Expensive black-box combinatorial optimization

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Permutation problems

A solution is a permutation of objects

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- Traveling Salesman Problem (TSP)

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  - $53! \approx 4.27e69$

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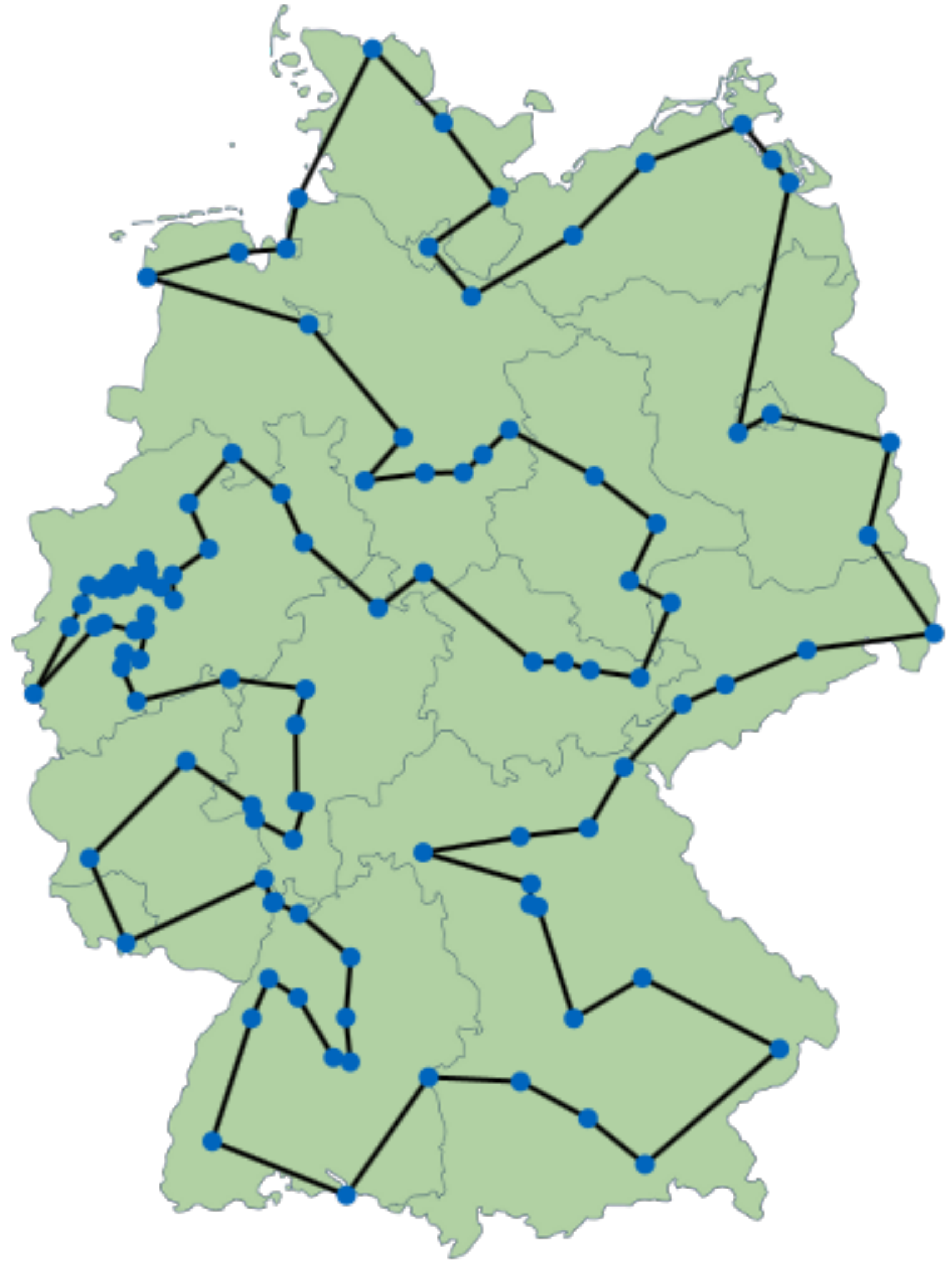
Number of atoms in the galaxy



