Model-based Optimization with Normalizing Flows

Sara Karami

IFT Seminars

April 2024

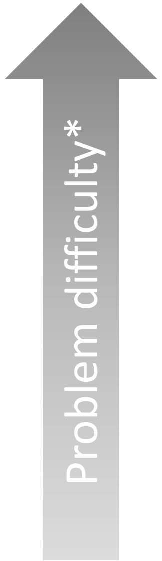
Outline

- Introduction and Background
- Proposed approach
- Experiments and Results
- Conclusion and Future work

Optimization

General form: $\min_{x}\{f(x) : x \in \Omega\}$

Selecting method according to $f(x)$



- Blackbox Optimization (BBO)
- Derivative Free Optimization (DFO)
- Gradient Descent
- Analytical Solvers

*Problem difficulty: Less information / assumptions available

Optimization

General form: $\min_{x} \{ f(x) : x \in \Omega \}$

Selecting method according to $f(x)$

Problem difficulty*

- Blackbox Optimization (BBO) $\rightarrow$ Only gives output values when gets some input queries
- Derivative Free Optimization (DFO) $\rightarrow$ No direct access to derivatives but they exist and there is a level of **smoothness**
- Gradient Descent $\rightarrow$ No regular form but there is a formulation to calculate the derivatives
- Analytical Solvers $\rightarrow$ Formulating the problem and its constraints in specific forms

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- Blackbox Optimization (BBO)
- Derivative Free Optimization (DFO)
- Gradient Descent
- Analytical Solvers

→ Only if derivatives do not exist or are too costly to compute

Black Box Optimization

Function characteristics:

- Complexity: non-smooth, discontinuous, highly multimodal, noisy
- Dimensionality: large search space
- Separability: dependence between objective variables

$$\min_x \{ f(x) : x \in \Omega \}$$

Schematic of a Black Box [1]

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Real-world examples:

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Real-world examples:

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Goal: Find a good enough solution with **minimum number of sample evaluations**

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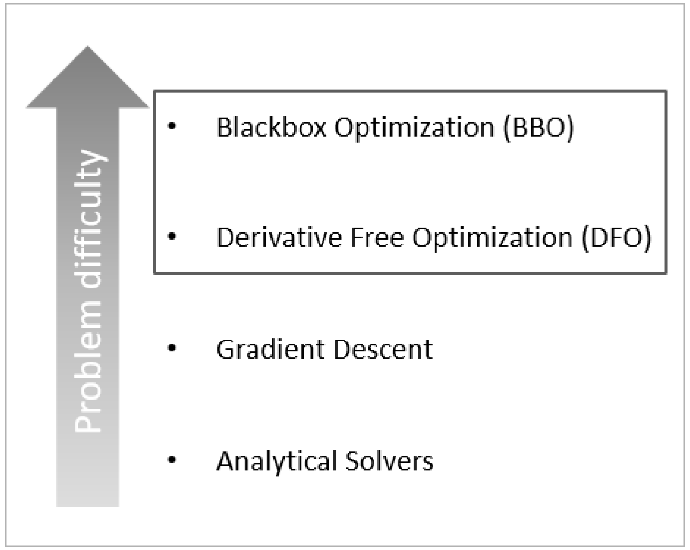
BBO vs DFO

Black-box optimization

- Typically, no assumptions of any form of continuity, differentiability or smoothness on the function
- More on the **heuristic side** without mathematical support
- Main approaches are **Evolutionary Algorithms** (EA) and **Randomized based** methods

Derivative free optimization

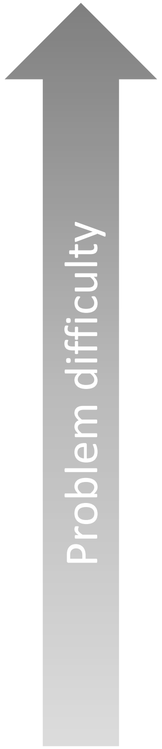
- More mathematically supported: prove of **convergence** and/or **stopping criterion**
- More on the **deterministic** side
- Direct search and surrogate-based



BBO Methods

Deciding BBO method

- Complexity and characteristics of $f(x)$
- Cost of evaluation or evaluation budget



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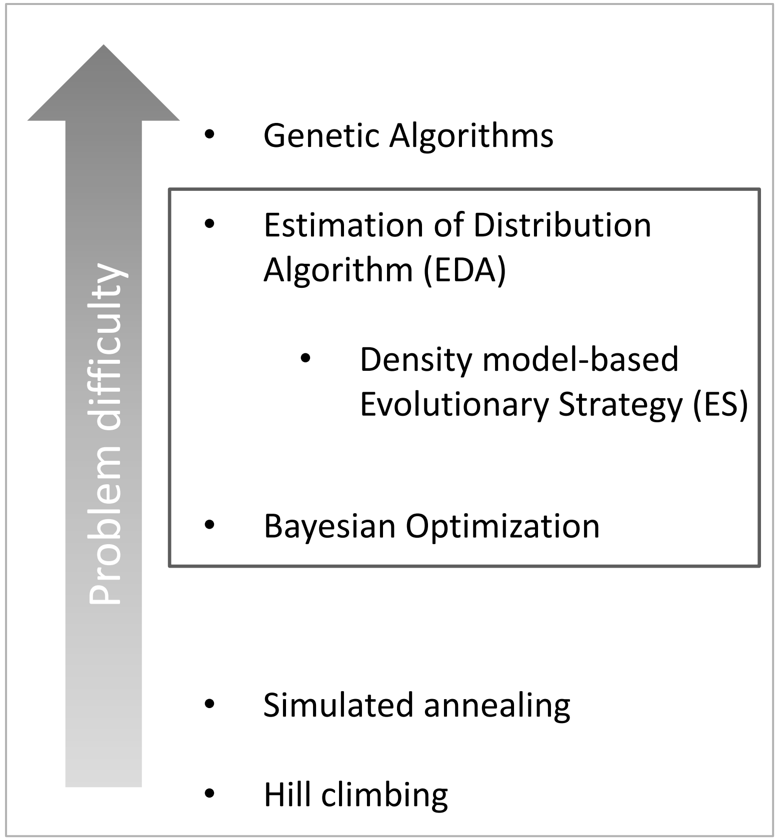
Model-based BBO

- View optimization as a series of incremental updates of a model
    - Gaussian process
    - Probabilistic distribution
- Initialize the model
- Sample candidate solutions
- Evaluate the samples and update the model



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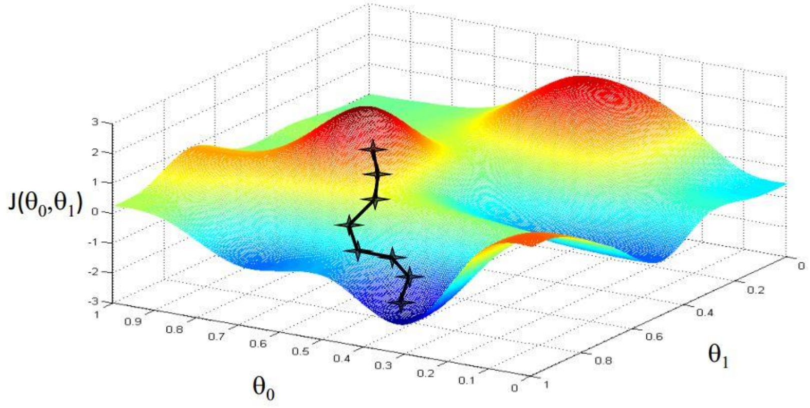
Hill Climbing



- Starts from a random point
- Randomly selects a neighbor with **better** value

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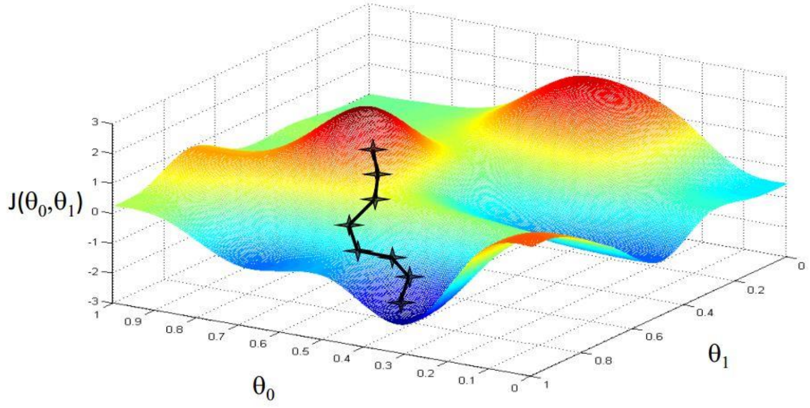

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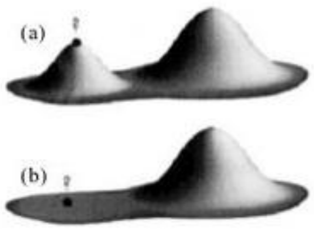

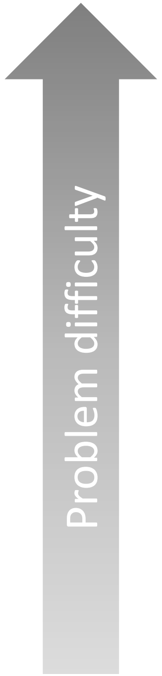

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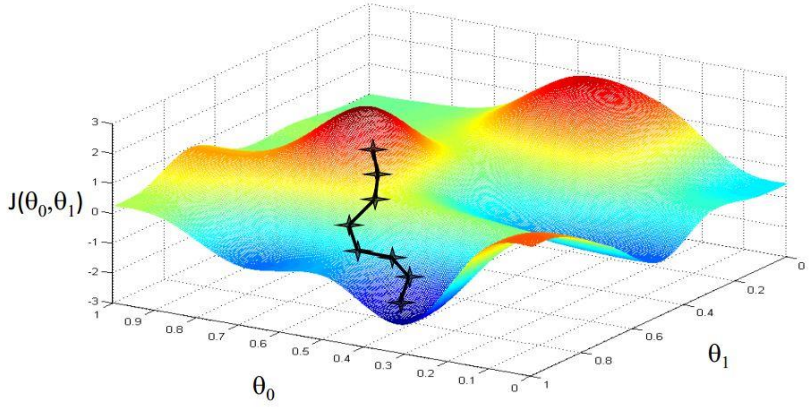

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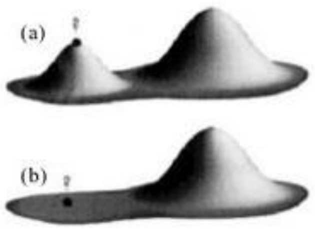

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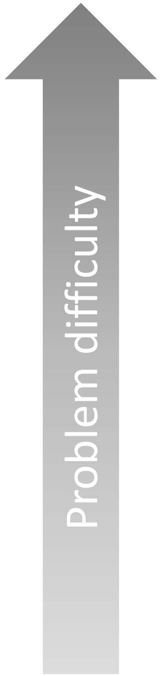
- Hill climbing vs Gradient descent?



