Distribution Algorithms

Both: iteratively

- sample points from the distribution and evaluate them
- update the distribution by using the evaluated points

Differences

- EDA: maximum likelihood estimation to fit distribution of sampled points
- NES: natural gradient method for expected function value

- While design principles are different, update equations sometimes coincide

Part 2:
Theoretical Foundations

Rethinking NES in view of Natural Gradient Method

- Derivation of NES started with the natural gradient for expected objective:

$$J(\theta) = \mathbb{E}_{x \sim p(x;\theta)}[f(x)]$$

- With fitness shaping, it no longer makes sense as the original natural gradient

$$f(x_{1:\lambda})/\lambda, \cdots, f(x_{\lambda:\lambda})/\lambda \Longrightarrow w_1, \cdots, w_\lambda$$

  - **Can NES no longer be considered a natural gradient method?**

- NES estimates the natural gradient for another objective
  - This is formalized by **Information Geometric Optimization**

Information Geometric Optimization [OAAH17]

- Information Geometric Optimization (IGO):
  - stochastic optimization framework that uses probability distribution
  - IGO formalizes several popular BBO methods
    - e.g., NES, rank-μ CMA-ES, PBIL, cGA
- From IGO perspective, we can derive NES as a natural gradient method

IGO: Formulation

- IGO objective: $J_{\theta^{(t)}}(\theta) = \mathbb{E}_{x \sim p(x;\theta)}[W^f_{\theta^{(t)}}(x)]$

Objective function depends on the current parameter $\theta^{(t)}$

- Quantile function q(x) for weight*:

$$q^{\geq}_{\theta^{(t)}}(x) = \Pr_{y \sim p(y;\theta^{(t)})}[f(y) \geq f(x)]$$

0 for the best
1 for the worst

- With a non-increasing function $w : [0,1] \to \mathbb{R}$, weight function is defined:

$$W^f_{\theta^{(t)}}(x) = w(q^{\geq}_{\theta^{(t)}}(x))$$

* Assuming Lebesgue measure of level-set of objective is 0, which is common in continuous optimization

IGO: Natural Gradient

- Natural gradient of IGO: Let us denote $\tilde{\nabla}_\theta \log p(x;\theta) = F^{-1}\nabla_\theta \log p(x;\theta)$

$$\tilde{\nabla}_\theta J_{\theta^{(t)}}(\theta) = \mathbb{E}_{x\sim p(x;\theta)}[W^f_{\theta^{(t)}}(x)\tilde{\nabla}_\theta \log p(x;\theta)]$$

$$\approx \frac{1}{\lambda}\sum_{i=1}^{\lambda} W^f_{\theta^{(t)}}(x)\tilde{\nabla}_\theta \log p(x;\theta)$$

- We also need to estimate the weights $W^f_{\theta^{(t)}}(x) = w(q^{\geq}_{\theta^{(t)}}(x))$

  q(x) is the prob. of sampling a solution that is better than x =>

$$W^f_{\theta^{(t)}}(x) \approx w((\mathrm{rk}(x) - 1/2)/\lambda)$$ rk() is the ranking of x wrt. f

Other Distributions

- IGO principle can be applied to other distributions
- For many distributions belonging to the exponential family, (inverse of) FIM can be computed in a closed form (i.e. without estimating FIM)
  - Bernoulli distribution (PBIL, cGA)
  - MGD (xNES, rank-μ update CMA-ES)
  - Categorical distribution
- There are cases where estimating FIM is necessary (e.g. restricted Boltzmann machines; RBM)

xNES is an Instance of IGO

- Let $\Sigma = AA^\top$
- When parameterizing the Gaussian distribution by

$$\theta = (m, R), \quad R = \ln(A^{-1}\Sigma(A^\top)^{-1})$$

R is a kind of 'local' coordinate

- IGO Update:

$$m^{(t+1)} = m^{(t)} + \eta_m \sum_{i=1}^{\lambda} w_i (x_{i:\lambda} - m^{(t)})$$

$$R^{(t+1)} = \eta_\Sigma \sum_{i=1}^{\lambda} w_i (z_{i:\lambda} z_{i:\lambda}^\top - I)$$

- By transforming it to cov. in 'global' coordinate, i.e., $\Sigma^{(t+1)} = A^{(t)} \exp(R^{(t+1)}) A^{(t)\top}$ we obtain the same update as xNES

CMA-ES [HMK03,Han16]: Quick Overview

- one of the most powerful methods for BBO
- also uses MGD parameterized by N(m, σ^2 C)
  - m: d-dim mean vector, σ: (scalar) step-size, C: pos. def. matrix
- Update for each parameter:
  - m: **weighted recombination (natural gradient update)**
  - σ: specific method such as cumulative step-size adaptation
  - C: **rank-μ update (natural gradient update)** & rank-one update
- CMA-ES = **natural gradient update** + step-size adaptation + rank-one update

the relationship with the natural gradient was discovered after the development of CMA-ES [ANOK10]

Rank-μ update CMA-ES = natural gradient update
(combination of weighted recombination & rank-μ update)

Rank-μ Update CMA-ES is an Instance of IGO

- Natural gradient Update with MGD:

$$m^{(t+1)} = m^{(t)} + \eta_m \sum_{i=1}^{\lambda} w_i (x_{i:\lambda} - m^{(t)})$$

$$\Sigma^{(t+1)} = \Sigma^{(t)} + \eta_\Sigma \sum_{i=1}^{\lambda} w_i ((x_{i:\lambda} - m^{(t)})(x_{i:\lambda} - m^{(t)})^\top - \Sigma^{(t)})$$

- This precisely corresponds to the rank-μ update CMA-ES
  - The natural gradient plays a crucial role in CMA-ES

Cautions regarding Natural Gradient Update

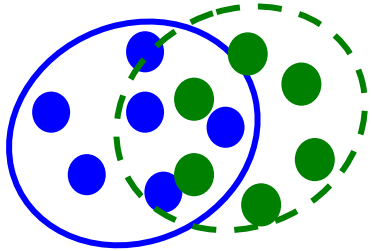
- The natural gradient does **not** explain everything in the efficiency
- The step-size adaptation & rank-one update in the CMA-ES are **not** explained from natural gradient perspective, but they drastically improve performance
  - evolution path (i.e. a sum of consecutive) is quite effective, especially for small population size setting
- Recognizing the limitations of the natural gradient method contributes to the development of practically useful algorithms

Part 3:
Recent Advances

Improving Natural Gradient Estimation by Sample Reuse

- Usually, IGO algorithms *discard* solutions after evaluation once
  - This is a waste, so can't we reuse such old samples in some way?
- IGO includes two components that should be estimated
  - Quantile (prob. of sampling a better point than x)
  - Natural gradient
- For this purpose, **importance sampling** has been utilized [SAOO15]

current samples
& distribution



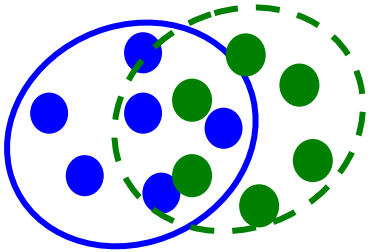
old samples
& distributions

Estimation Target and Monte-Carlo Estimation

- Estimation target: $\mathbb{E}_{x\sim p(x;\theta^{(t)})}[g(x)]$
  - for quantile $q^{\geq}_{\theta^{(t)}}(x_i^{(t-k)})$: $g(x) = \mathbb{1}\{f(x) > f(x_i^{(t-k)})\} \quad (\because \mathbb{E}[\mathbb{1}\{\cdot\}] = \Pr[\cdot])$
  - for natural gradient : $g(x) = W^f_{\theta^{(t)}}(x)\tilde{\nabla}_\theta \log p(x;\theta^{(t)})$

current samples & distribution

old samples & distributions



- (Naive) Monte-Carlo estimation:

$$\frac{1}{\lambda}\sum_{i=1}^{\lambda} g(x_i^{(t)})$$

  - This uses only current samples, and **discards old samples**

Sample Reuse via Importance Sampling [SAOO15]

- Importance sampling: utilize obs. in previous *K* iterations

current distribution

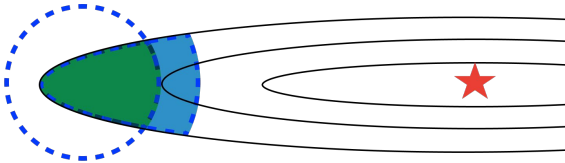
$$\frac{1}{\lambda(K+1)} \sum_{k=0}^{K} \sum_{i=1}^{\lambda} g(x_i^{(t-k)}) \frac{p(x_i^k; \theta^{(t)})}{p(x_i^k; \theta^{(t-k)})}$$

old distributions

- Assign large values to samples that seem to be drawn from the p(θ^t)
  - old samples that are ***similar*** to current => ***utilized***
  - old samples that are ***far*** to current => ***ignored***
- More sophisticated estimator was also used in [SAOO15]

Performance Issues of xNES

- Performance of xNES degrades on ill-conditioned problems
- Why?
  - More promising regions are located inside the distribution
  - As a result, step-size tends to be shrinked
- This is reasonable considering the improvement of the function value in **one step**



- But our ultimate goal is to improve the quality of the solution obtained by repeating this process, not necessarily the result in a single step

Practical Improvements for xNES

- To address the inefficiency, several improvements have been proposed:

- **Distance weight** [FNKO11]:
  - Modifying weight function to speed-up moving and enlarging distribution in the direction of promising regions
- **Emphasis on distribution expansion** [NSFO21]:
  - Faster adaptation of the distribution by emphasizing the enlargement in the direction in which it occurs

How to Design Weight Function?

- Weights are often used in NES and CMA-ES:
  - For the upper solution, $w_i \propto \log\left(\frac{\lambda}{2}+1\right) - \log(i)$
  - For the lower solution, values such as 0 or -1/λ are used
- Quality gain analysis [Arn05,AAH20]:
  - analyze expected improvement of function value at one step
  - optimal weight is similar to the above weight* $\Sigma = \sigma^2 I$
    - **Note:** the optimal weight is derived for **isotropic** Gaussian distribution
    - Not clear whether the weight is good for **'general'** Gaussian

* the result is obtained on (infinite dimensional) sphere [Arn05] and convex quadratic [AAH20] functions

DX-NES: Distance Weight [FNKO11]

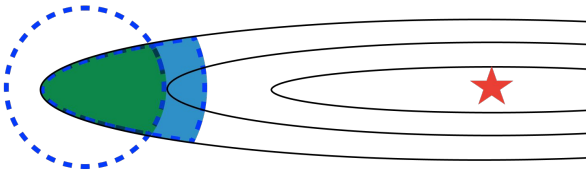
- New weighting strategy for 'general' Gaussian distribution
- **Core idea**: Moving mean vector and/or enlarging distribution in the direction of outer promising distribution

$$w_i^{\mathrm{dist}} \propto \hat{w}_i \exp(\alpha \| A^{-1}(x - m) \|)$$

① Mahalanobis distance from mean

$$\hat{w}_i = \max\left(0, \log\left(\frac{\lambda}{2} + 1\right) - \log(i)\right)$$

② assign 0 for bad solutions by 'max(0,・)' operation



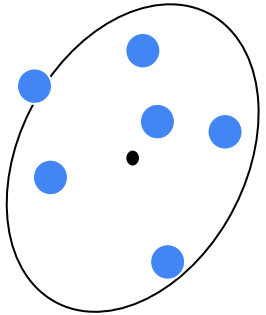
Give larger weight to solutions generated in the outer promising region (**blue** region)