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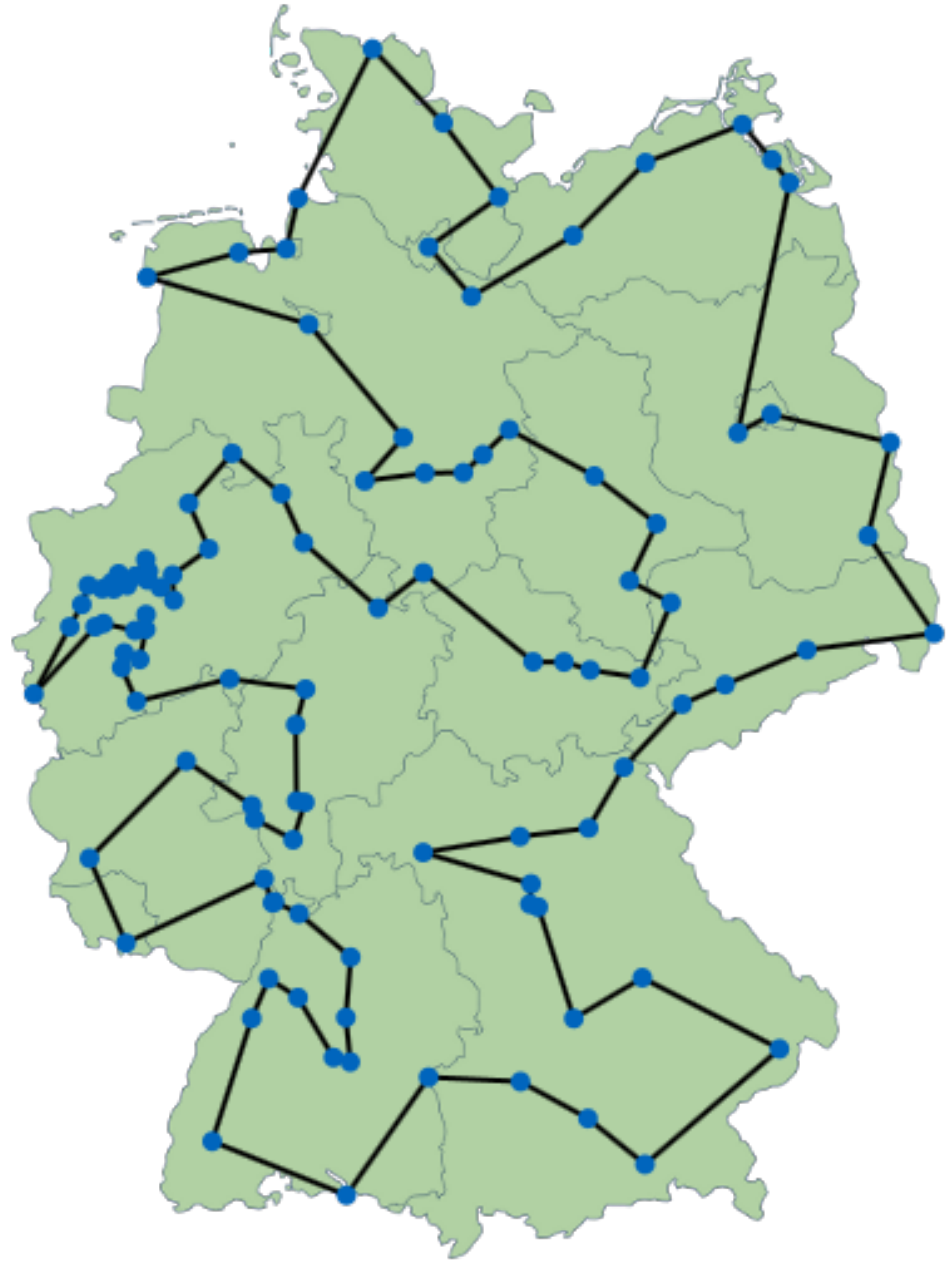