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https://umu.to/blog/2018/06/29/hill-climbing-irl
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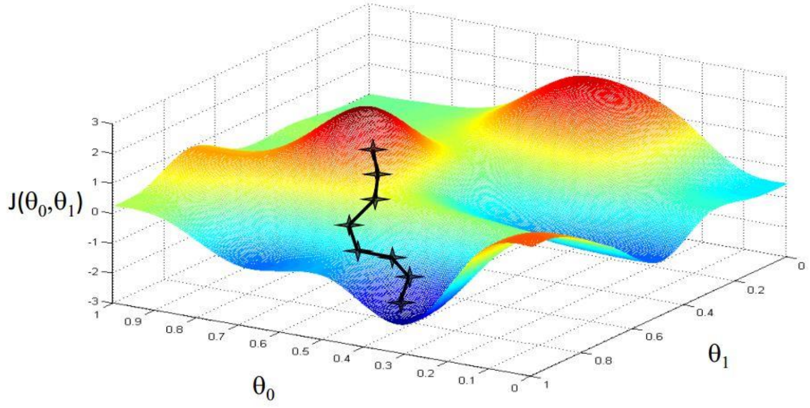

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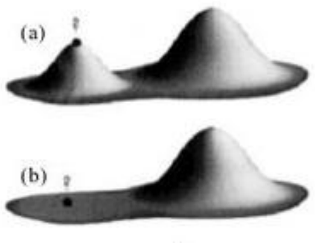

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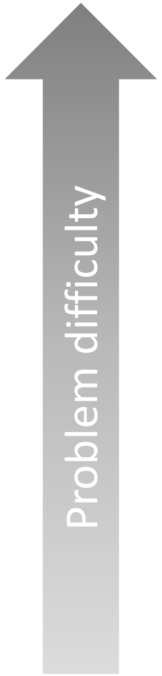
- Hill climbing vs Gradient descent? **Greedy** choice the next point based on **immediate local information** regardless of gradient amount or direction



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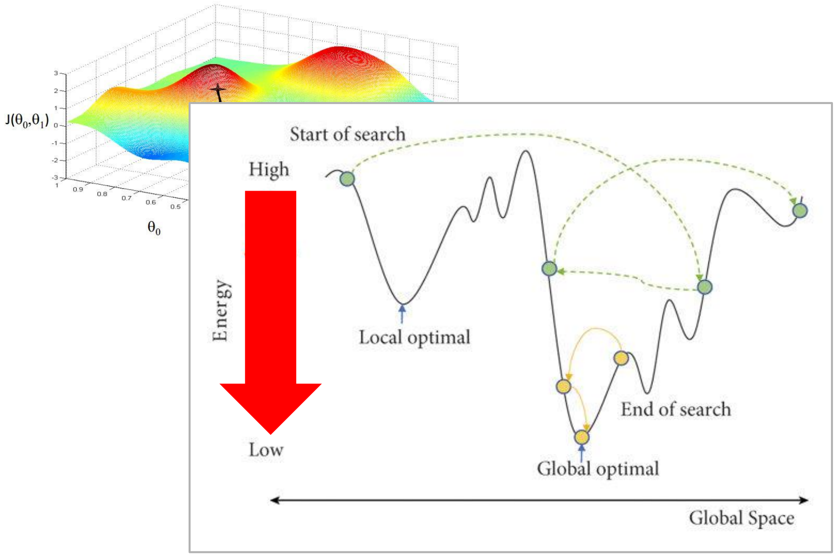
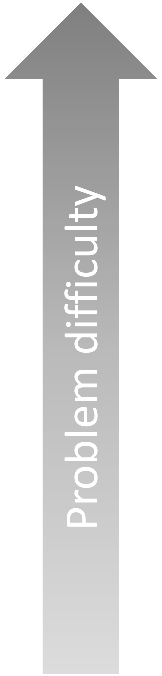
Simulated Annealing



- Accepts **suboptimal** solutions with a probability relative to a **temperature** parameter and has an **adaptive step size**
- Provides better exploration and possibility of jumping out of local optima



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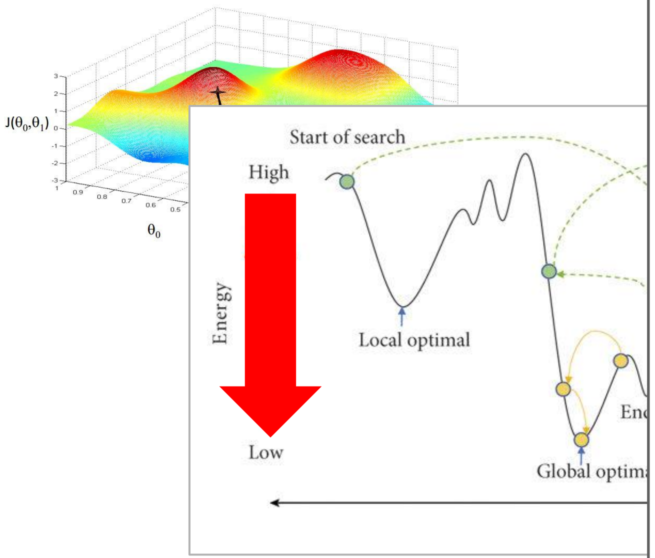

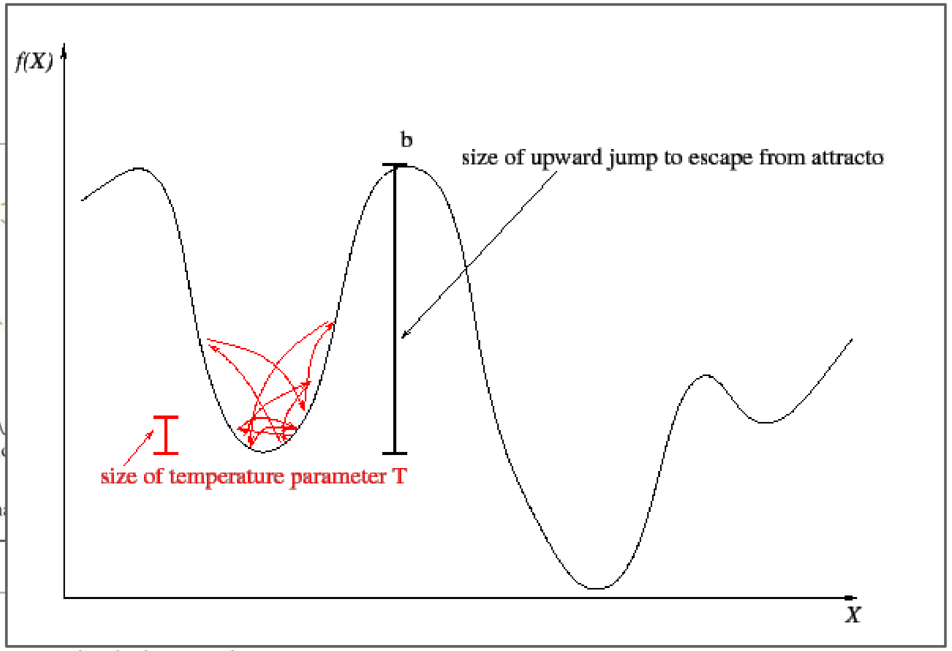

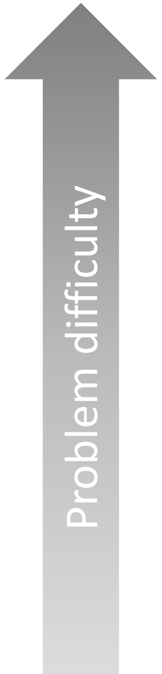

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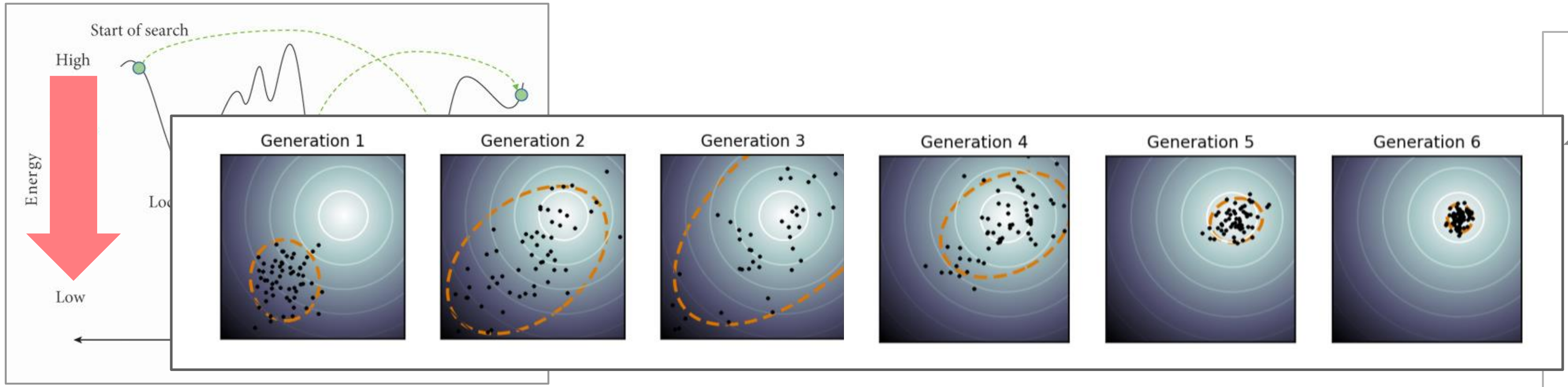
- **One sample at a time** gives a very limited view of the optimization landscape and scheduled temperature leads to premature convergence

https://www.researchgate.net/figure/Principle-of-the-simulated-annealing-algorithm_fig5_360434054
https://www.researchgate.net/figure/Simulated-Annealing-if-the-temperature-is-very-low-wrt-the-jump-size-SA-risks-a_fig4_30531067

Density Model-Based ES



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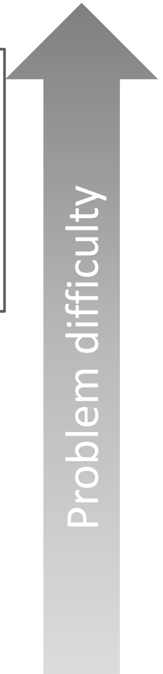

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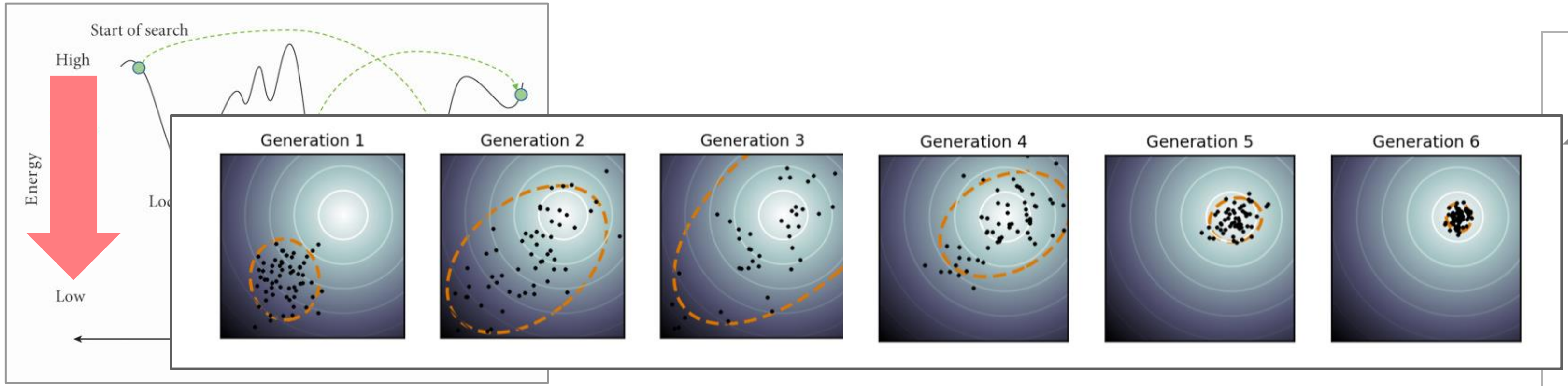