Mirrored sampling

Naive Sampling

- All λ samples are generated i.i.d (i=1,...,λ)

$$z_i \sim \mathcal{N}(0, I), \quad x_i = m + \sigma B z_i$$

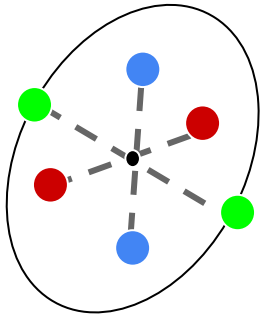


Mirrored Sampling

- Generates pairs of solutions symmetrically with respect to the mean vector (i=1,...,λ/2)

$$z_{2i-1} \sim \mathcal{N}(0, I), \; z_{2i} = -z_{2i-1}$$

$$x_{2i-1} = m + \sigma B z_{2i-1}, \; x_{2i} = m + \sigma B z_{2i}$$



Additional Discussions on Mirrored Sampling

- Empirical mean of samples matches the mean vector
  - may enable accurately estimating natural gradient wrt mean
    - DX-NES(-IC) shows superior performance in multimodal problems
  - more detailed investigation is interesting work

- Note: direct application for CMA-ES is not straightforward
  - causes bias for step-size adaptation [ABH11]
  - debiasing (e.g. by modifying strategy parameters [GK20]) is needed

Emphasizing Expansion [NSFO21]

- Key observation: Shrink is typical, but expansion is relatively rare
  - To fully utilize the information of expansion, we emphasize it!
- We quantify the amount of change in each direction of distribution

  Second moment change (e_i: eigenvector, i=1,..,d):

$$\tau_i = \frac{e_i^\top (B^{(t+1)} B^{(t+1)\top} - B^{(t)} B^{(t)\top}) e_i}{e_i^\top B^{(t)} B^{(t)\top} e_i}$$

$\tau_i > 0$ => distribution has been **expanded** in the direction of e_i

Emphasizing Expansion [NSFO21] (2)

- Expansion matrix Q: (γ is hyperparameter)

$$Q := \gamma \sum_{i=1}^{d} \mathbb{1}\{\tau_i > 0\} e_i e_i^\top + I$$

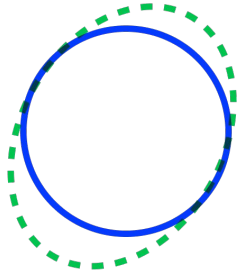
- Emphasizing expansion is performed:

$$B^{(t+1)} \leftarrow Q B^{(t+1)} / \sqrt[d]{\det(Q)}$$

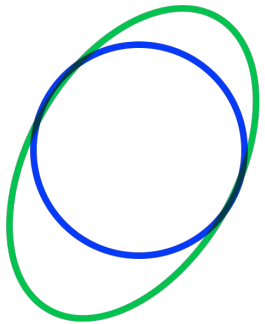
$$\sigma^{(t+1)} \leftarrow \sigma^{(t+1)} \cdot \sqrt[d]{\det(Q)}$$

To keep det(B)=1, normalization is performed

(blue) before cov.
(green) after cov.



Emphasizing Expansion



for High-Dimensional Problems

- The complexity:
  - time complexity*: $\mathcal{O}(d^3 + \lambda d^2)$ (decomposition, update cov.)
  - space complexity: $\mathcal{O}(d^2 + \lambda d)$ (matrix, population)
  - difficult to apply it for high-dimensional (e.g. 1000) problems
- Main reason of this complexity:
  - # of params. (i.e. degree of freedom) of covariance is $\mathcal{O}(d^2)$
- Basic policy: reducing # of params. of covariance (i.e. restricting the representation of covariance)

* This complexity is reduced to O(λd^2) if we decompose covariance at every O(d/λ) iteration

Pros. and Cons. of Restricted Representation

- Advantage:
  - reducing (time and space) complexity
  - making learning efficient
    - according to # params. O(d^2), learning rate is set to O(1/d^2)
    - reduction of # params. enables to set higher learning rate
- Disadvantage:
  - variable dependencies cannot be captured if restriction is not sufficient
    - optimization can fail or be inefficient on problems with strong variable dependencies

Use of Diagonal Covariance Matrix [RH08]

- Simple and effective form of covariance: Diagonal representation

$$\Sigma = D$$ (D is diagonal matrix)

- Natural gradient corresponds to extracting the diagonal components of the natural gradient in the case of full covariance matrix
  - This update corresponds to rank-μ update of *Sep-CMA** scalable variant
- Efficient for ill-conditioned problems
- **Limitation**: variable dependencies are completely ignored in cov.

* In Sep-CMA, Σ = σ^2 D is used because step-size adaptation is performed

VD-CMA [AAH14]

- VD-CMA represents the covariance matrix using 2d parameters:

$$\Sigma = \sigma^2 D(I + vv^\top)D$$

d-dim vector diagonal matrix

- Thanks to vector v, *VD-CMA partially addresses variable dependencies*
- v and D are updated by natural grad.* (+ rank-one update and step-size adapt.):

$$v^{(t+1)} = v^{(t)} + \eta_v \tilde{\nabla}_v J_{\theta^{(t)}}(\theta)$$

$$D^{(t+1)} = D^{(t)} + \eta_D \tilde{\nabla}_D J_{\theta^{(t)}}(\theta)$$

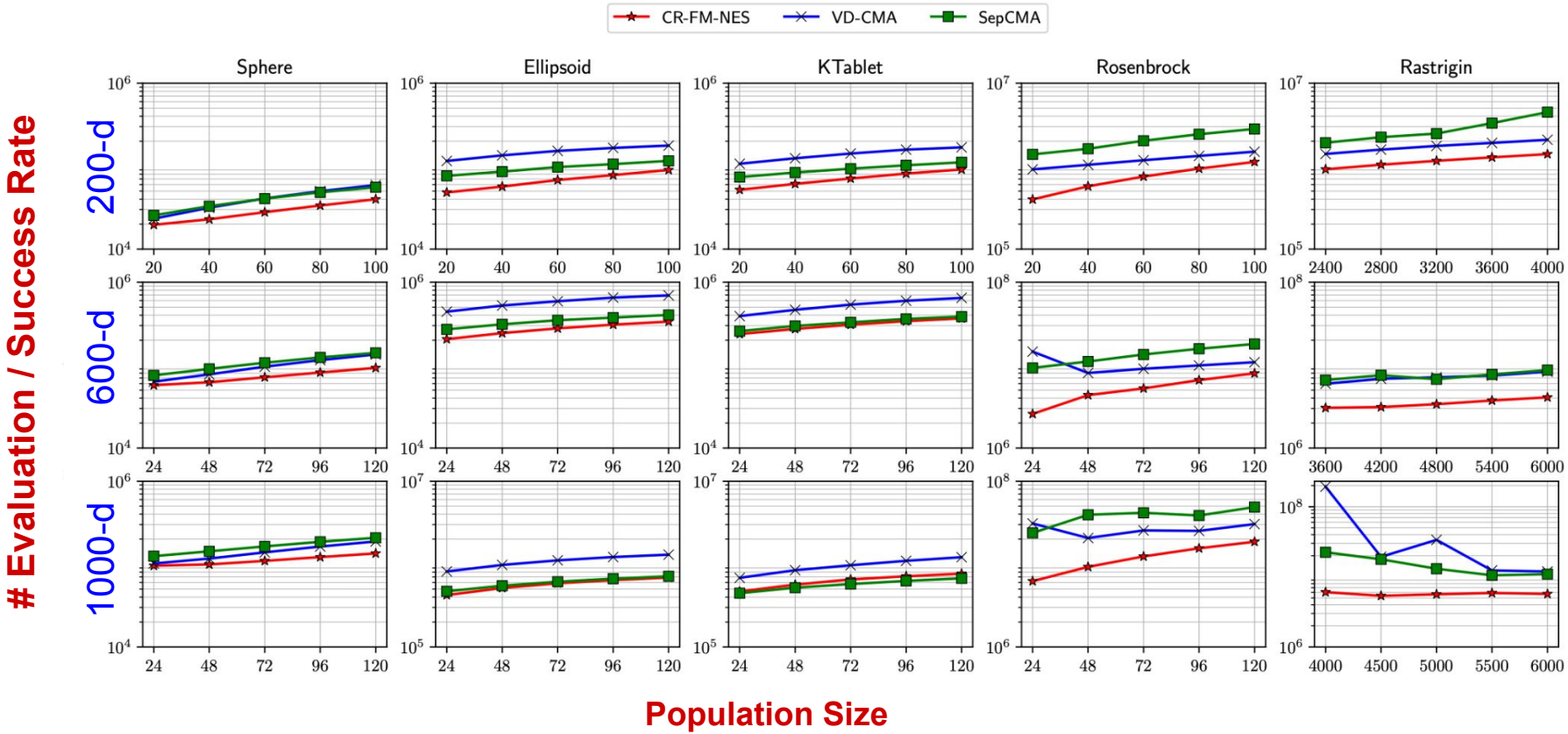
All computations are performed in **linear** time O(d)

* To avoid singularity of the FIM, a modified FIM is used in VD-CMA

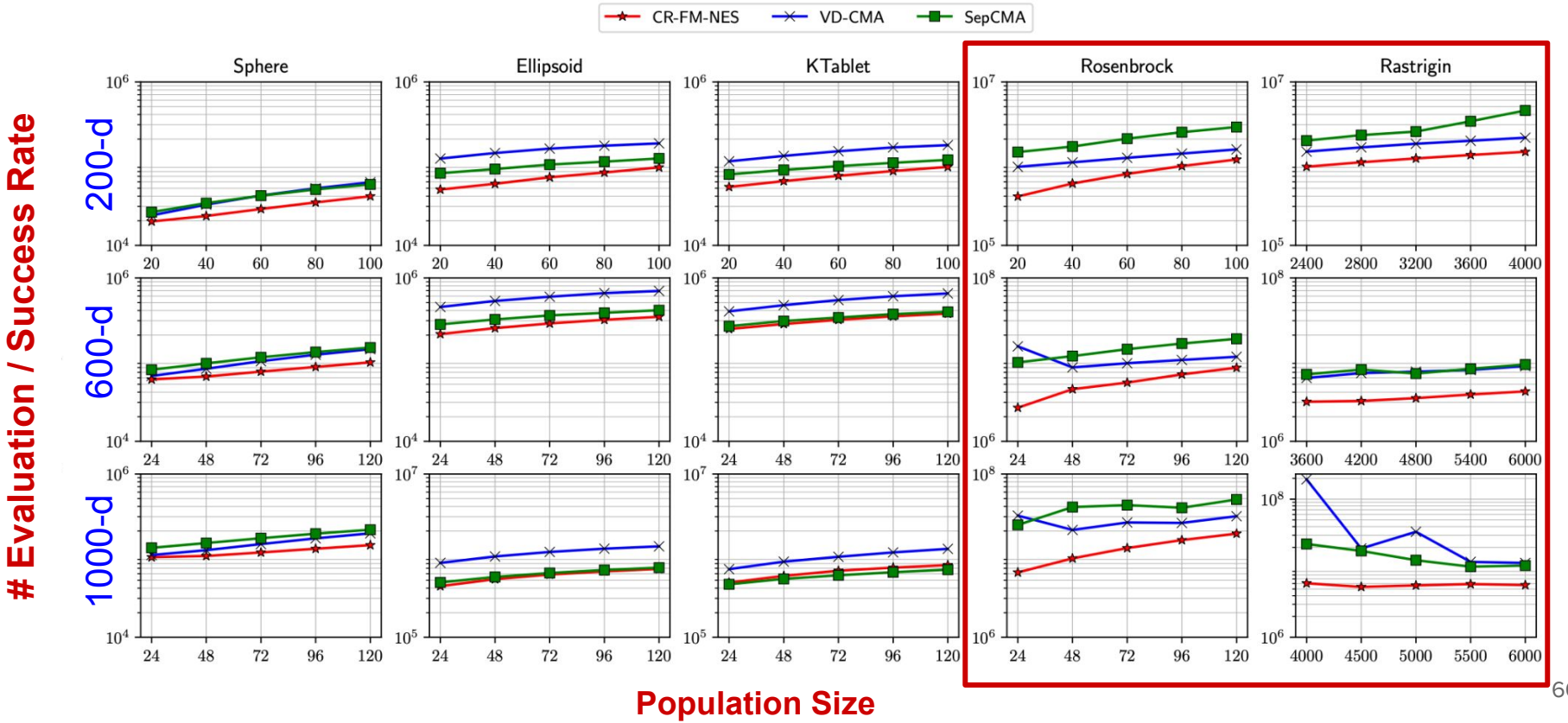
CR-FM-NES [NO22]

- CR-FM-NES uses the same representation as VD-CMA
  - all computations are also performed in linear time
- Instead of step-size adaptation for σ, natural gradient update is used
- Several recent improvements are included
  - distance weight
  - mirrored sampling
  - rank-one update

Comparison: CR-FM-NES vs. VD-CMA vs. Sep-CMA



Comparison: CR-FM-NES vs. VD-CMA vs. Sep-CMA



Towards Completely Hyperparameter-Free Methods

- Internal parameters often have recommended values
  - They are set to ensure they perform well across a wide range of problems
  - However, in ***difficult*** problems (e.g. multimodal and noisy), these settings are often insufficient
- Increasing population size often helps to solve such difficult problems
  - It is difficult to know the appropriate values beforehand in BBO scenarios
  - Tuning can be expensive, so it would be preferable to avoid

Can we adapt the hyperparameter online?