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Classical setting

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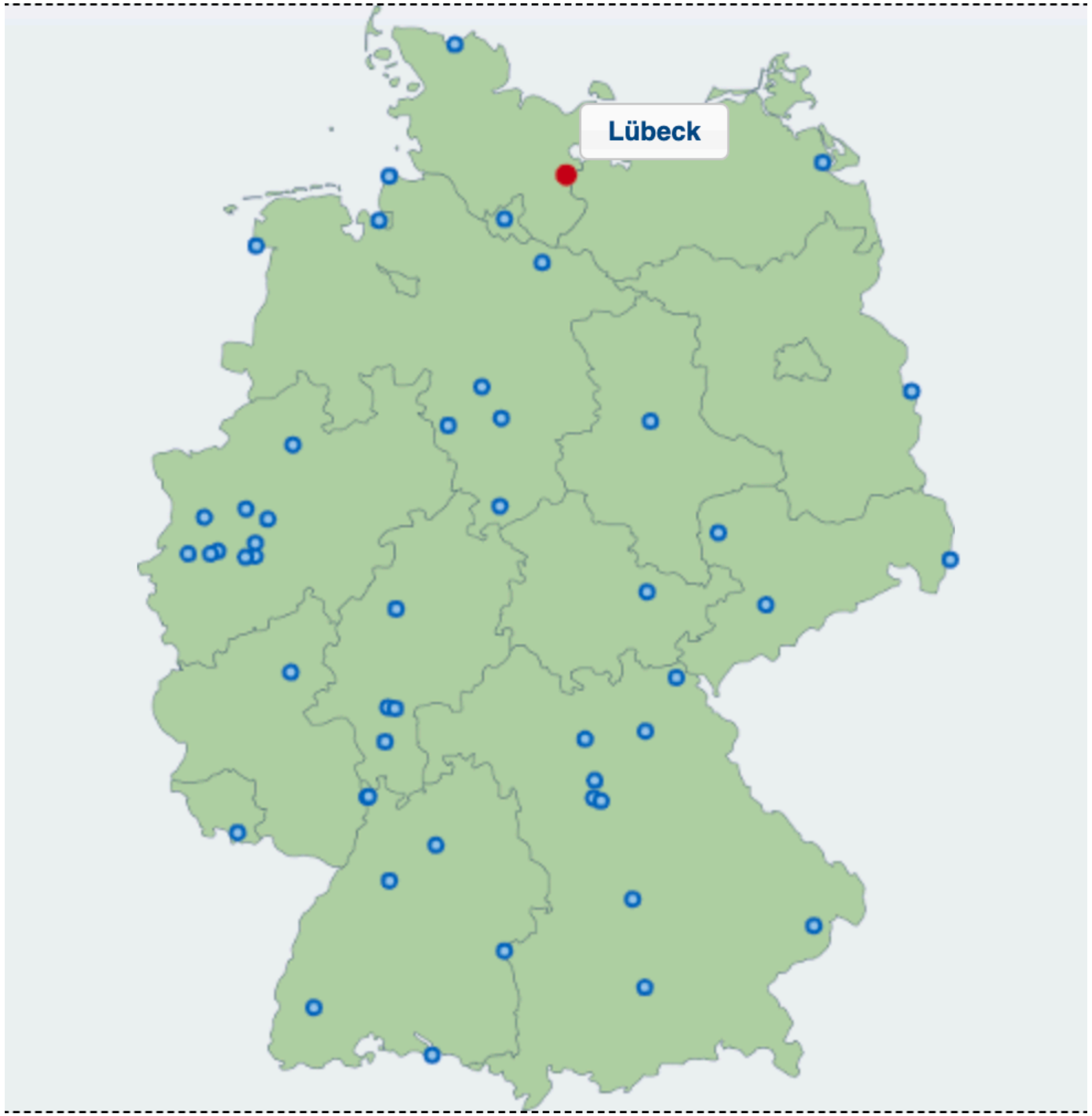
Go to the closest city