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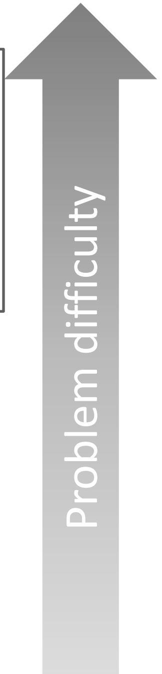

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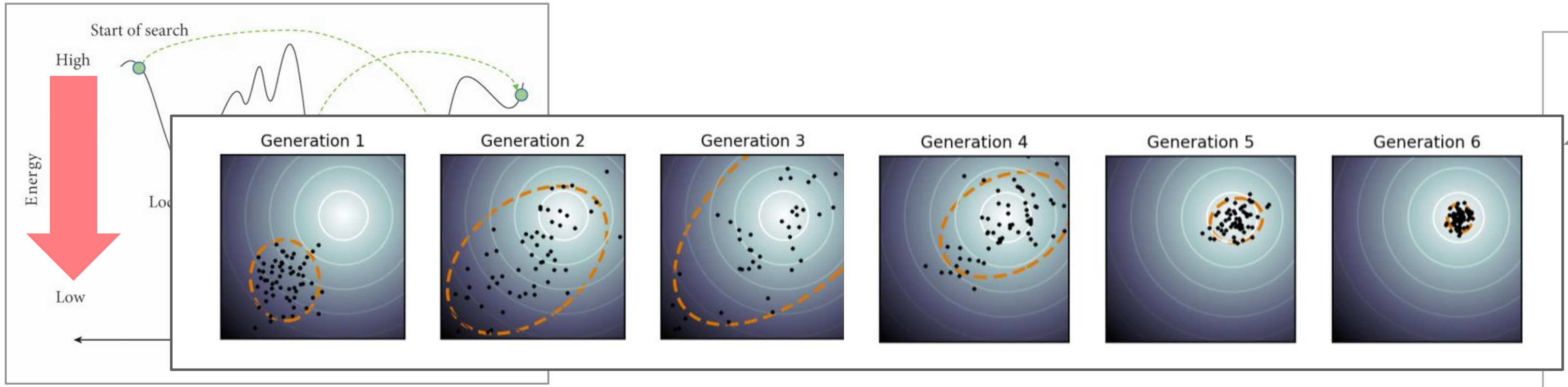

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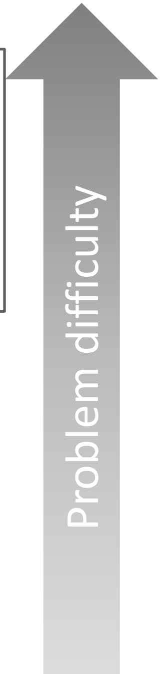
- **Evaluation:** Calculating the function value **(Fitness)** for each individual



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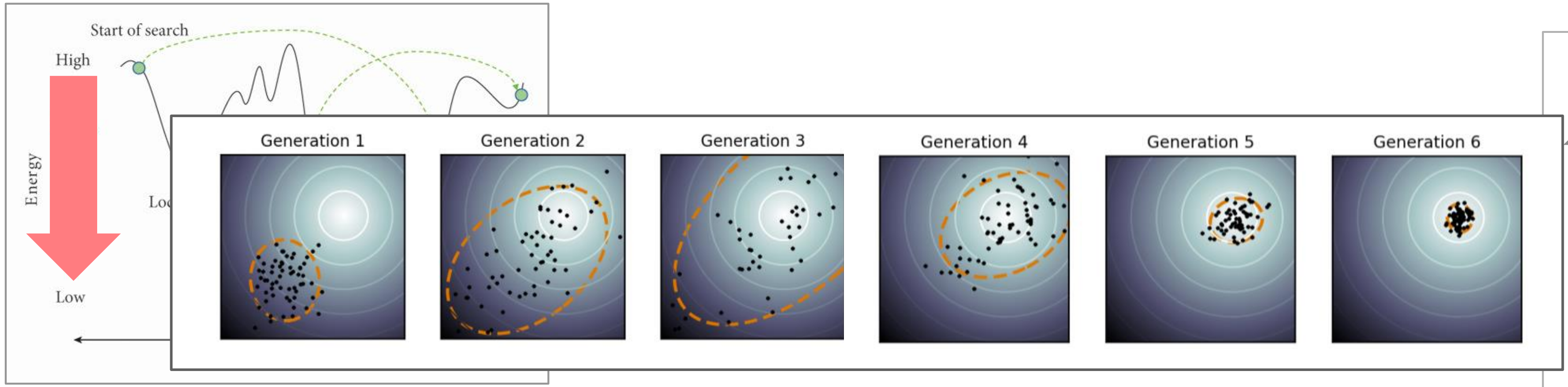

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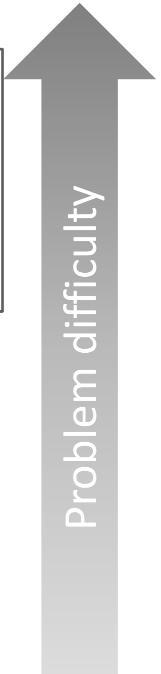

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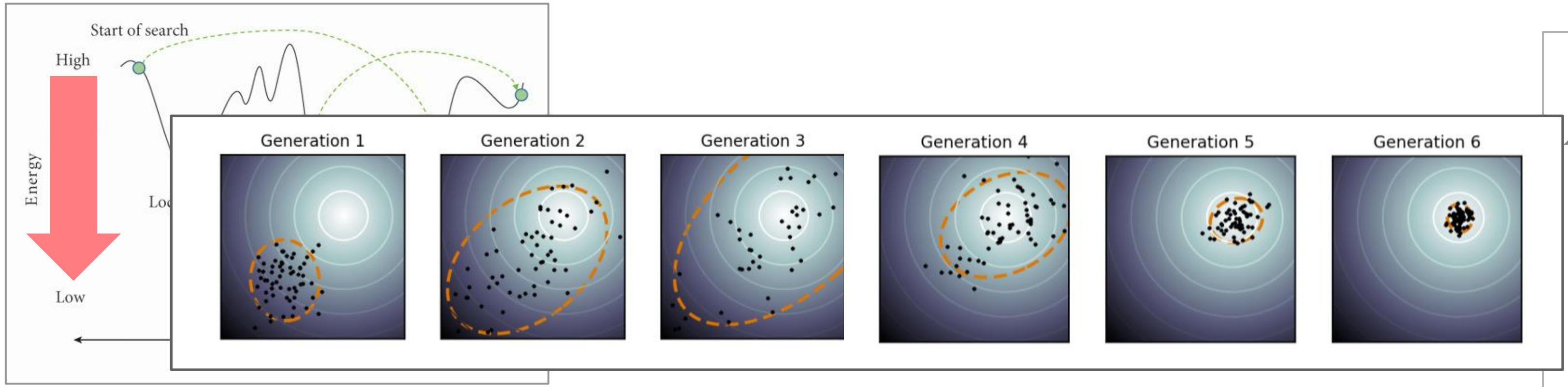

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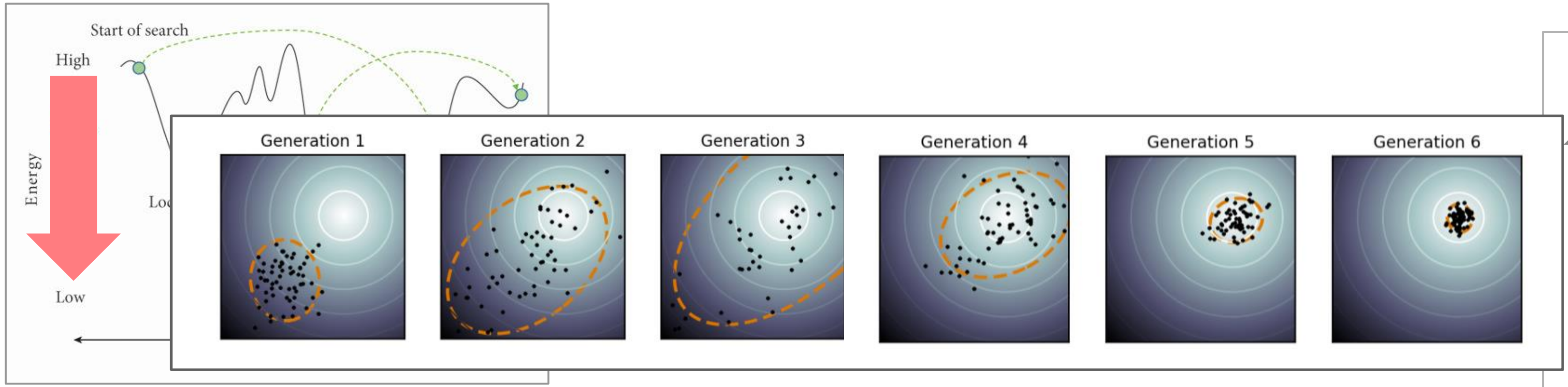

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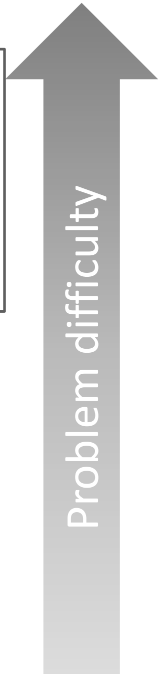

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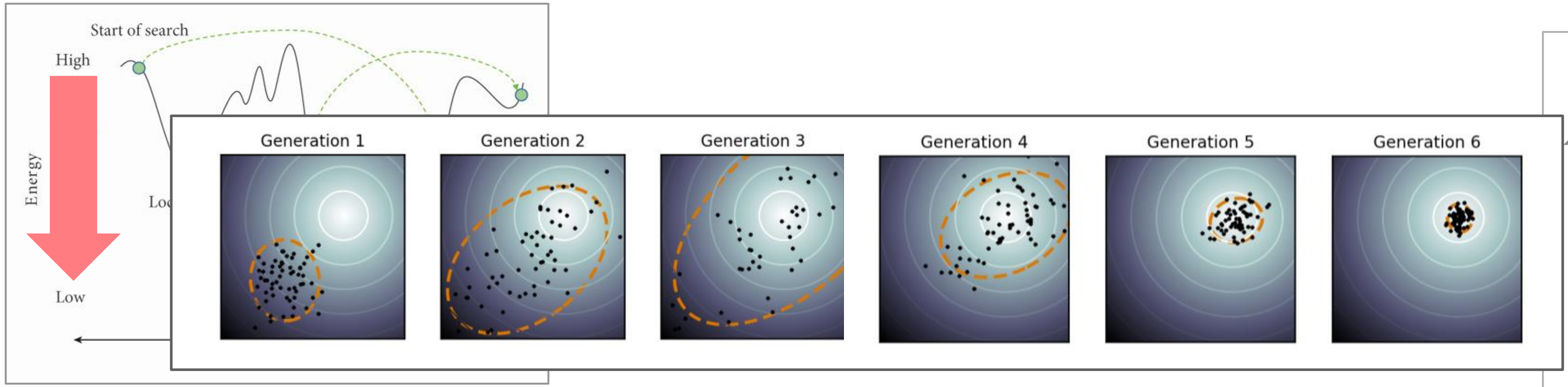