Learning Rate Adaptation vs. Population Size Adaptation

- Important observation: Increasing population size has effect similar to decreasing mean-vector learning rate [MA17]
  - CMA-ES with a small population size solves multimodal problems, through (fixed) appropriate setting of learning rate
- **Learning rate adaptation** vs. **population size adaptation**
  - Learning rate adaptation is more practically useful
  - E.g. parallel implementation (population size may be set to # of workers)
- Introduction of latest LRA [NAO23] (GECCO'23, best paper nominated)
  - While this focus LRA for CMA, but same principle is applicable to NES

Learning Rate Adaptation: Setup

- Notations:
  - distribution parameters: $\theta_m = m, \theta_\Sigma = \mathrm{vec}(\Sigma)$
    - "vec" is the vectorization operator
  - original updates: $\Delta_m^{(t)} = m^{(t+1)} - m^{(t)}, \Delta_\Sigma^{(t)} = \mathrm{vec}(\Sigma^{(t+1)} - \Sigma^{(t)})$
  - learning rate factors: $\eta_m^{(t)}, \eta_\Delta^{(t)}$
- Modified updates for mean and covariance:
  - $\theta_m^{(t+1)} = \theta_m^{(t)} + \eta_m^{(t)} \Delta_m^{(t)}$
  - $\theta_\Sigma^{(t+1)} = \theta_\Sigma^{(t)} + \eta_\Sigma^{(t)} \Delta_\Sigma^{(t)}$

Learning Rate Adaptation: Main Concept

- We adapt the learning rate based on the signal-to-noise ratio (SNR):

$$\mathrm{SNR} := \frac{\|\mathbb{E}[\Delta]\|_F^2}{\mathrm{Tr}(F\,\mathrm{Cov}[\Delta])} = \frac{\|\mathbb{E}[\Delta]\|_F^2}{\mathbb{E}[\|\Delta\|_F^2] - \|\mathbb{E}[\Delta]\|_F^2}$$

F: Fisher information matrix

- **Insight**: in noisy problems, when noise becomes dominant, SNR -> 0
  - To improve function value, maintaining a positive SNR is crucial
  - If we consider (well-structured) multimodal problems as a kind of noisy problems, similar arguments can be applied
- We keep SNR = αη (α: hyperparameter)

Learning Rate Adaptation: Main Concept (2)

- Assume LR is sufficiently small over *n* iterations
  - param. don't change much ⇒ updates are considered to be i.i.d
- *n* steps update:

$$\theta^{(t+n)} = \theta^{(t)} + \eta \sum_{k=0}^{n-1} \Delta^{(t+k)}$$

$$\approx \theta^{(t)} + \mathcal{D}\left(n\eta\mathbb{E}[\Delta], n\eta^2 \mathrm{Cov}[\Delta]\right)$$

- *n* = *1/η* & small *η* ⇒ more concentrated update than *η=1*
- The SNR over *n* iterations: $\frac{\|\mathbb{E}[\Delta]\|_F^2}{\eta \,\mathrm{Tr}(F\,\mathrm{Cov}[\Delta])} = \frac{1}{\eta}\mathrm{SNR}$
- Keeping SNR = *αη* ...
  - Keeping the SNR as *α* over *n* = *1/η* iterations **independently** of *η*

Learning Rate Adaptation: SNR Estimation

- We introduce moving averages for each m and Σ

$$\mathcal{E}^{(t+1)} = (1-\beta)\mathcal{E}^{(t)} + \beta\tilde{\Delta}^{(t)},$$
$$\mathcal{V}^{(t+1)} = (1-\beta)\mathcal{V}^{(t)} + \beta\|\tilde{\Delta}^{(t)}\|_2^2$$

local coordinate

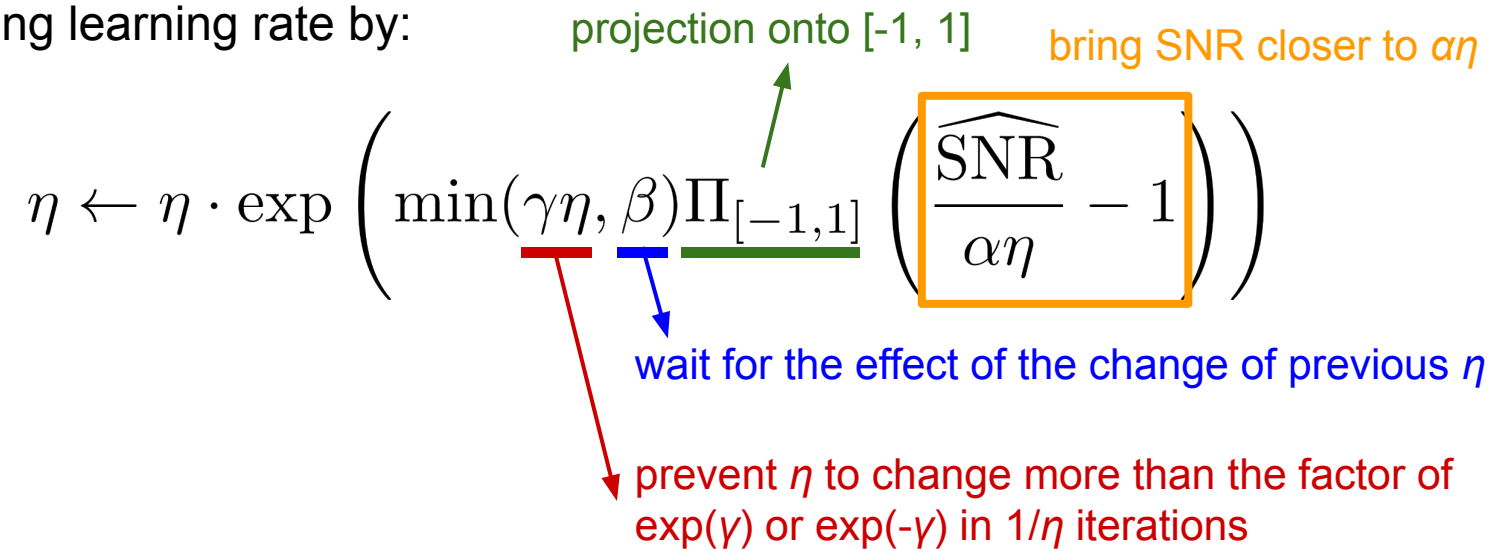
$$\tilde{\Delta}_m = \sqrt{\Sigma}^{-1}\Delta_m$$
$$\tilde{\Delta}_\Sigma = 2^{-\frac{1}{2}}\mathrm{vec}(\sqrt{\Sigma}^{-1}\mathrm{vec}^{-1}(\Delta_\Sigma)\sqrt{\Sigma}^{-1})$$

- The SNR is estimated as:

$$\mathrm{SNR} := \frac{\mathbb{E}[\tilde{\Delta}]^2}{\mathrm{Tr}(\mathrm{Cov}[\tilde{\Delta}])} = \frac{\mathbb{E}[\tilde{\Delta}]^2}{\mathbb{E}[\|\tilde{\Delta}\|^2] - \|\mathbb{E}[\tilde{\Delta}]\|^2},$$
$$\approx \frac{\|\mathcal{E}\|_2^2 - \frac{\beta}{2-\beta}\mathcal{V}}{\mathcal{V} - \|\mathcal{E}\|_2^2} =: \widehat{\mathrm{SNR}}$$

Update Equation of Learning Rate Adaptation

- Adapting learning rate by:

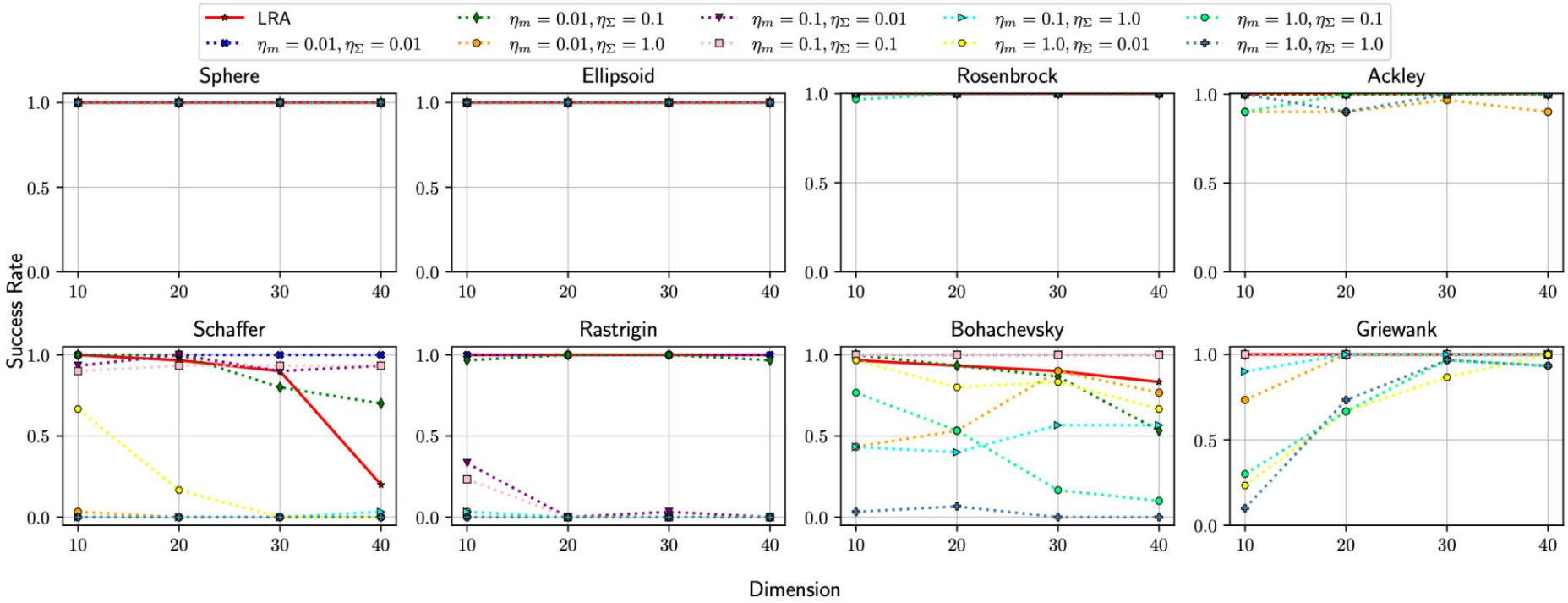


- We set the upper bound to 1 to prevent unstable behavior

Experiments: Research Questions and Setups

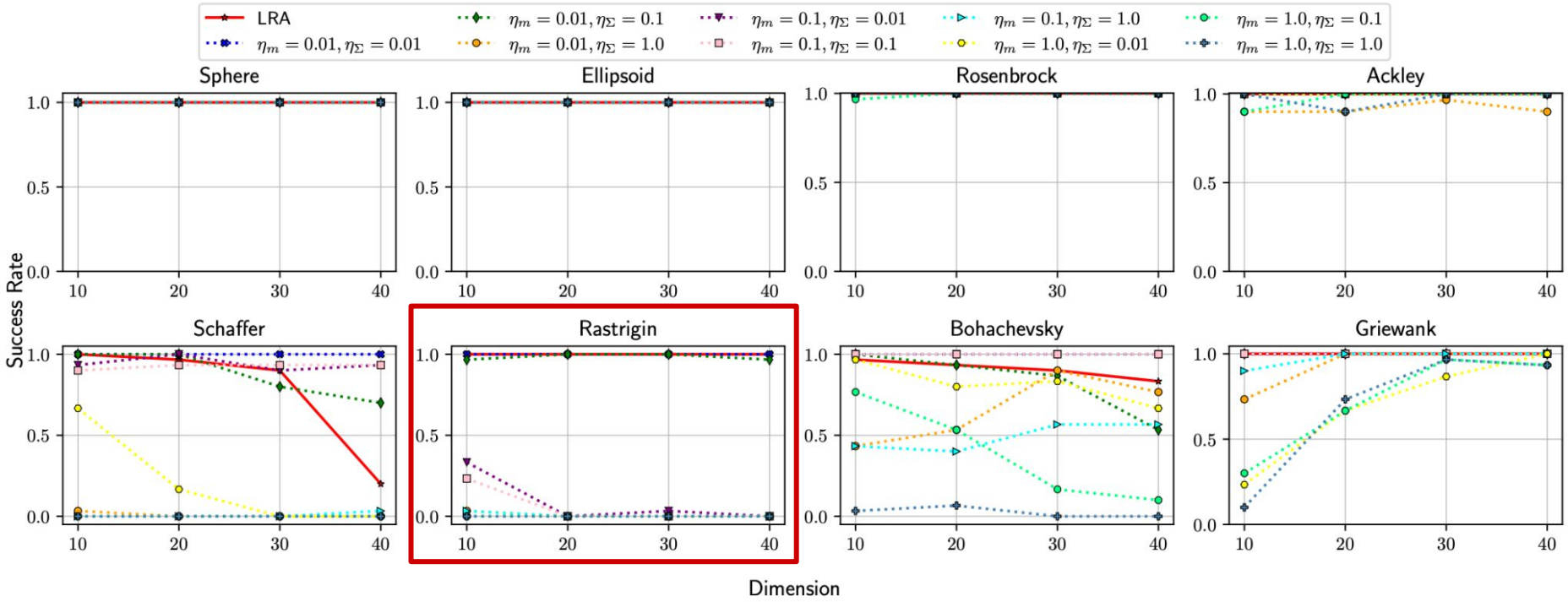
- We compare *LRA-CMA* with CMA with fixed learning rates
- Benchmark problems
  - unimodal (Sphere, Ellipsoid, Rosenbrock) and multimodal (Ackley, Schaffer, Rastrigin, Bohachevsky, Griewank)
  - In noisy problems, we considered additive Gaussian noise
- Population size: recommended value $\lambda = 4 + \lfloor 3 \ln d \rfloor$

Success Rate versus (10-40)Dim. (Noiseless Problems)



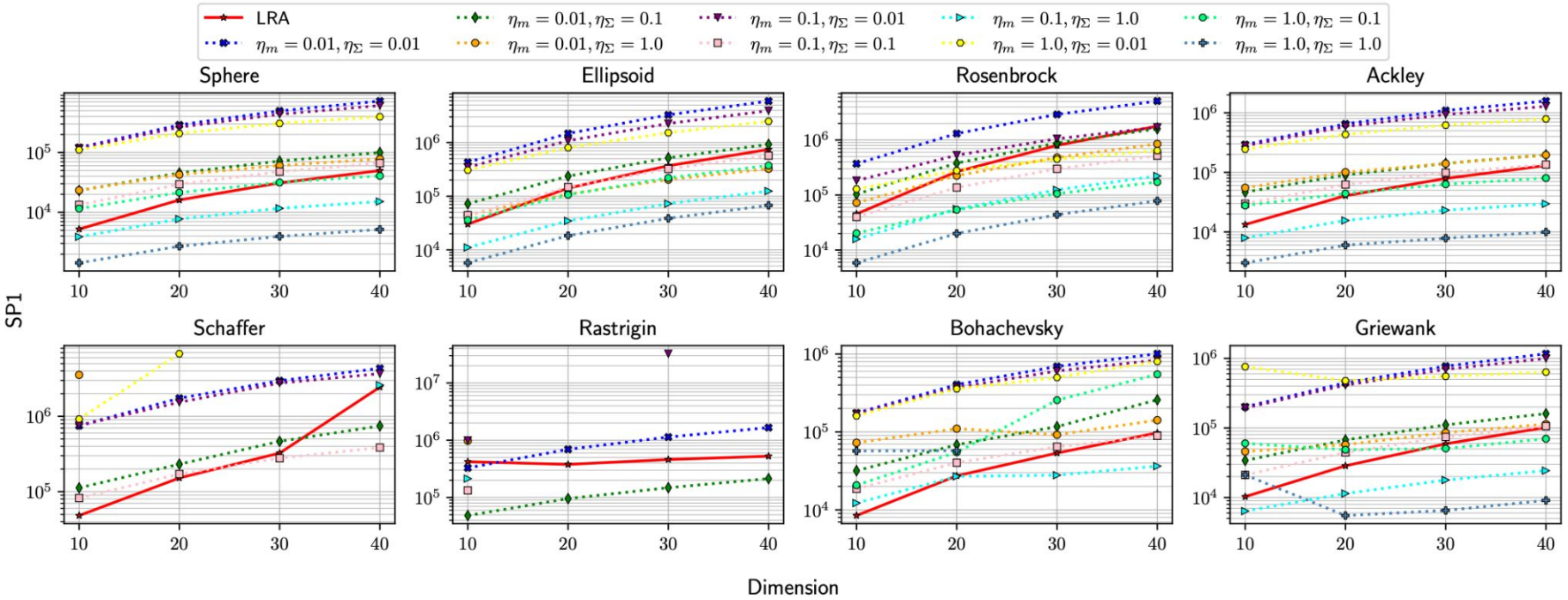
For multimodal, CMA with high η often *failed*, but CMA with small η had a high SR
LRA-CMA had a relatively *good SR without tuning*

Success Rate versus (10-40)Dim. (Noiseless Problems)



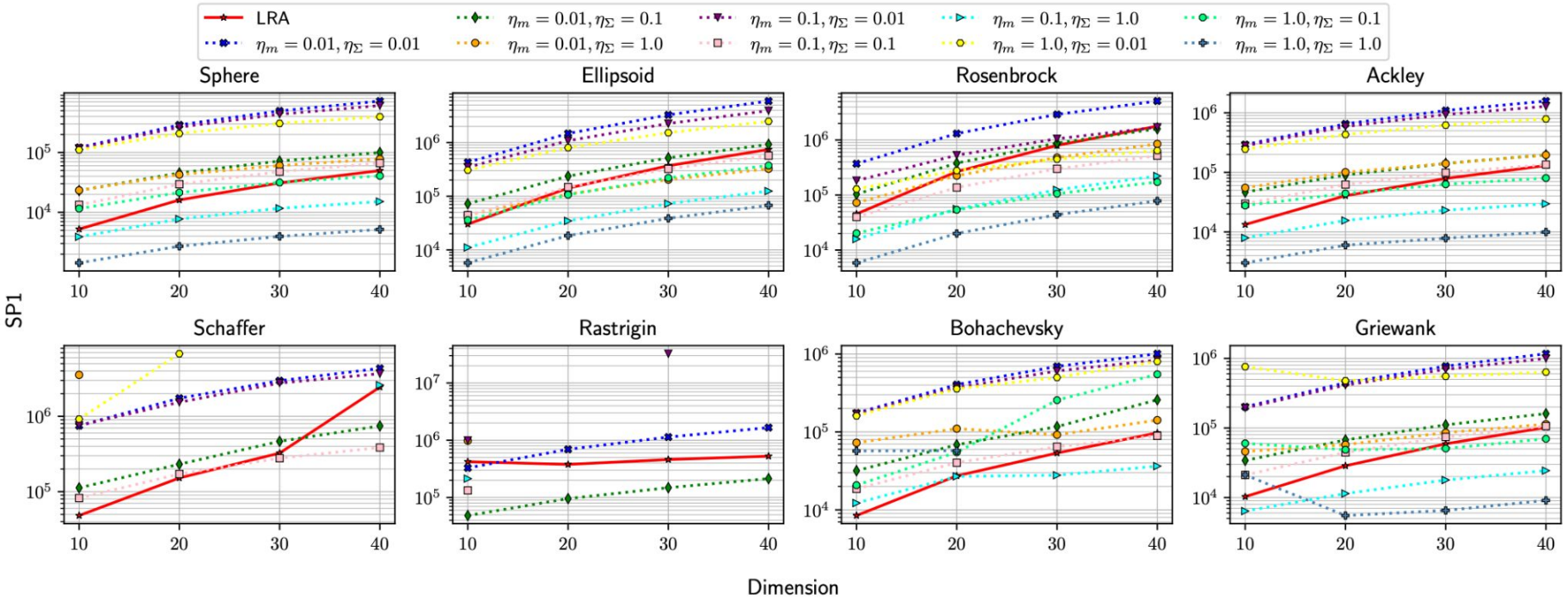
LRA with default pop. (e.g. λ=15 for d=40) succeeded in all trials on the Rastrigin

SP1 versus (10-40)Dim. (Noiseless Problems)



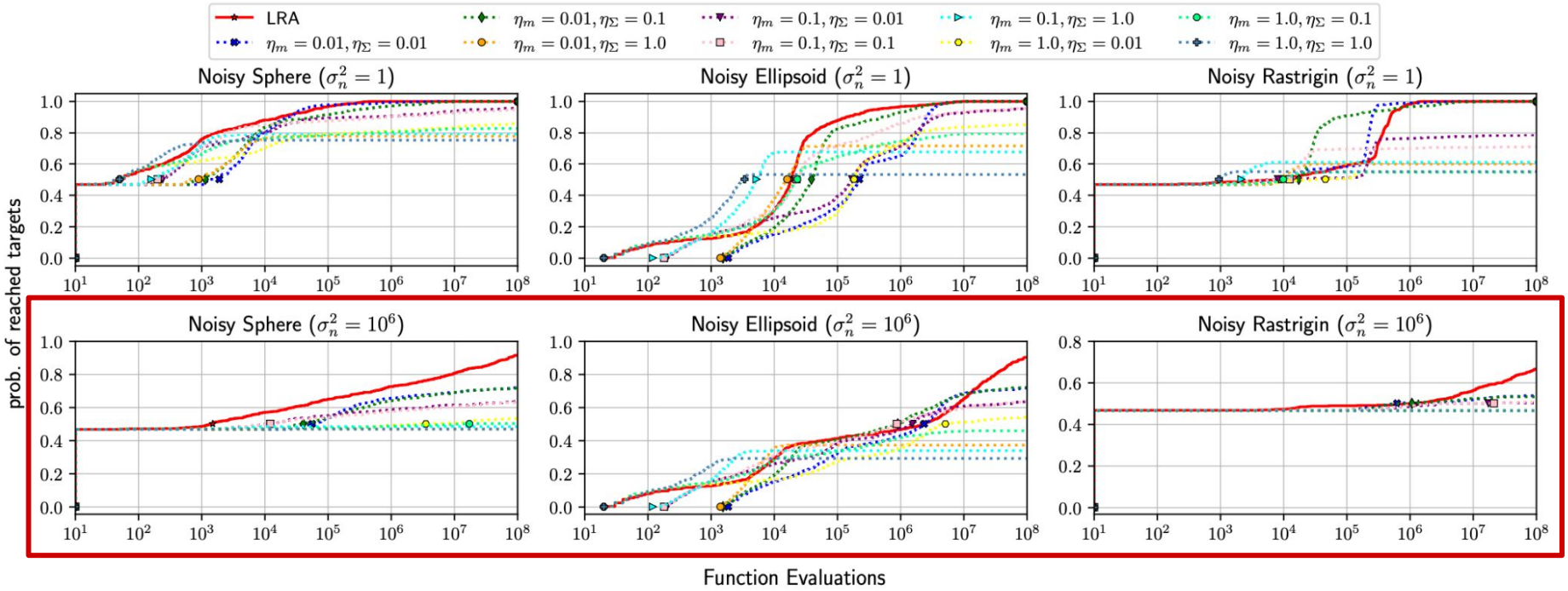
CMA with high η ⇒ worse on multimodal, CMA-ES with small η ⇒ slow on unimodal
Clear trade-off in efficiency exists depending on η