Classic greedy strategies



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- Deterministic but there are probabilistic variants
- Easy to implement, easy to justify
- Your first option!
- White-box: We need to have access to the particular instance

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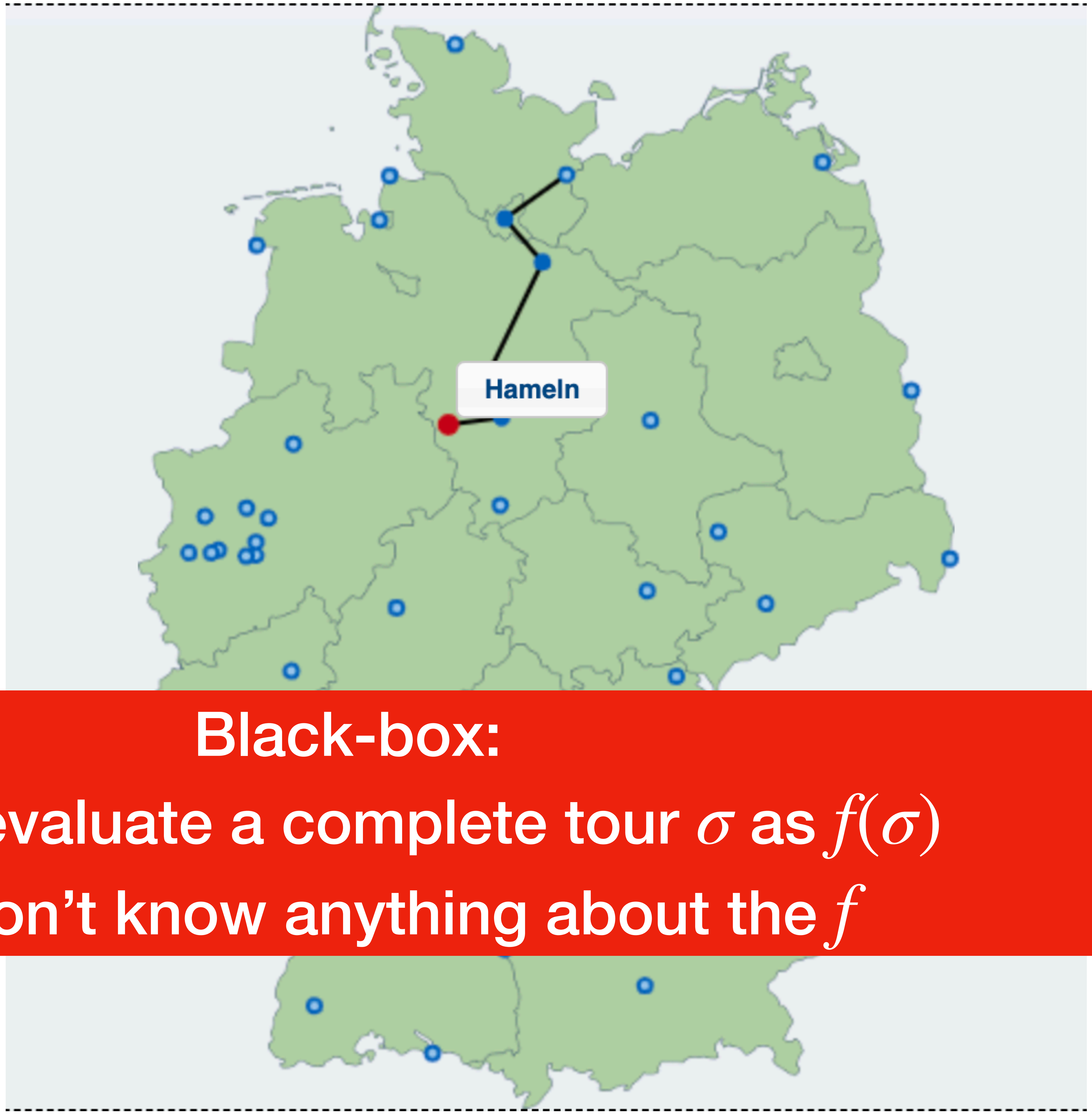