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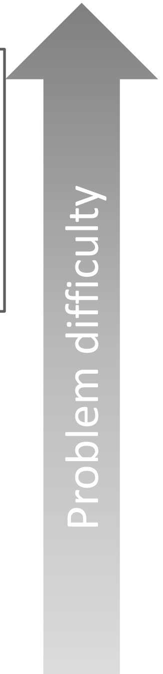

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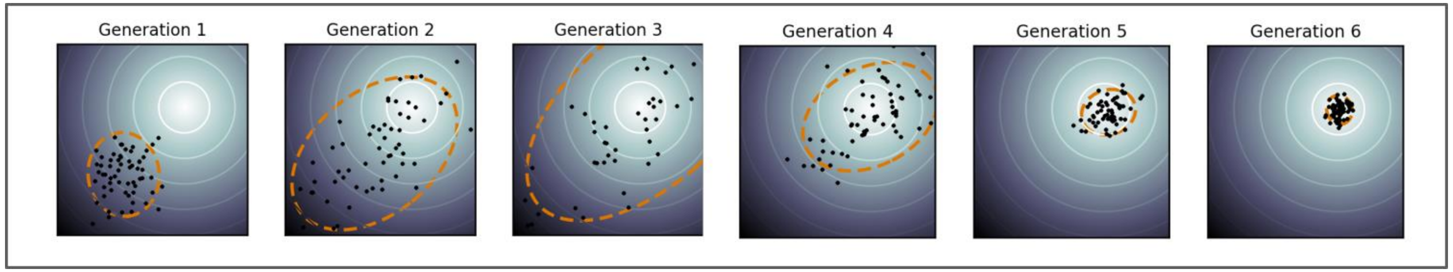
Covariance Matrix Adaptation Evolution Strategy (CMA-ES), a popular Density Model-Based ES



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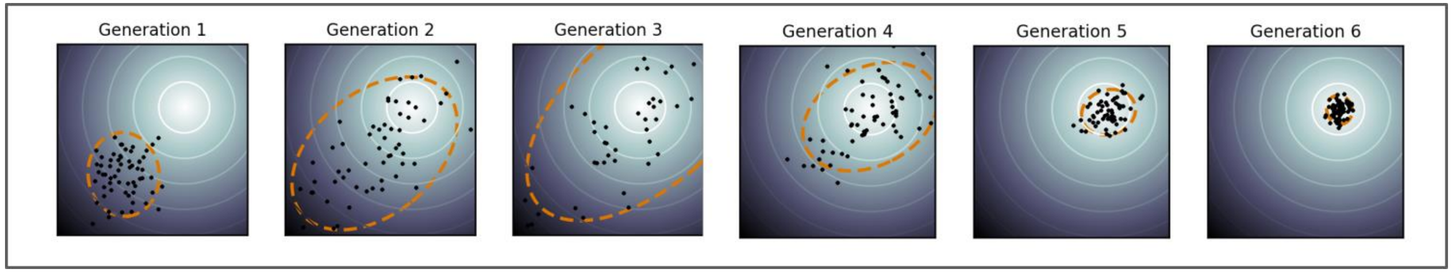
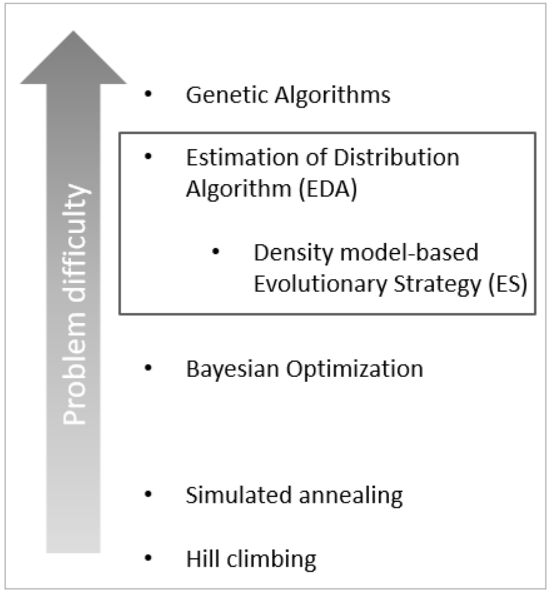


- Randomly sampling the 1st generation from a standard **Gaussian** distribution
- Evaluation: calculating fitness for each individual
- Selection: selecting the fitter individuals
- Updating covariance matrix and mean of the Gaussian
- Creating next generation from the updated Gaussian



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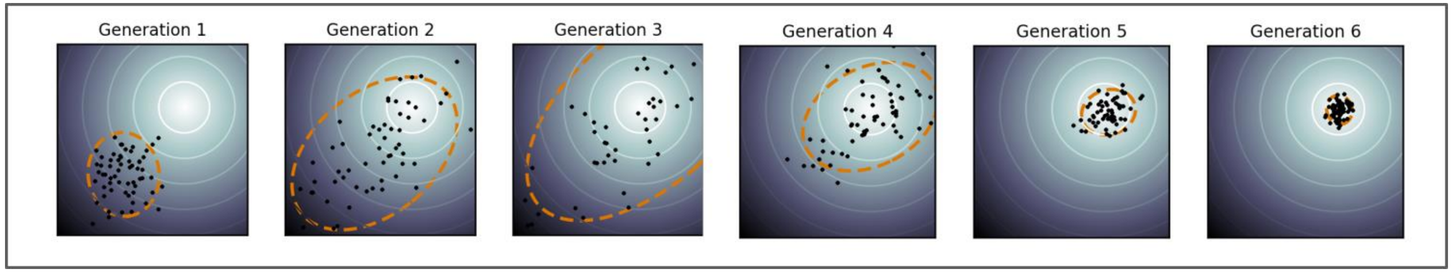

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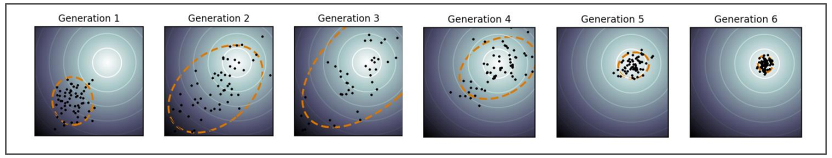
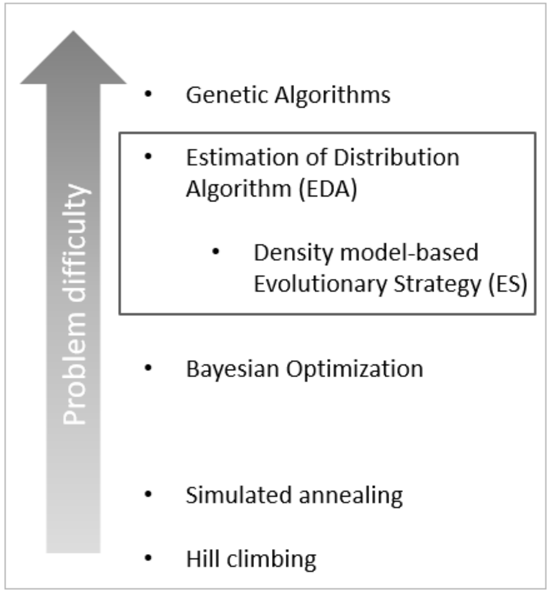


Drawbacks of CMA-ES:

- Arbitrary choice of distribution limits performance



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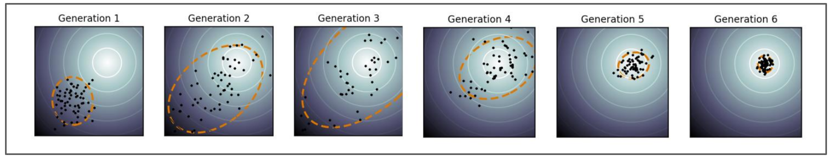

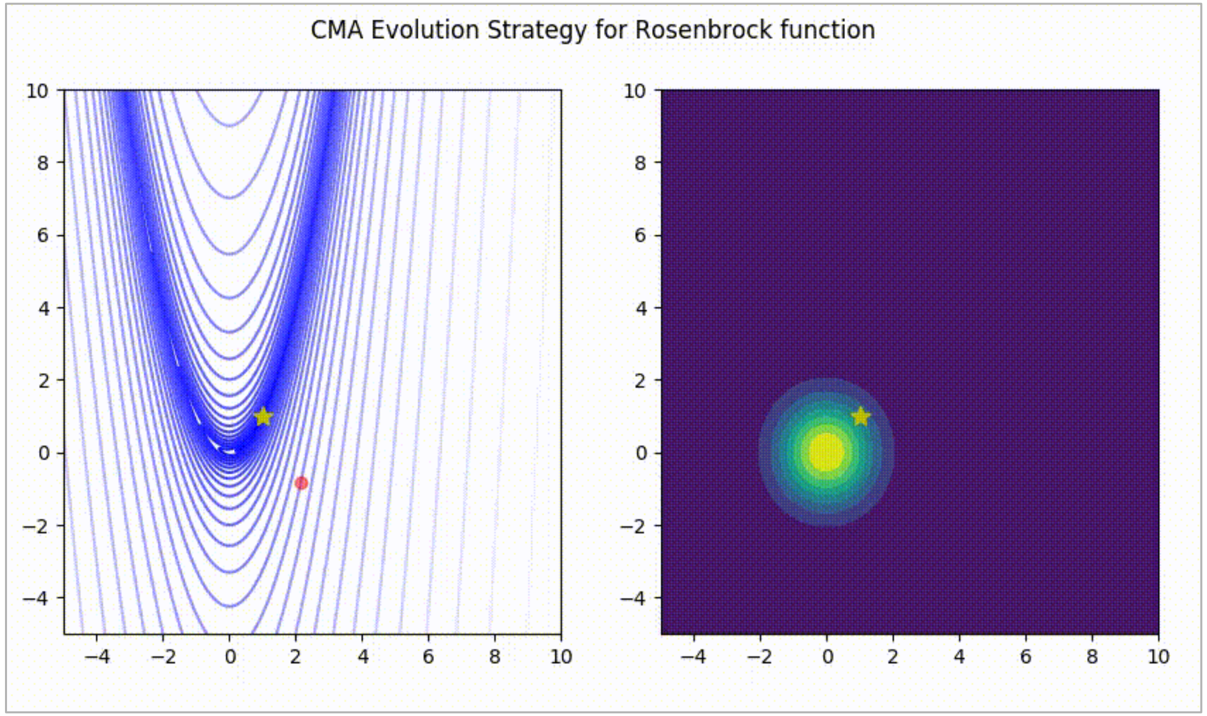

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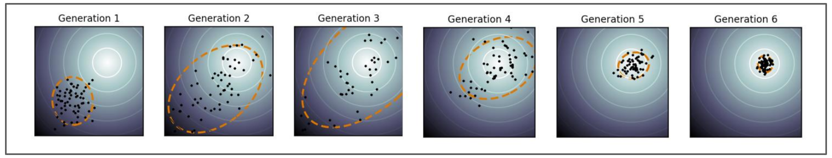