SP1 versus (10-40)Dim. (Noiseless Problems)



LRA shows stable and relatively good performance without expensive tuning

Empirical cumulative density function on noisy problems



CMA with fixed η had stopped improving the function value
In contrast, *LRA continued to improve* it even in strong noise

Part 4:
Practical Guide

Topics of this part

- How to understand behavior of NES/CMA-ES?
  - typical metrics for logging
  - typical behavior on benchmark problems
- How to run NES/CMA-ES in practical situations?
  - popular Python libraries
  - how to set initial configurations
    - injecting domain knowledge for efficient optimization
    - automatic determination by using results on similar tasks
- The content of this part is inspired by [akimotolab/CMAES_Tutorial]

Logging Metrics

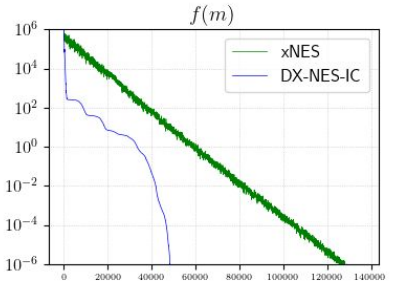
- Function value f(x)
  - may not be sufficient to judge whether optimization is finished
- Mean vector
  - useful for checking validity of range of box constraint
- Step-size σ
  - useful for checking convergence
- ratios of (sqrt) eigenvalues
  - if ratios significantly differ, normalizing scaling variables may be needed

Our Focus: DX-NES-IC

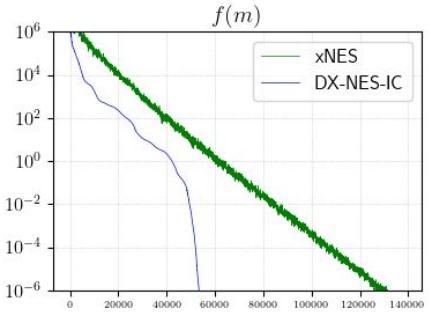
- DX-NES-IC shows better performance than xNES
  - Distance weight
  - Mirrored sampling
  - Switching learning rate
  - Emphasizing expansion

- Note: The behavior to be examined now do not differ significantly across NES/CMA-ES methods

40-Dim. k-Tablet



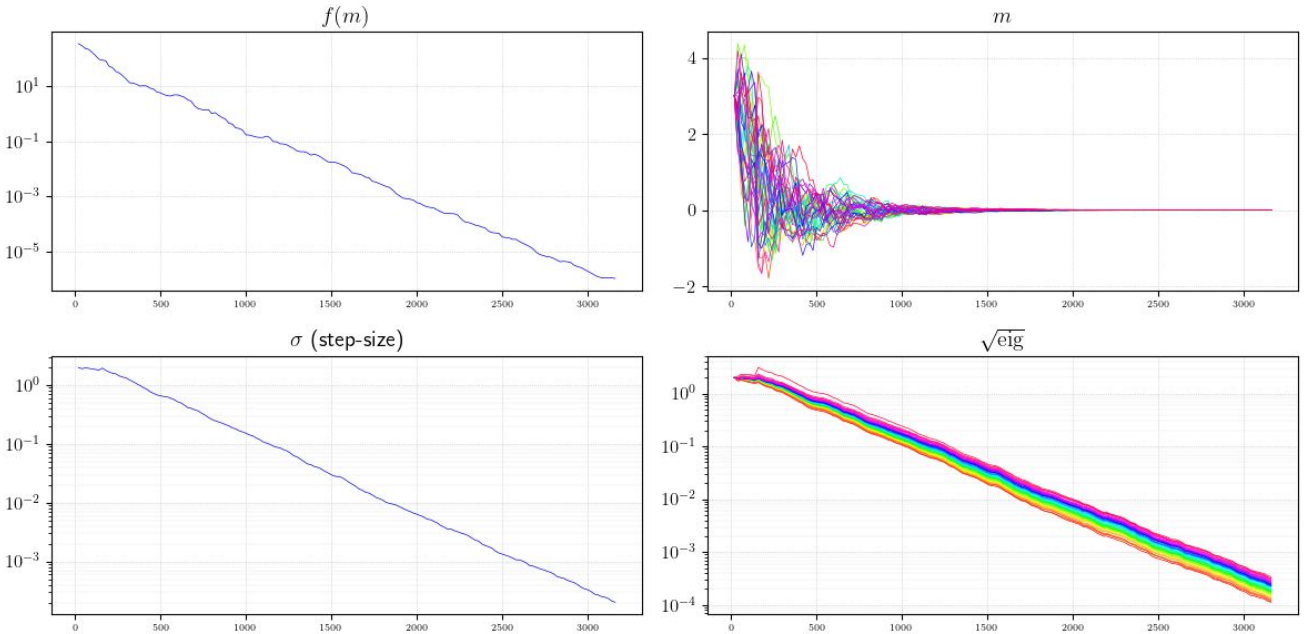
40-Dim. Ellipsoid

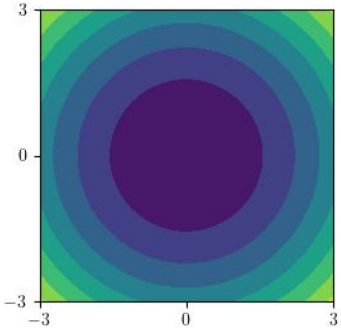


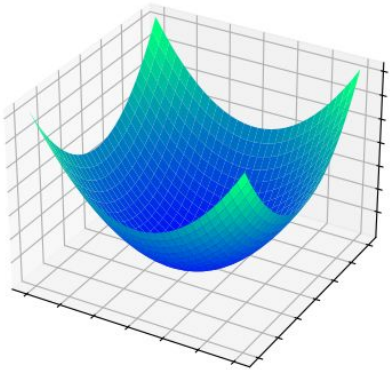
Easy Problem: Sphere Function

$$f_{\text{Sphere}}(x) = \sum_{i=1}^{d} x_i^2$$

importance of each variable is the ***same***







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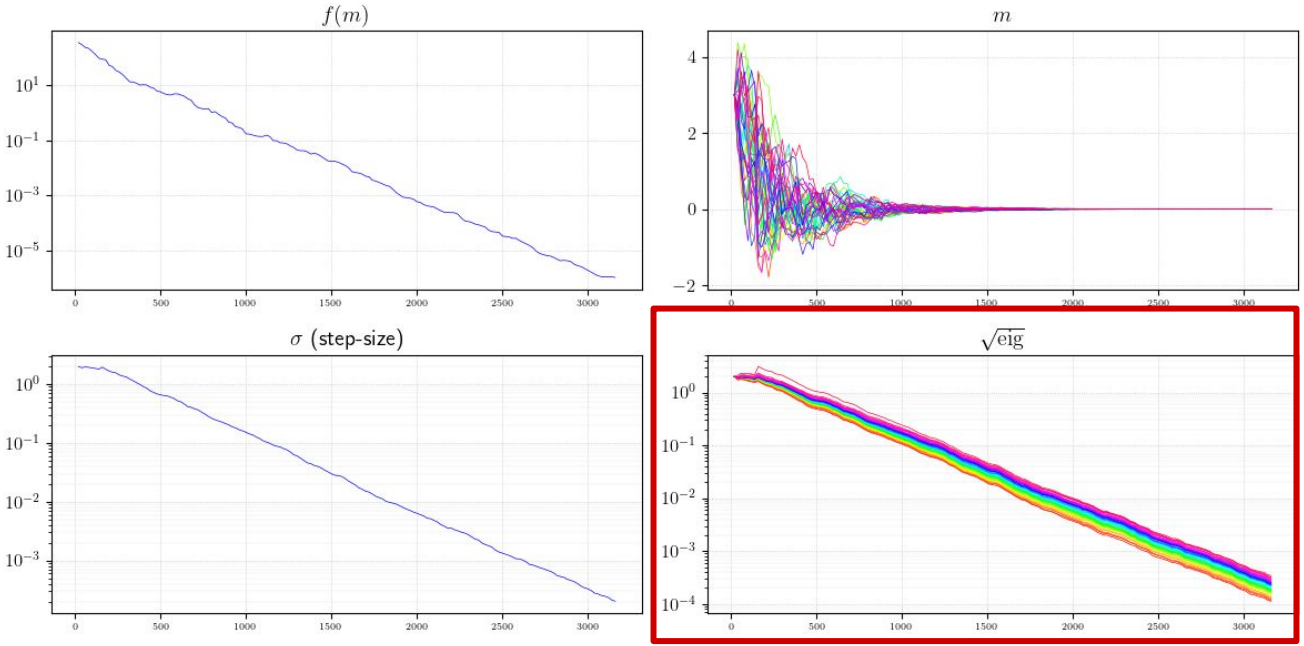
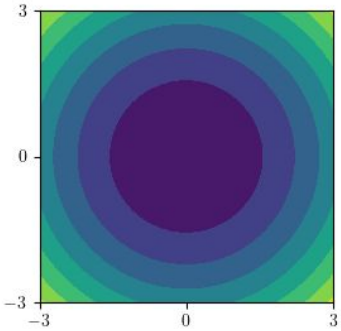
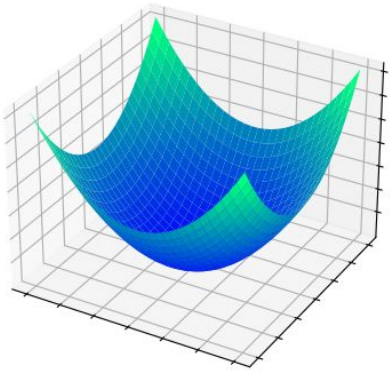