Black-box:
we can evaluate a complete tour σ as $f(\sigma)$
but don't know anything about the f

Genetic algorithms are black-box optimizers

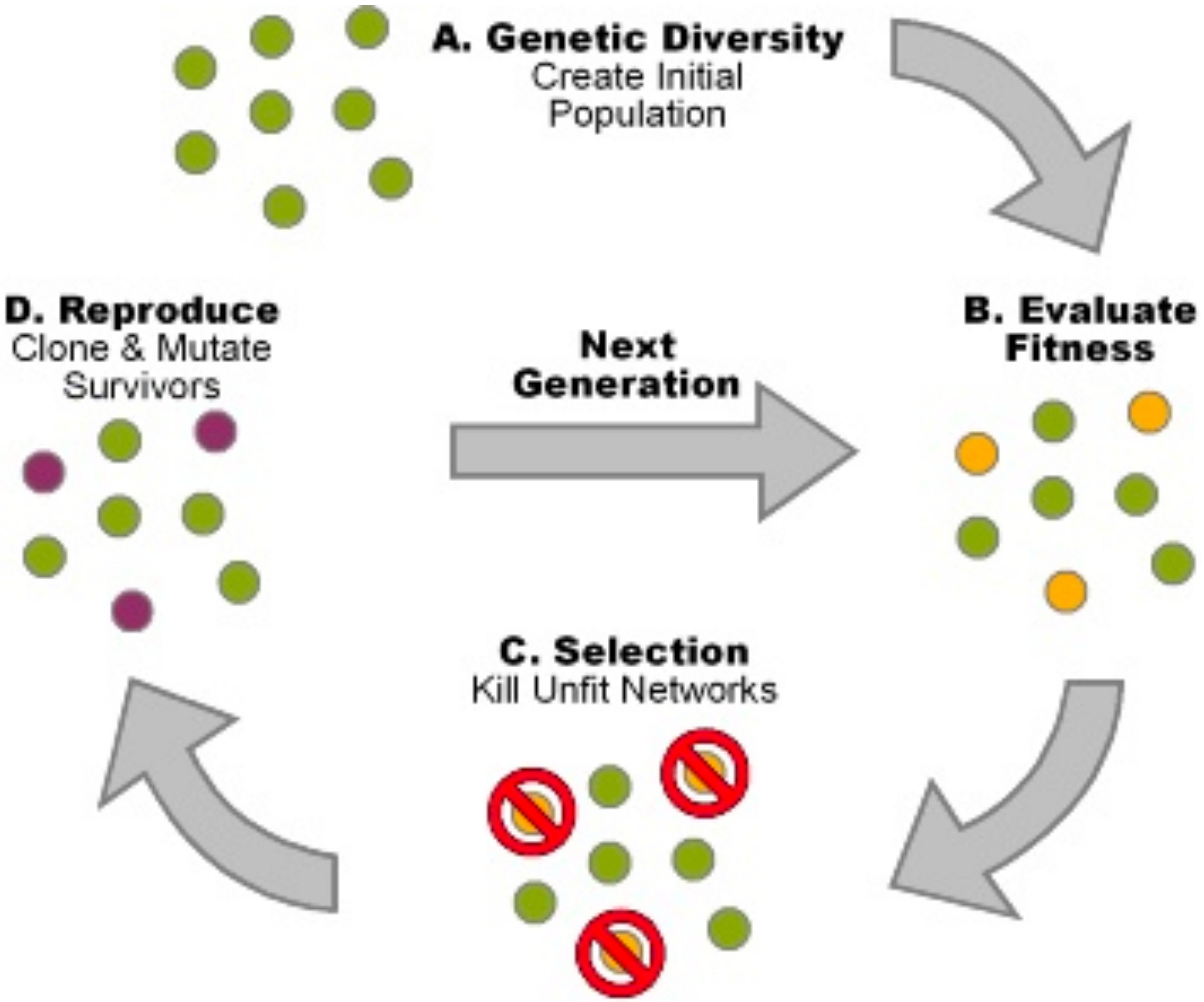

Image by https://quantdare.com