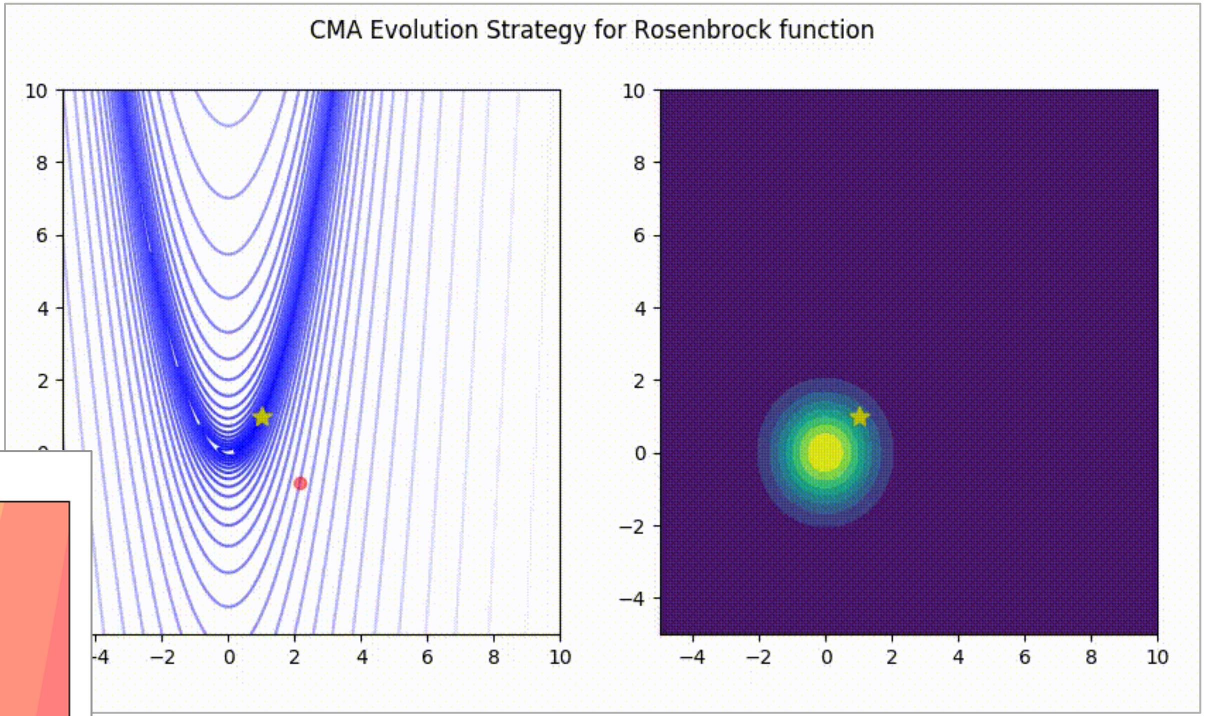

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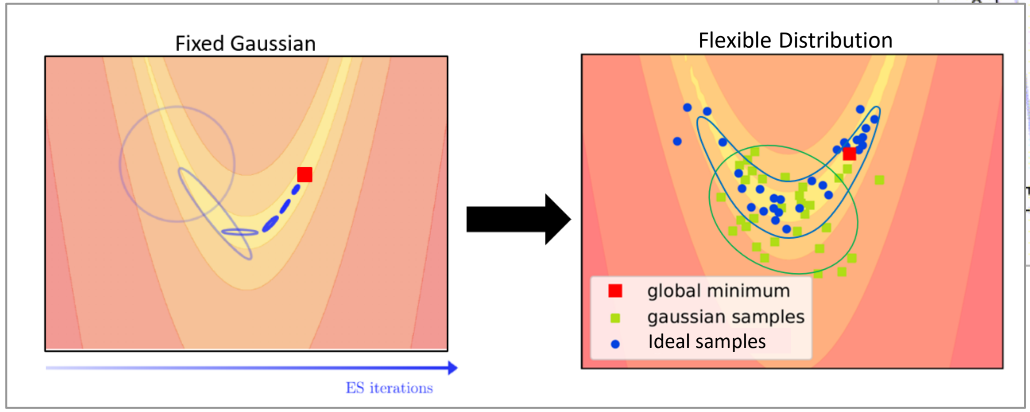

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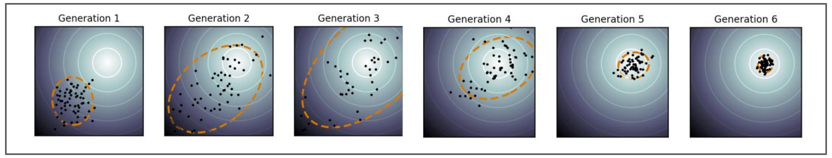
CMA-ES

Covariance Matrix Adaptation Evolution Strategy (CMA-ES), a popular Density Model-Based ES



Drawbacks of CMA-ES:

- Arbitrary choice of distribution limits performance
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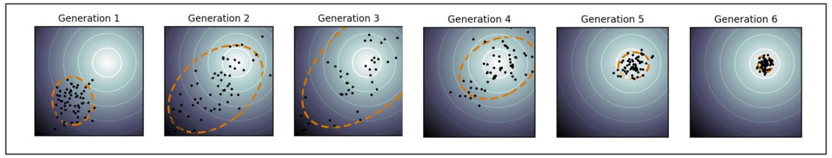

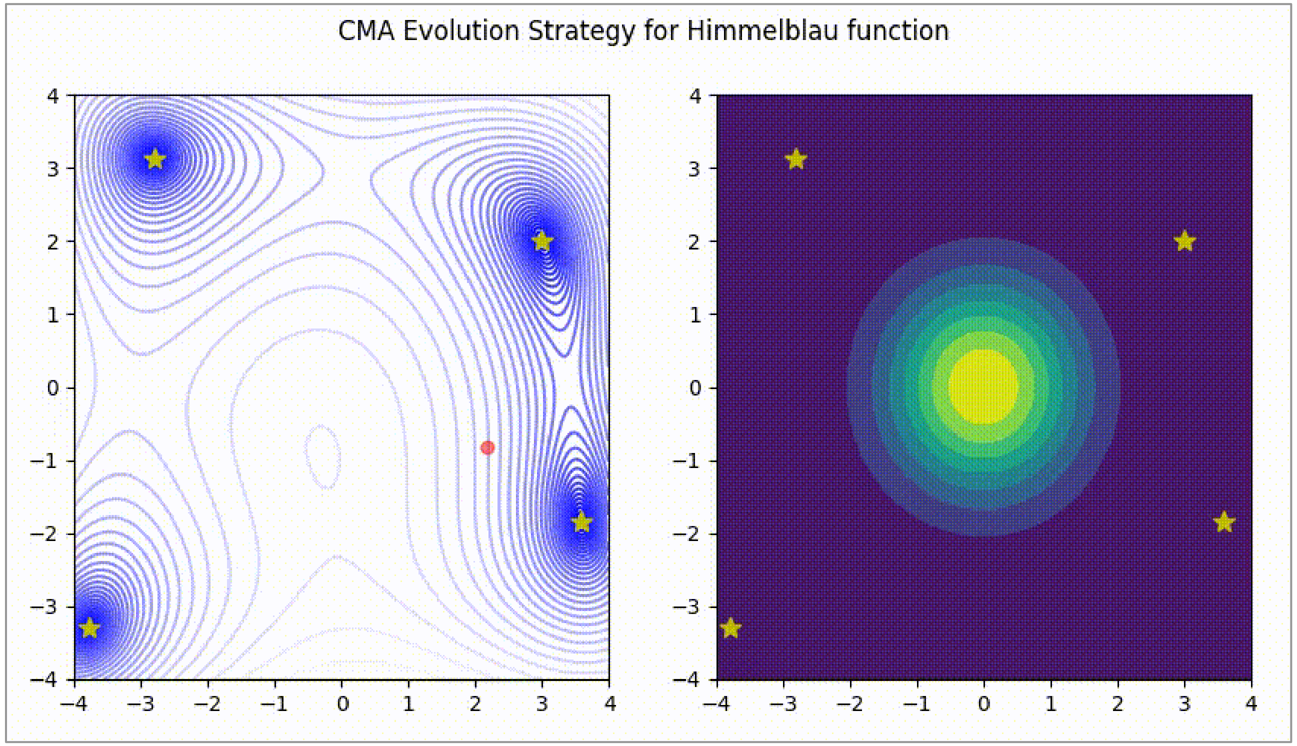

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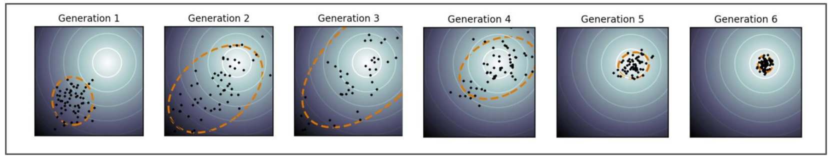

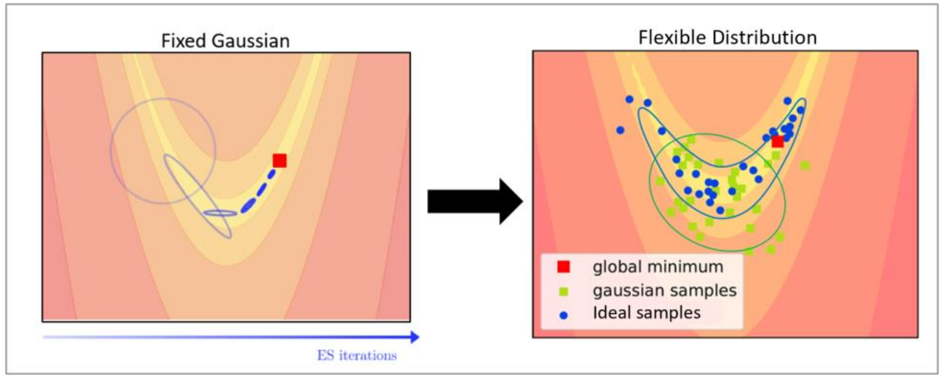

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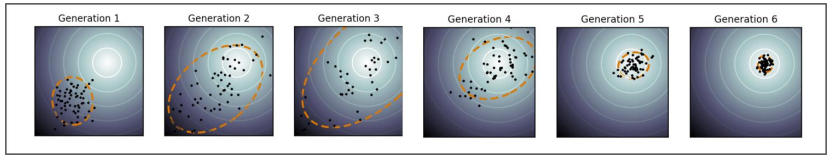

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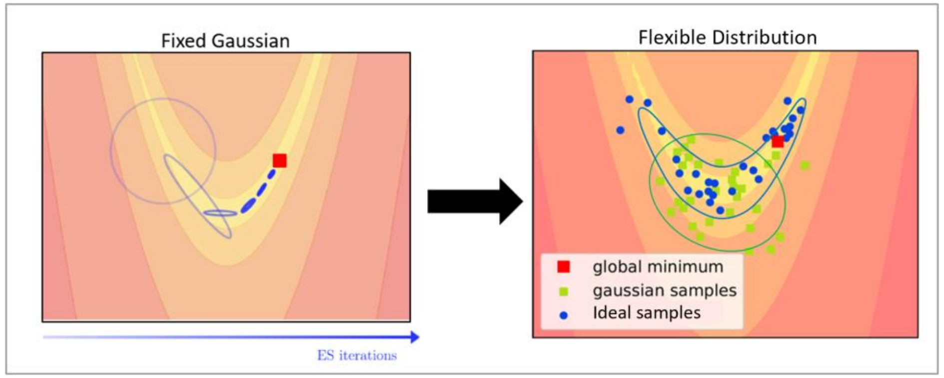

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Learn probability distribution $p_x(x)$ over a random variable X from observations