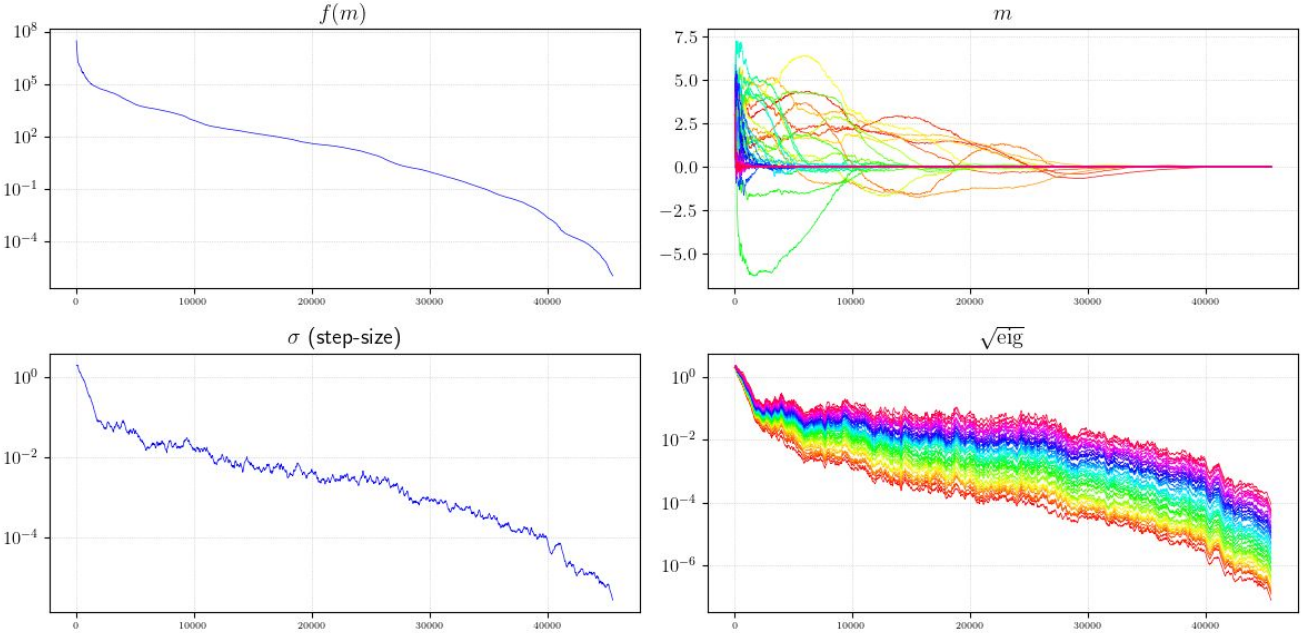


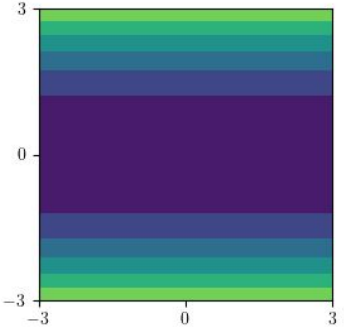


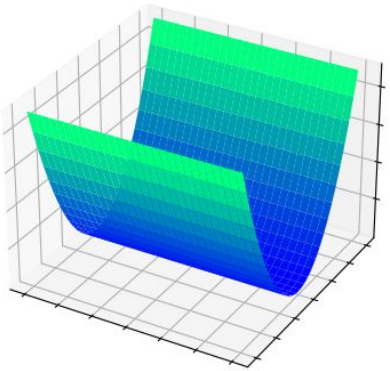
Ill-Conditioned Problem: Ellipsoid Function

$$f_{\text{Ellipsoid}}(x) = \sum_{i=1}^{d} (1000^{\frac{i-1}{d-1}} x_i)^2$$

importance of each variable is ***different***







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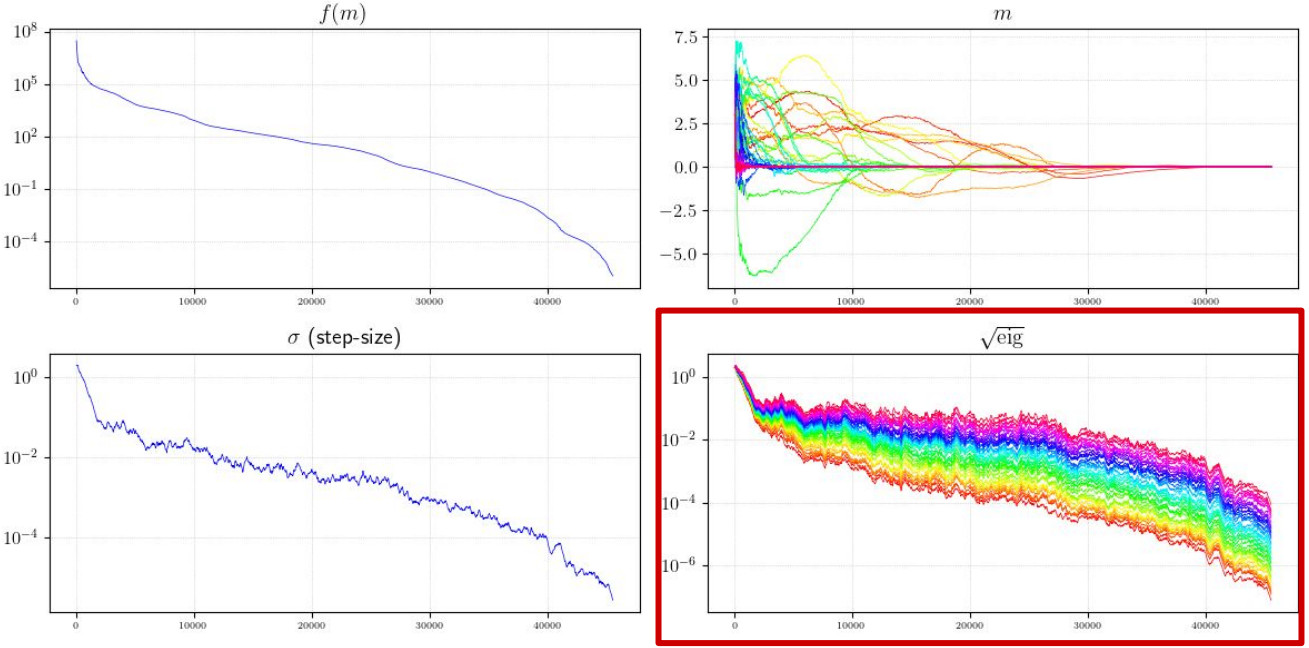
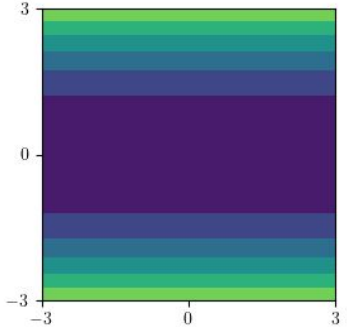
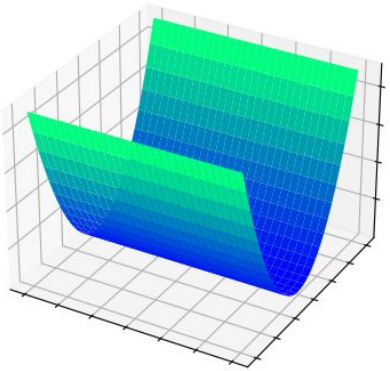


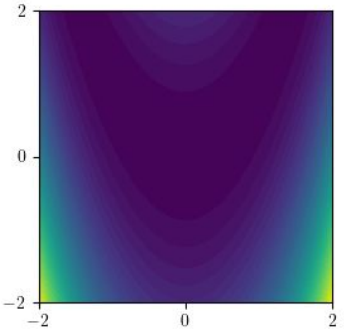


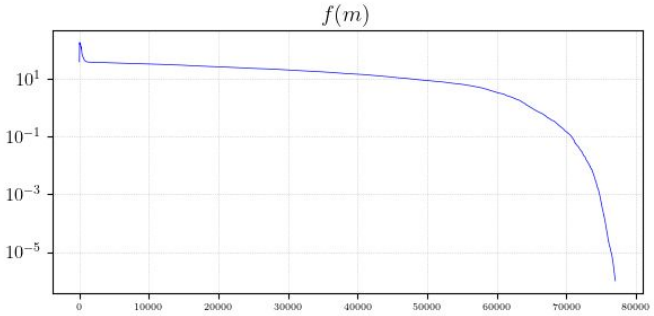


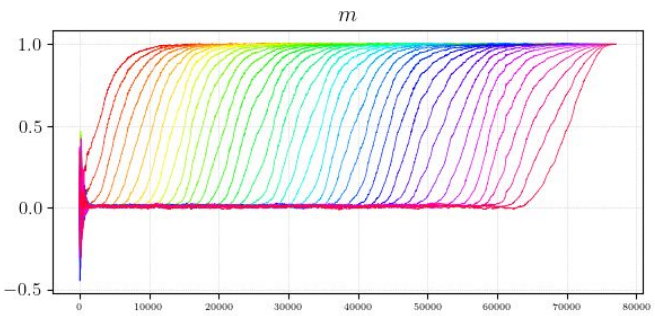
Non-Separable Problem: Rosenbrock Function

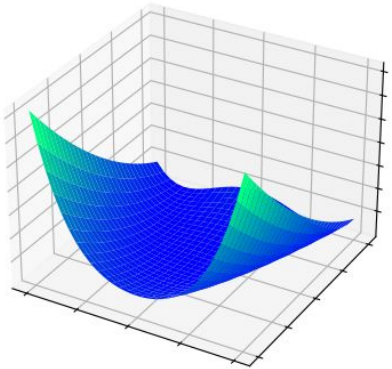
$$f_{\text{Rosenbrock}}(x) = \sum_{i=1}^{d-1} (100(x_{i+1} - x_i^2)^2 + (x_i - 1)^2)$$

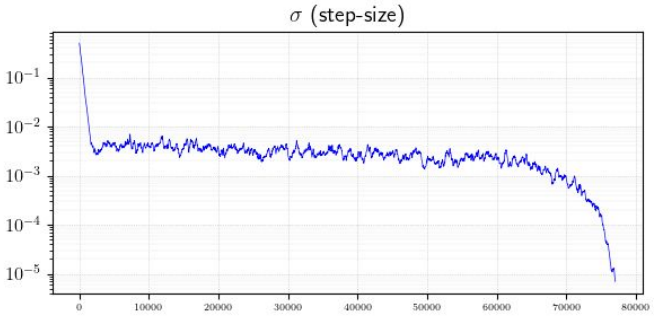
variable dependencies

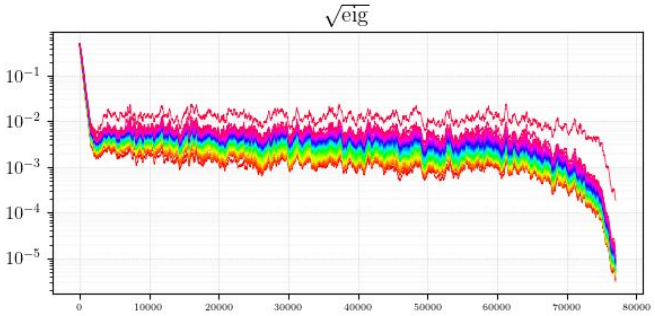








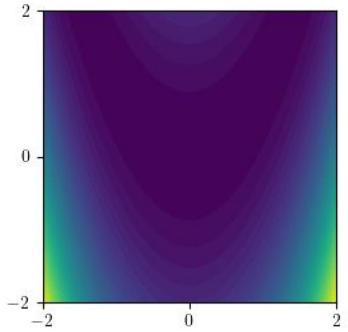


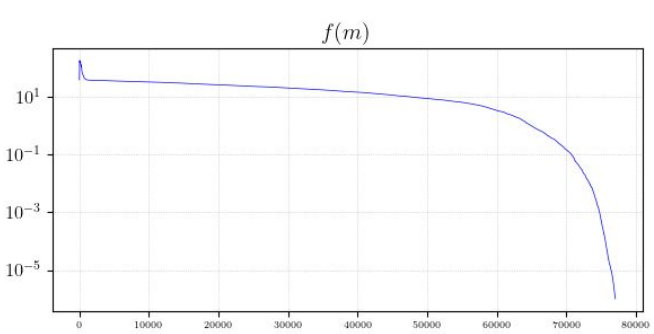


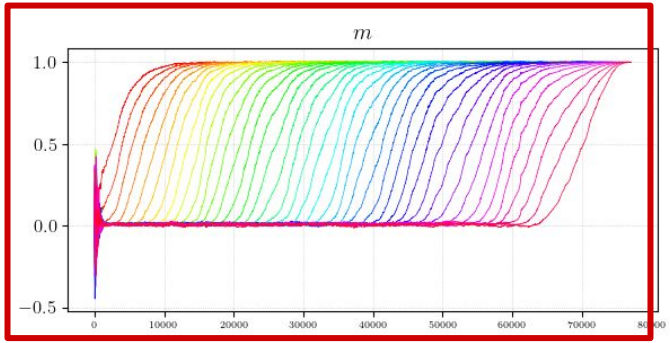
Non-Separable Problem: Rosenbrock Function