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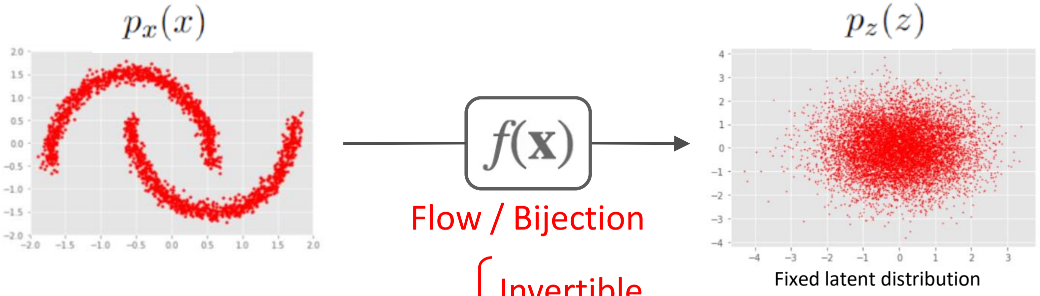

$$p_{\mathbf{X}}(\mathbf{x}) = p_{\mathbf{Z}}(f(\mathbf{x})) \left| \det Df(\mathbf{x}) \right|$$

Invertible
Differentiable

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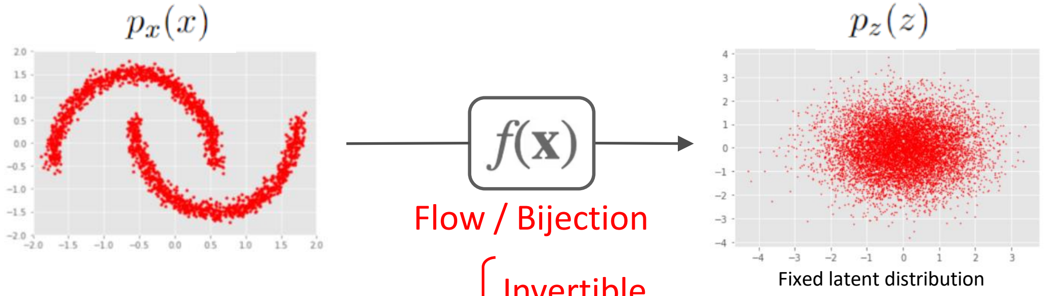

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Designing flows is the core research problem in NFs

- Each flow layer in NF is a simple invertible, differentiable function
- The overall flow network is a composition of simple flow layers

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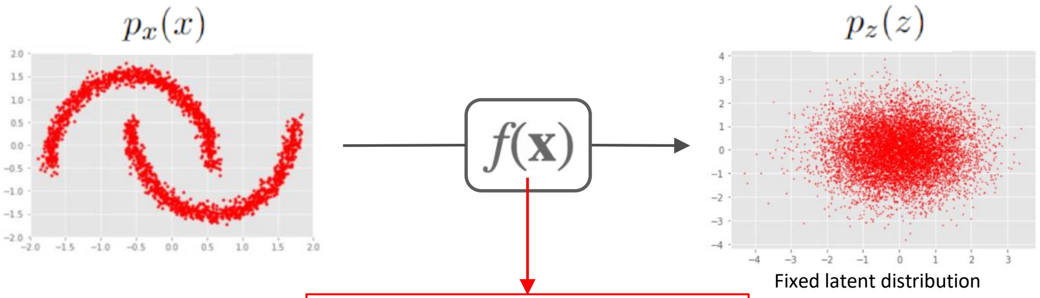

$$f = f_K \circ f_{K-1} \circ \cdots \circ f_2 \circ f_1$$

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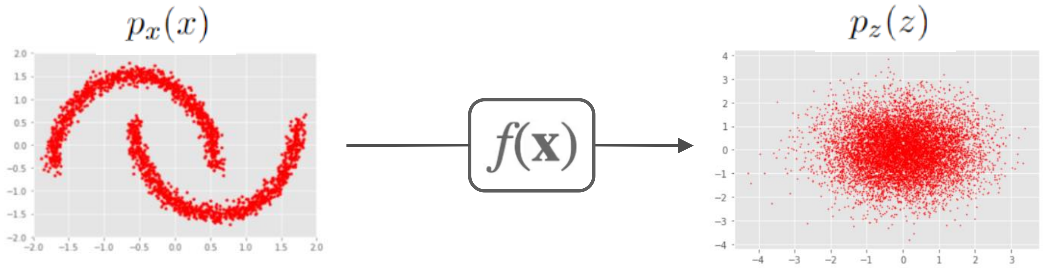
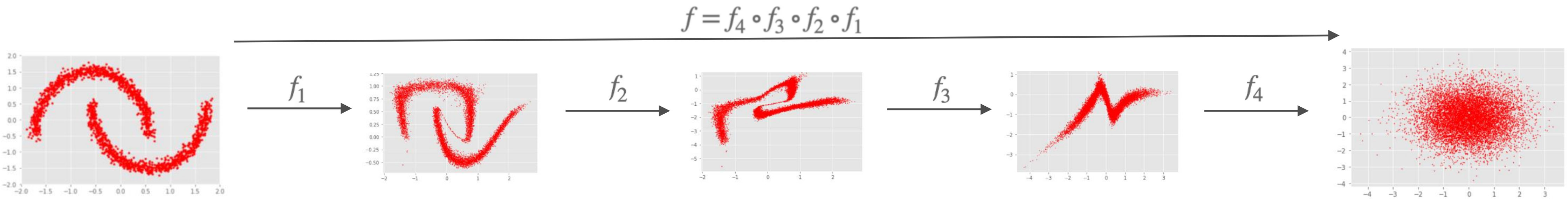


Fixed latent distribution



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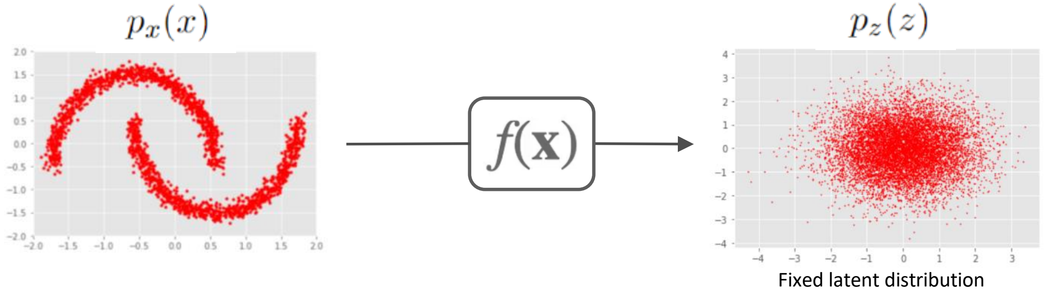

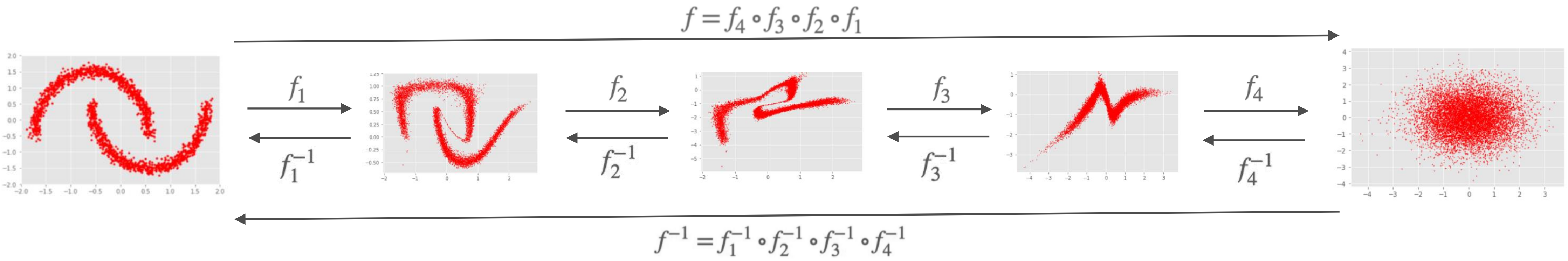

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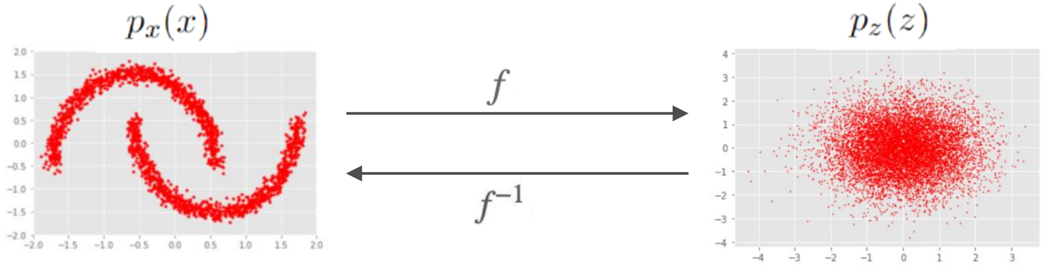

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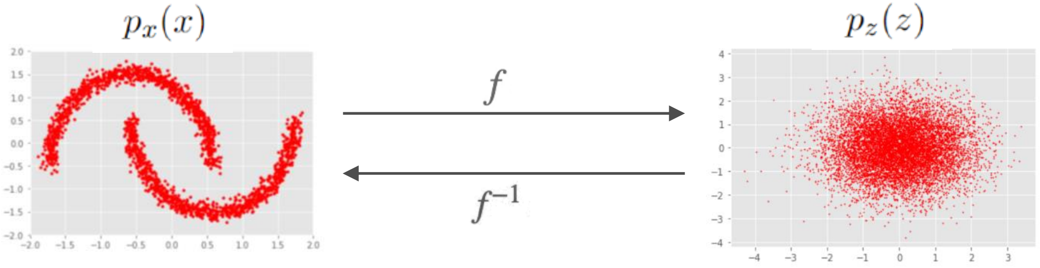

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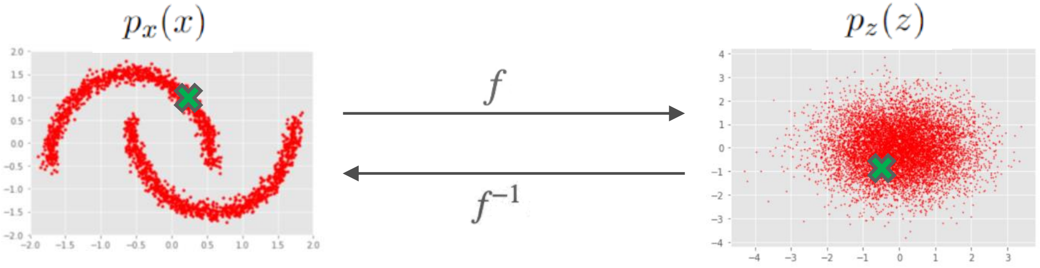

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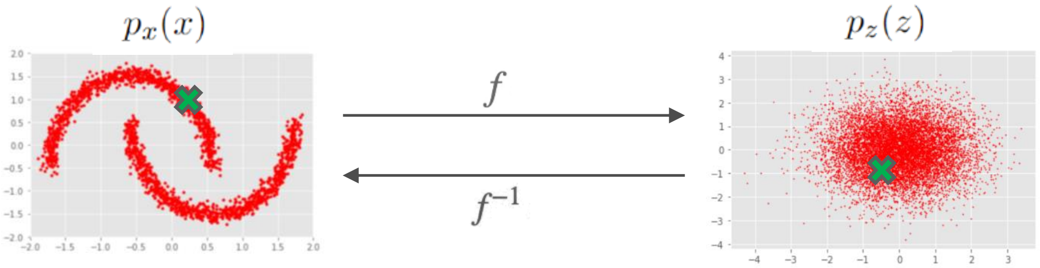

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- **Experiments and Results**
- Conclusion and Future steps
- Conclusion / PhD Plan

Recap

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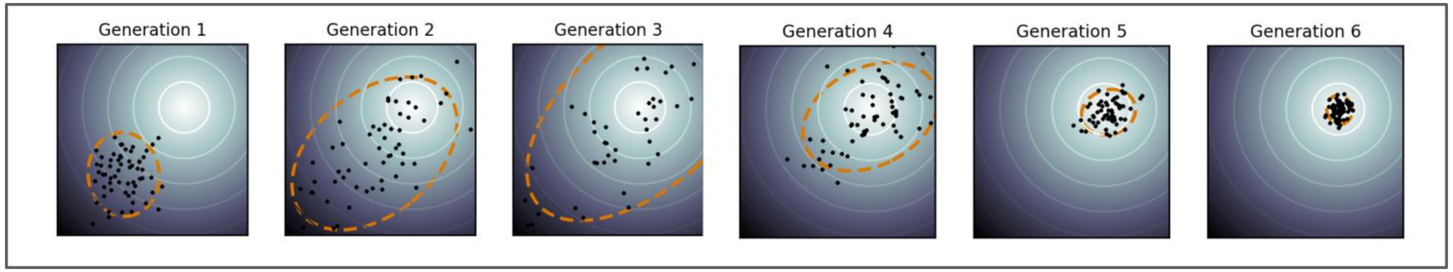

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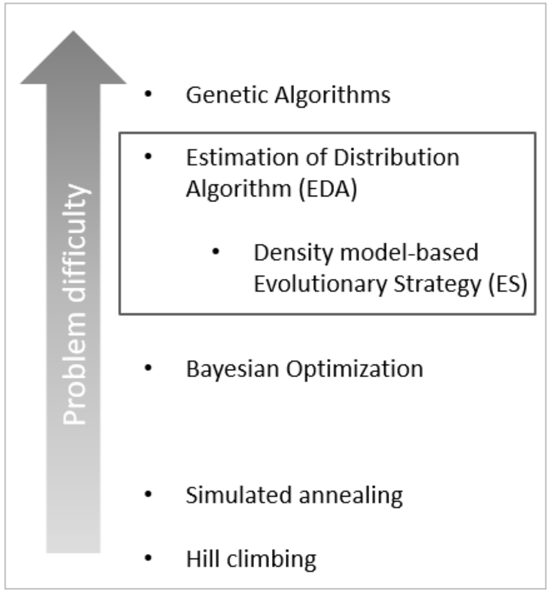

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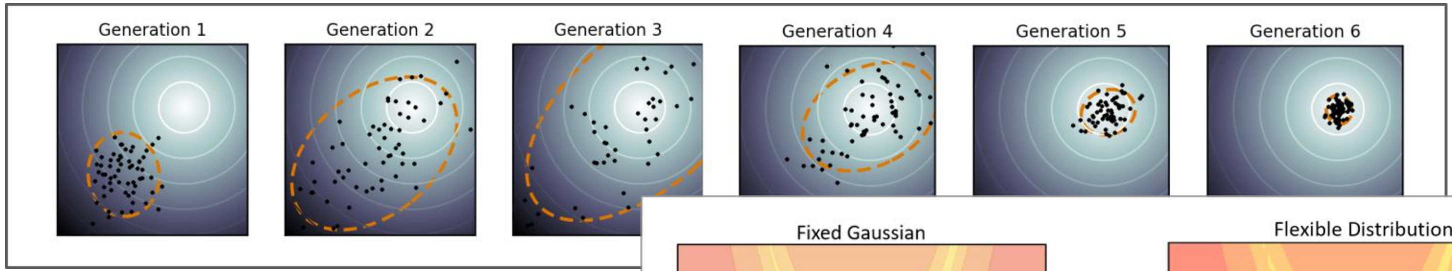

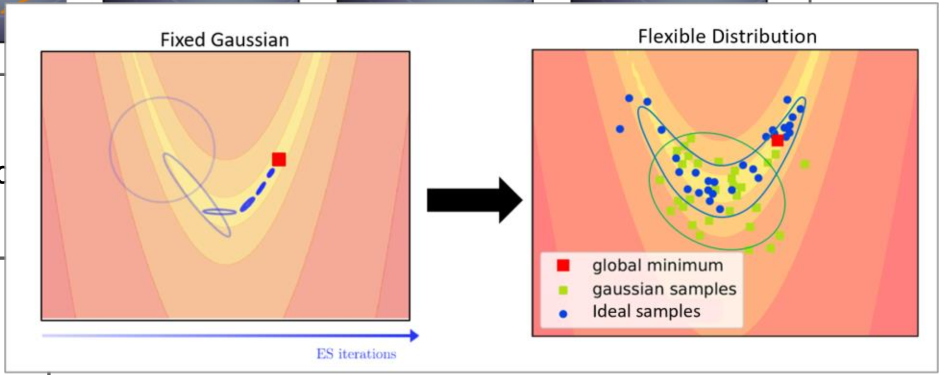

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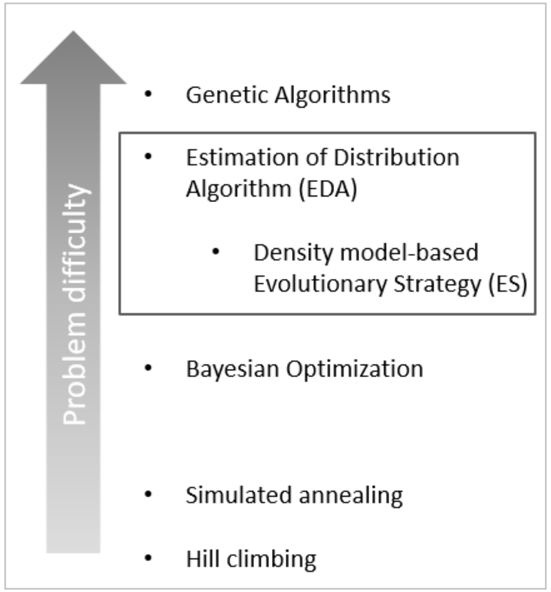

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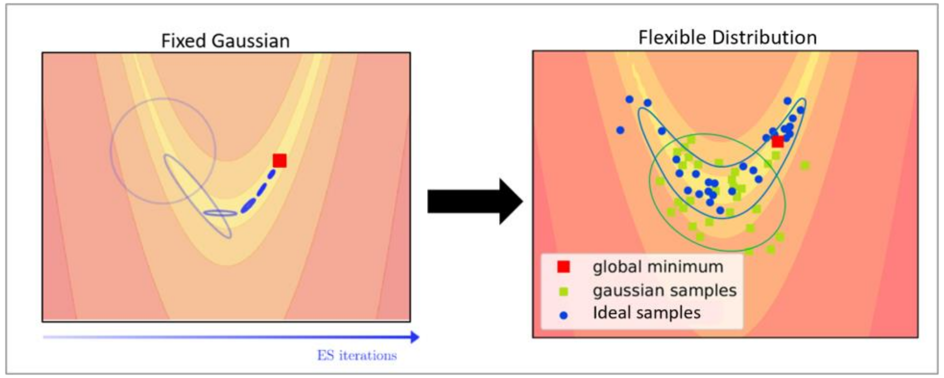

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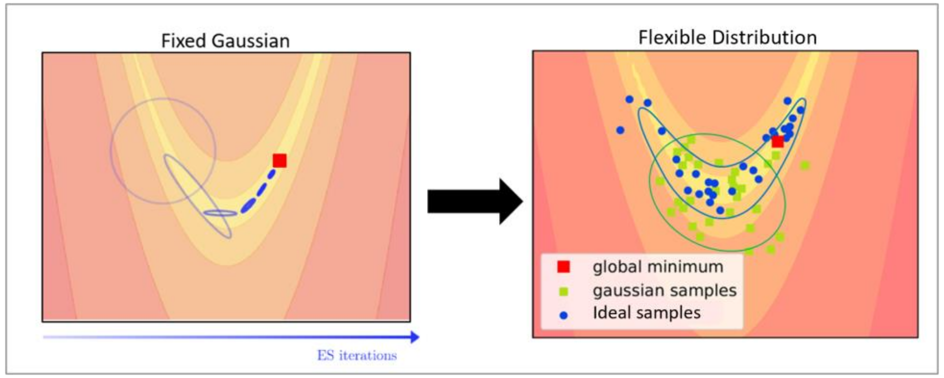

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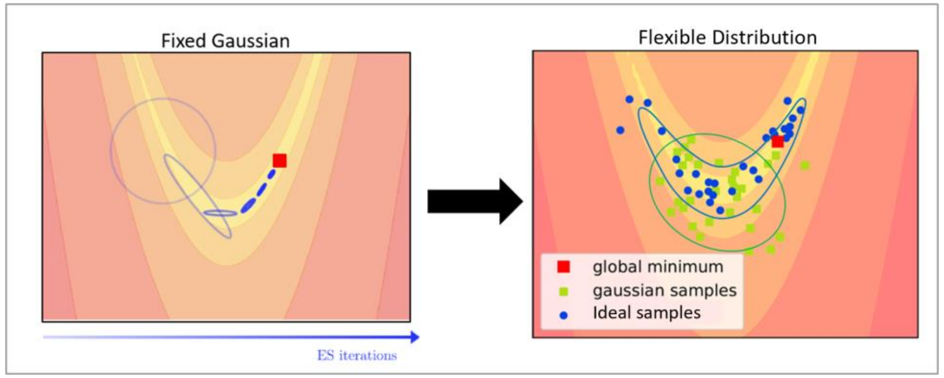

Integrating RealNVP in EDA (Estimation of Distribution Alg.)

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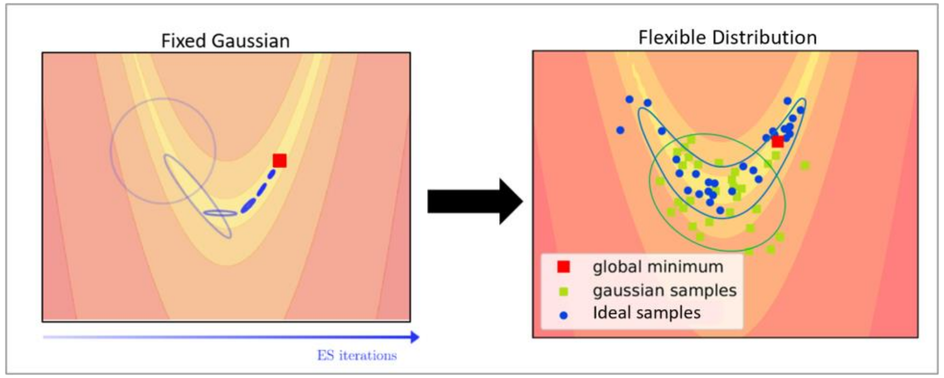