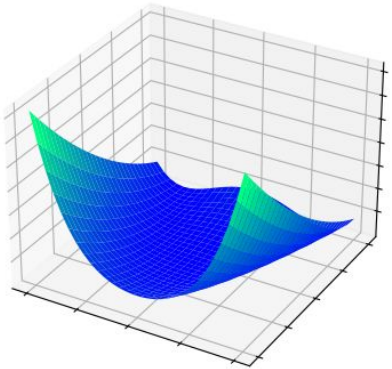
$$f_{\text{Rosenbrock}}(x) = \sum_{i=1}^{d-1} (100(x_{i+1} - x_i^2)^2 + (x_i - 1)^2)$$

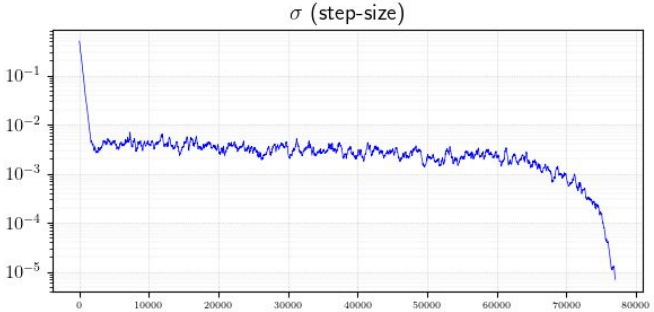
variable dependencies

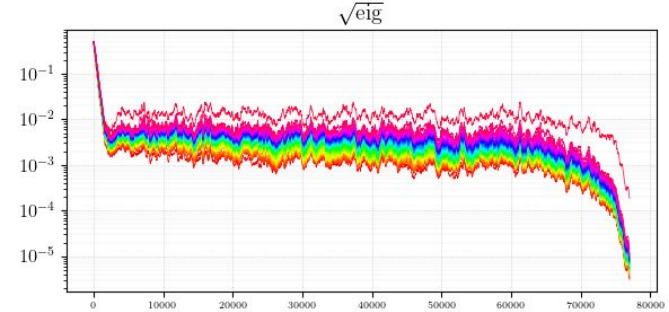






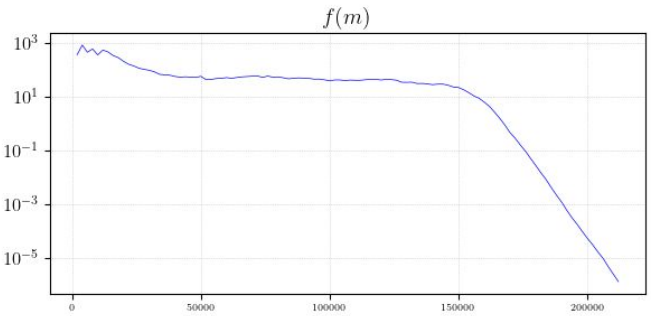


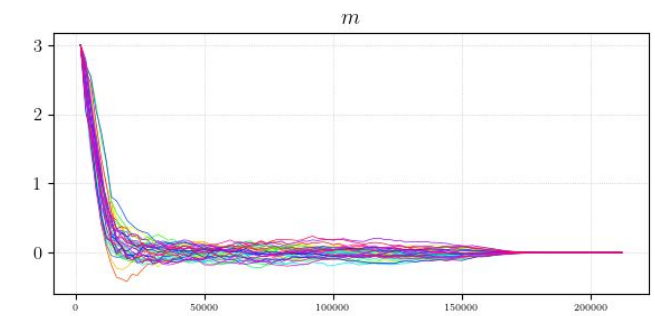


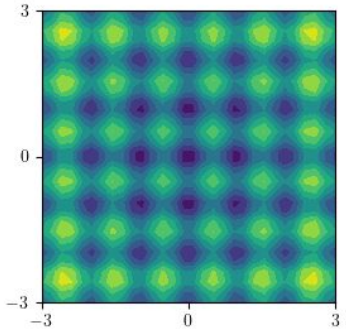


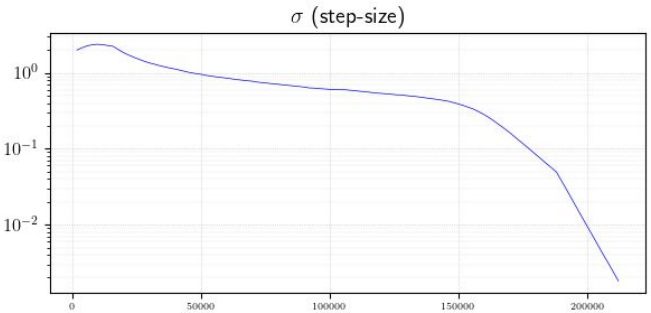
(Well-Structured) Multimodal Problem: Rastrigin Function

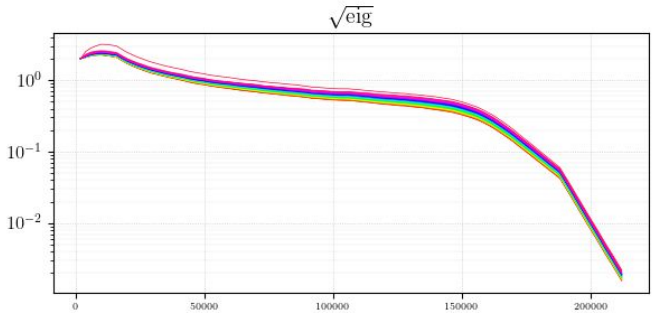
$$f_{\text{Rastrigin}}(x) = 10d + \sum_{i=1}^{d} (x_i^2 - 10\cos(2\pi x_i))$$

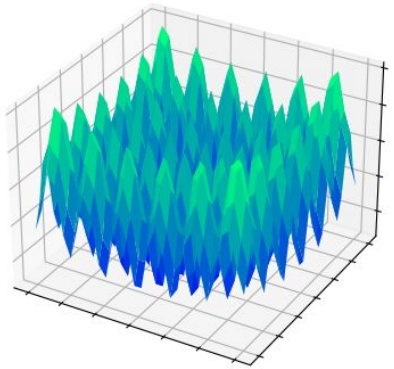








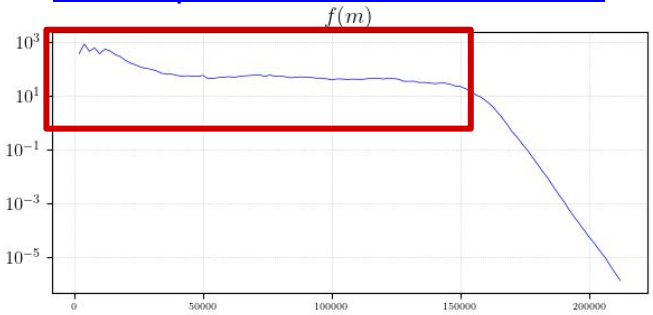


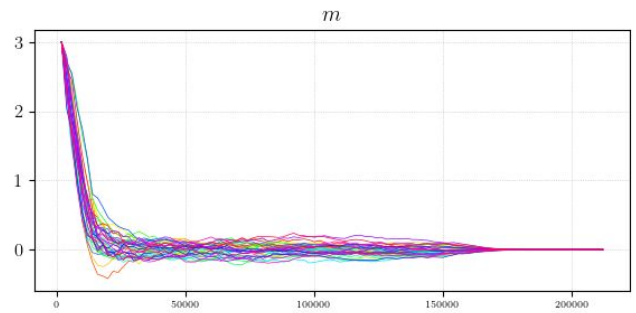


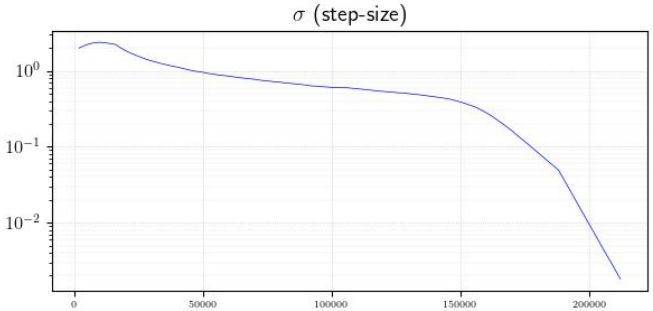
(Well-Structured) Multimodal Problem: Rastrigin Function

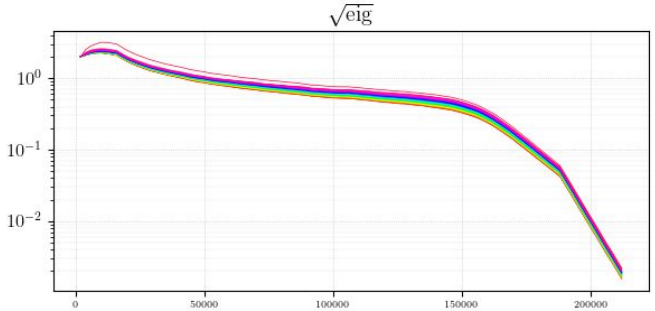
$$f_{\text{Rastrigin}}(x) = 10d + \sum_{i=1}^{d} (x_i^2 - 10\cos(2\pi x_i))$$

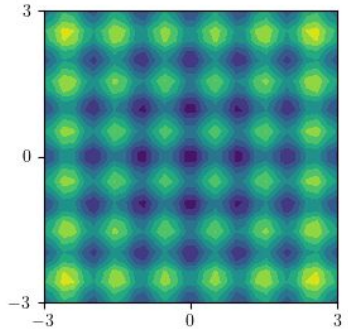
Is the optimization finished? - No!

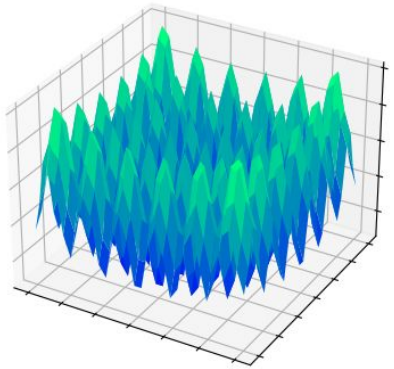












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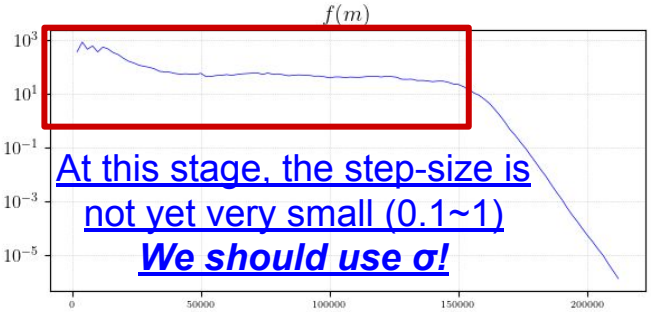
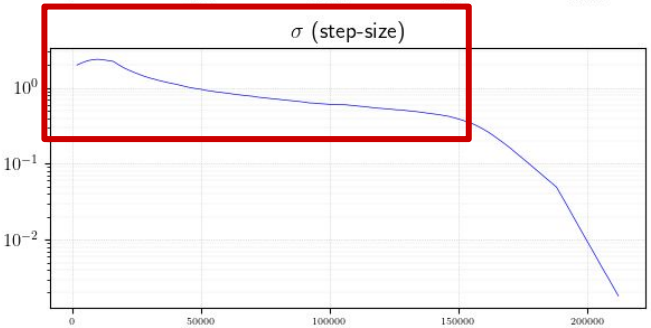
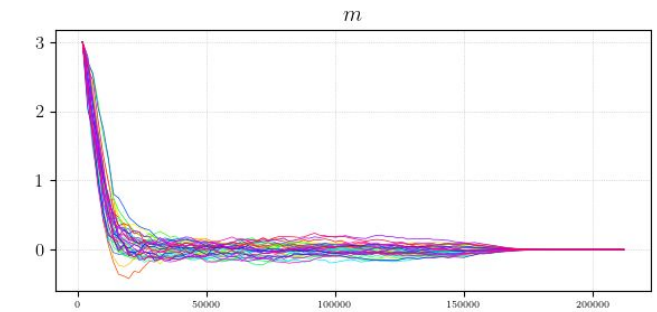
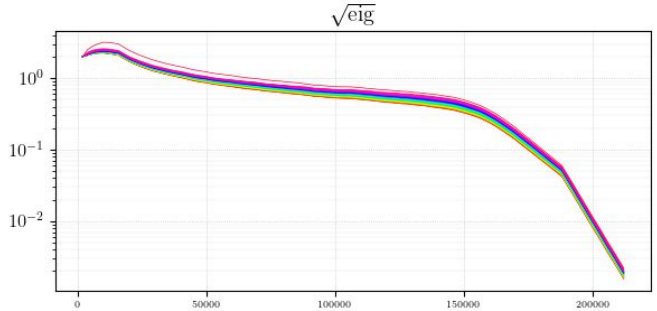