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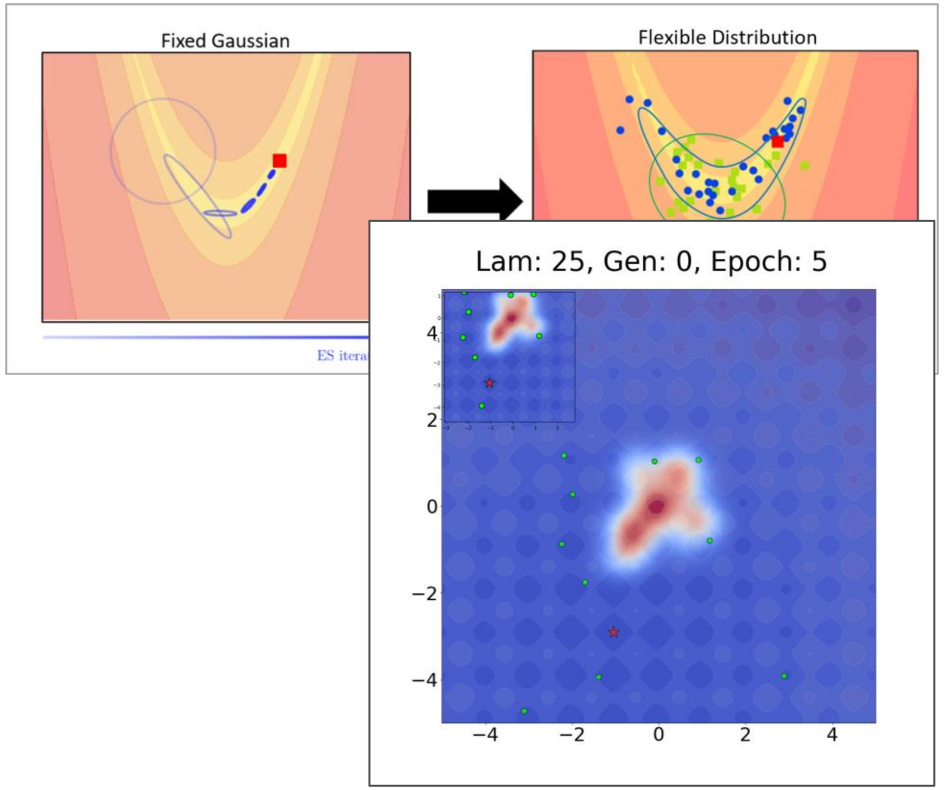

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- **Remapping** the selected samples to the latent space
- **Taking ES step in the latent space** to generate the next generation
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NF+ES is expected to outperform NF+EDA

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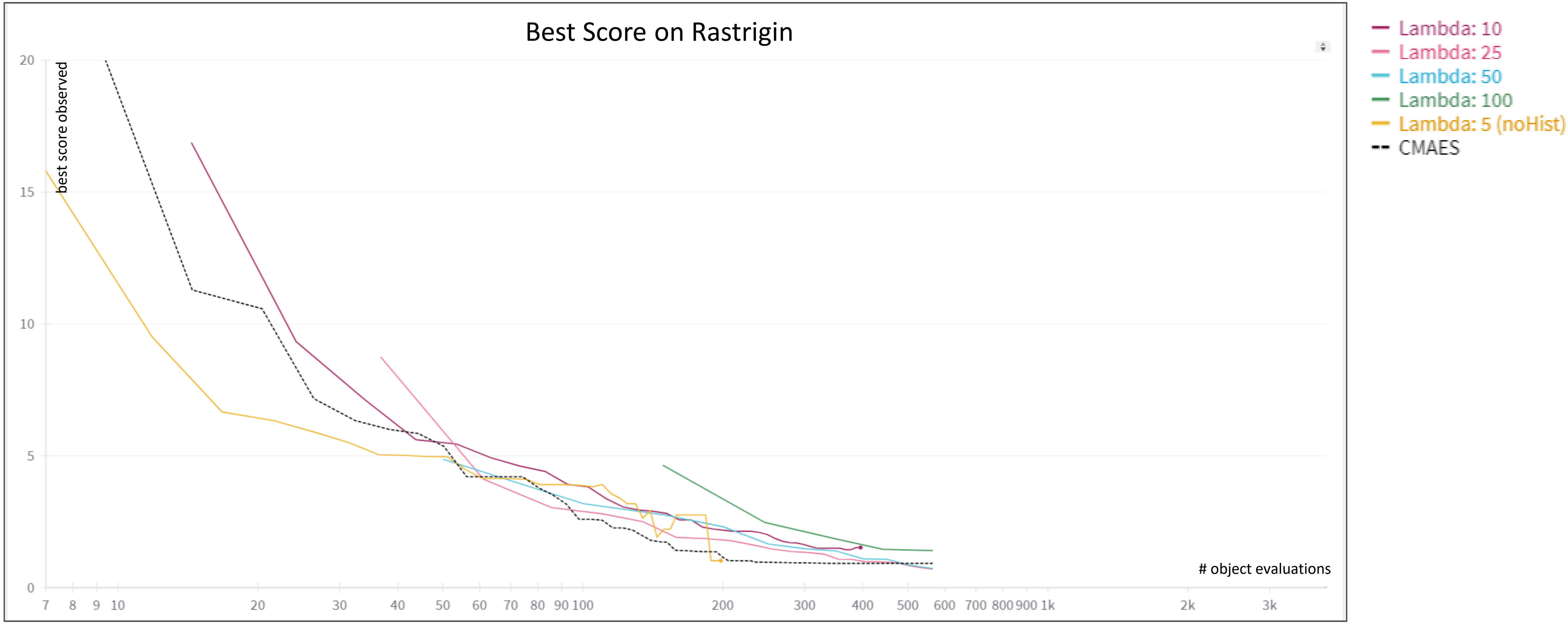

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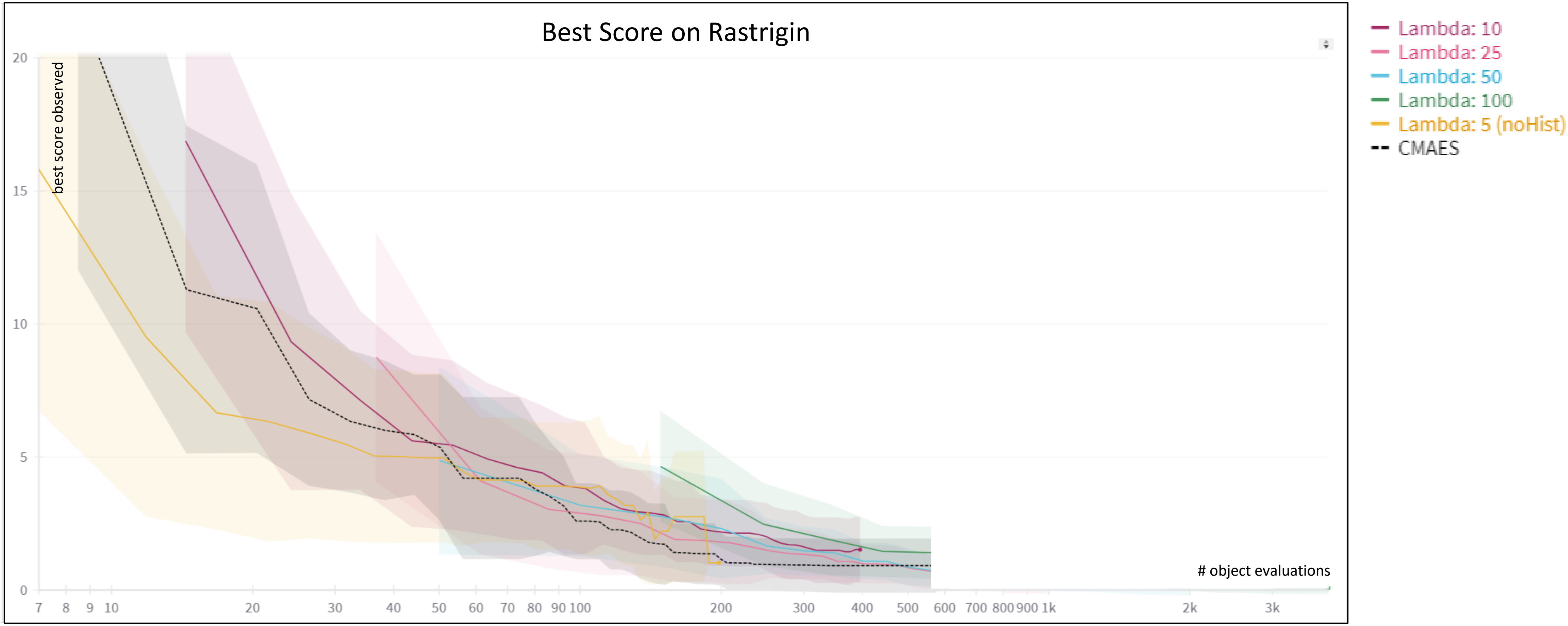
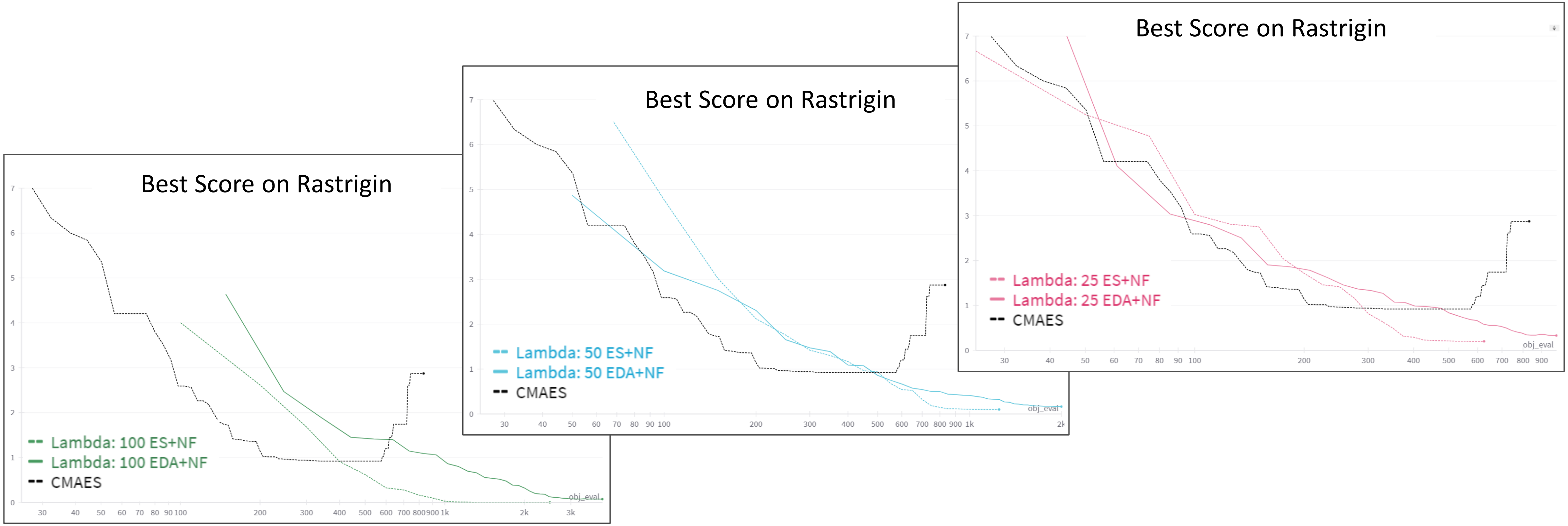


NF + ES (Evolutionary Strategy)

NF + ES model-based BBO vs NF + EDA Model-based BBO



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Conclusion and Future Steps

- Preliminary Results:
  - NF has the required capability to enhance model-based BBO
  - NF+EDA results are promising despite the simplicity of the method and with minimum hyperparameter tuning
  - NF+ES results outperform NF+EDA and are competent with CMA-ES even in the preliminary experiments without hyperparameter tuning
- Challenges ahead:
  - Model convergence and Exploration/Exploitation balance
  - Hyperparameter tuning
  - Conducting experiments on real-world data
- Next phase:
  - Applying Meta-optimization to further improve performance and sample efficiency