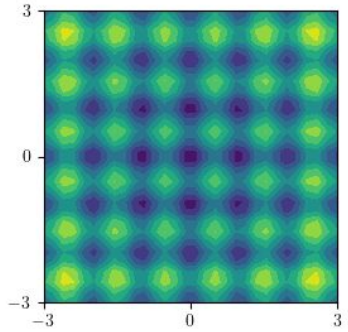
At this stage, the step-size is not yet very small (0.1~1)

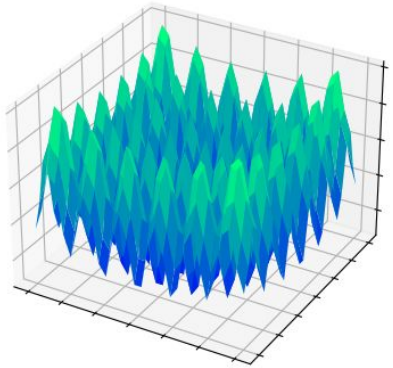
We should use σ!











Python OSS for NES/CMA-ES

- CMA-ES/pycma:
  - Most famous CMA-ES OSS, useful for research and practical purpose
- msu-coinlab/pymoo:
  - Many multi-objective optimization methods including CMA-ES
- google/evojax, RobertTLange/evosax:
  - Jax-based ES implementation
- CyberAgentAILab/cmaes (*focus of this tutorial*):
  - Lightweight implementation, suitable for educational purpose
  - Employed by optuna, which is a popular HPO software

Usage for CyberAgentAILab/cmaes

ask-and-tell interface

```python
import numpy as np
from cmaes import CMA

def quadratic(x1, x2):
    return (x1 - 3) ** 2 + (10 * (x2 + 2)) ** 2

if __name__ == "__main__":
    optimizer = CMA(mean=np.zeros(2), sigma=1.3)

    for generation in range(50):
        solutions = []
        for _ in range(optimizer.population_size):
            x = optimizer.ask()
            value = quadratic(x[0], x[1])
            solutions.append((x, value))
            print(f"#{generation} {value} (x1={x[0]}, x2 = {x[1]})")
        optimizer.tell(solutions)
```

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        optimizer.tell(solutions)
```

1: initialize optimizer

2: generate solutions

3: evaluate x on f

4: update distributions

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        optimizer.tell(solutions)
```

initial distribution
(mean, step-size, and cov.)

How to Set Initial Distribution?: Mean Vector

- If you know promising regions, it is reasonable to initialize the mean there
- E.g. hyperparameter optimization of deep neural networks
  - It is often the case that the paper proposing the network structure provides *recommended values*
    - may be beneficial to set the mean vector to the recommended values
  - However, a certain degree of unimodality is assumed

How to Set Initial Distribution?: Step-Size σ

- If you are somewhat confident that the optimum lies on near mean, it may be possible to reduce step-size

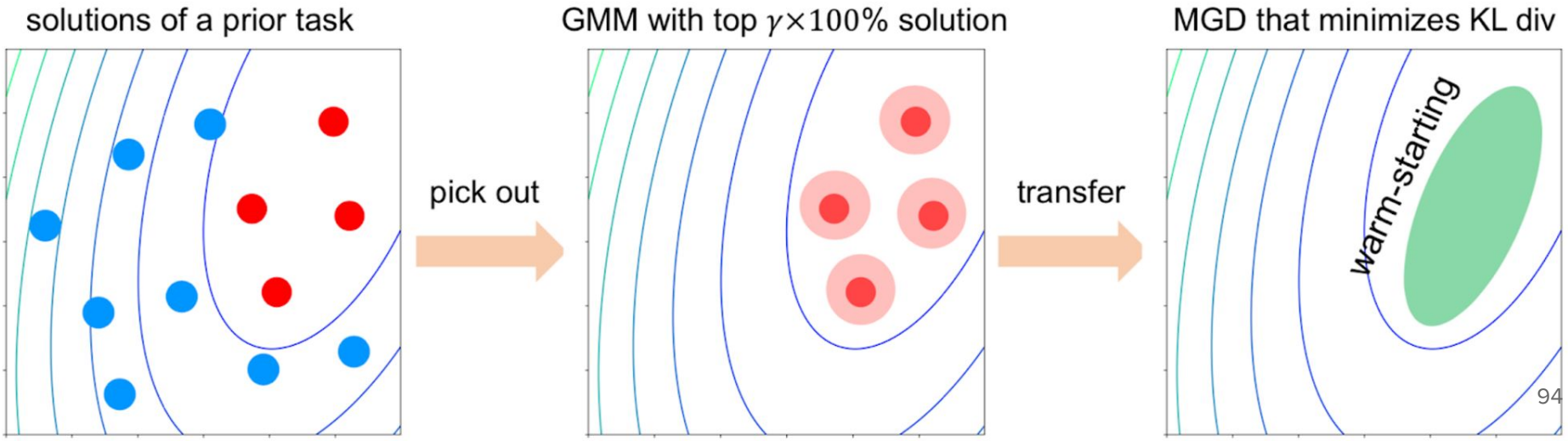
- In well-structured multimodal (i.e. big-valley) problems, setting a relatively large value is a reasonable choice
- However, in weakly-structured multimodal problems, a large step-size can be detrimental
- In BBO scenarios, trial-and-error cannot (or may not) be avoidable

Automatic Determination of Initial Distribution from Data

- In BBO scenarios, is it impossible to utilize information about the problem?
  - Not necessarily the case: we often have results on related (source) task
- Example 1: HPO with periodic execution
  - Updating model and running HPO *whenever* new data becomes available
  - Previous HPO can be considered as the source task
- Example 2: HPO with partial data
  - Before building model with large-scale data, performance are verified using *partial* data
  - HPO with partial data can be considered as the source task
- Example 3: HPO for different dataset
  - Model construction is performed *separately* for each dataset due to accuracy/size
  - HPO for different dataset can be considered as the source task

Warm Starting CMA-ES [NWA+21]: Overview

- Assumption:
  - The source task and target task are similar
- Basic idea:
  - Approaching the initial dist. of MGD to promising regions estimated from source task



Warm Starting CMA-ES [NWA+21]: Implementation

```
if __name__ == "__main__":
    # Generate solutions from a source task
    source_solutions = []
    for _ in range(1000):
        x = np.random.random(2)
        value = source_task(x[0], x[1])
        source_solutions.append((x, value))

    # Estimate a promising distribution of the source task,
    # then generate parameters of the multivariate gaussian distribution.
    ws_mean, ws_sigma, ws_cov = get_warm_start_mgd(
        source_solutions, gamma=0.1, alpha=0.1
    )
    optimizer = CMA(mean=ws_mean, sigma=ws_sigma, cov=ws_cov)
```

result on source task

hyperparameter for Warm Starting CMA: Default is sufficient

initial distribution

How to Set Hyperparameters?: Population Size λ

- Increasing pop. size is beneficial for well-structured multimodal problems
  - However, practitioners often wish to specify # workers as pop. size...
  - You can specify any pop. size by using *learning rate adaptation*
- without LRA (default)

```
optimizer = CMA(mean=np.ones(10) * 3, sigma=2.0)
```

- with LRA [NAO23]

only modification

```
optimizer = CMA(mean=np.ones(10) * 3, sigma=2.0, lr_adapt=True)
```

Part 5: Summary and Future Challenges

NES objective & Natural Gradient

- NES objective: the function of θ, not x

$$J(\theta) = \mathbb{E}_{x \sim p(x;\theta)}[f(x)]$$

- Natural gradient update with Monte Carlo method

$$\theta \leftarrow \theta + \eta \cdot F^{-1} \nabla_\theta J(\theta)$$

$$\approx \theta + \eta \cdot \frac{1}{\lambda} \sum_{i=1}^{\lambda} f(x_i) F^{-1} \nabla_\theta \log p(x_i; \theta)$$

Fitness Shaping

- Fitness shaping: introduce the weights $(w_i \geq \cdots \geq w_\lambda)$
  - rendering invariant under monotonically increasing transformation of f:

$$F^{-1}\nabla_\theta J(\theta) \approx \frac{1}{\lambda}\sum_{i=1}^{\lambda} f(x_i) F^{-1}\nabla_\theta \log p(x_i;\theta)$$

Fitness Shaping

$$\sum_{i=1}^{\lambda} w_i F^{-1}\nabla_\theta \log p(x_{i:\lambda};\theta)$$

$x_{i:\lambda}$: *i*-th best solution

NES uses only ranking rather than function value itself

Information Geometric Optimization (IGO)

- NES with fitness shaping is natural gradient method for another objective
- IGO objective: $J_{\theta^{(t)}}(\theta) = \mathbb{E}_{x \sim p(x;\theta)}[W^f_{\theta^{(t)}}(x)]$

Objective function depends on the current parameter $\theta^{(t)}$

- This framework generalizes some popular stochastic methods
  - continuous: xNES, Rank-μ update CMA-ES
  - binary: PBIL, cGA

Recent Advances

- **Sample Reuse via Importance Sampling**
  - Leveraging discarded ‘old’ samples for improving estimation accuracy
- **Addressing Inefficiency of xNES**
  - Distance weight & emphasis on distribution expansion
- **High-Dimensional Optimization**
  - Restricting representation of covariance matrix
- **Learning Rate Adaptation**
  - Solving difficult problems (e.g. multimodal and noisy) without tuning

Future Challenges (1)

- **Designing Weights (Fitness Shaping) for 'General' Gaussian Distribution**
  - Optimal weights for isotropic Gaussian are derived (quality gain analysis)
    - Not clear for Gaussian distribution with *general* cov. matrix
  - Distance weight addresses the issue, but theoretical validity is not clear
- **Towards Completely Hyperparameter-Free Optimizer**
  - Population size adaptation (PSA) and learning rate adaptation (LRA)
    - But experiments are still not exhaustive (e.g. hyperparameter)
  - Lack of comparison between PSA and LRA

Future Challenges (2)

- **BBO with Safety Constraints**
  - There is a need to optimize while maintaining fval. above a threshold
  - Active in areas such as bayesian optimization [SGBK15],
    but few studies in NES/CMA
- **Mutivariate Discrete BBO via Natural Gradient**
  - While there are BBO methods such as PBIL and cGA that use (*univariate*)
    Bernoulli distributions, there are hardly any that use multivariate ones
  - An example exists of applying the natural gradient method to an RBM
    (Restricted Boltzmann Machine), but empirical evaluation is limited

Thank you for listening!

contact: masahironomura5325@gmail.com

Tutorial materials: https://github.com/nomuramasahir0/cec2023-tutorial

CyberAgentAILab/cmaes: https://github.com/CyberAgentAILab/cmaes

Acknowledgements:

The design of this slide is based on these wonderful slides by Yuta Saito.

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