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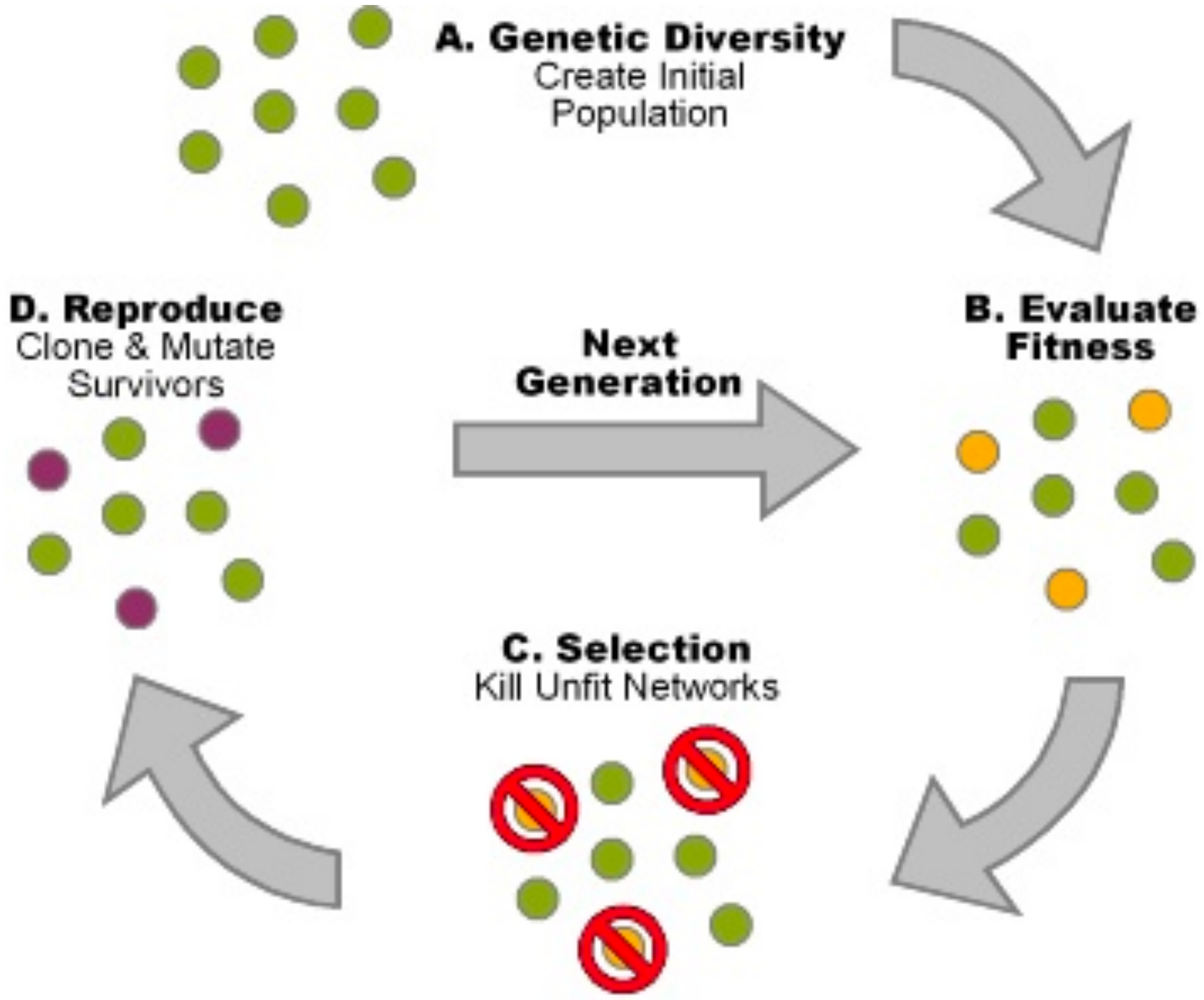

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- Millions of function evaluations

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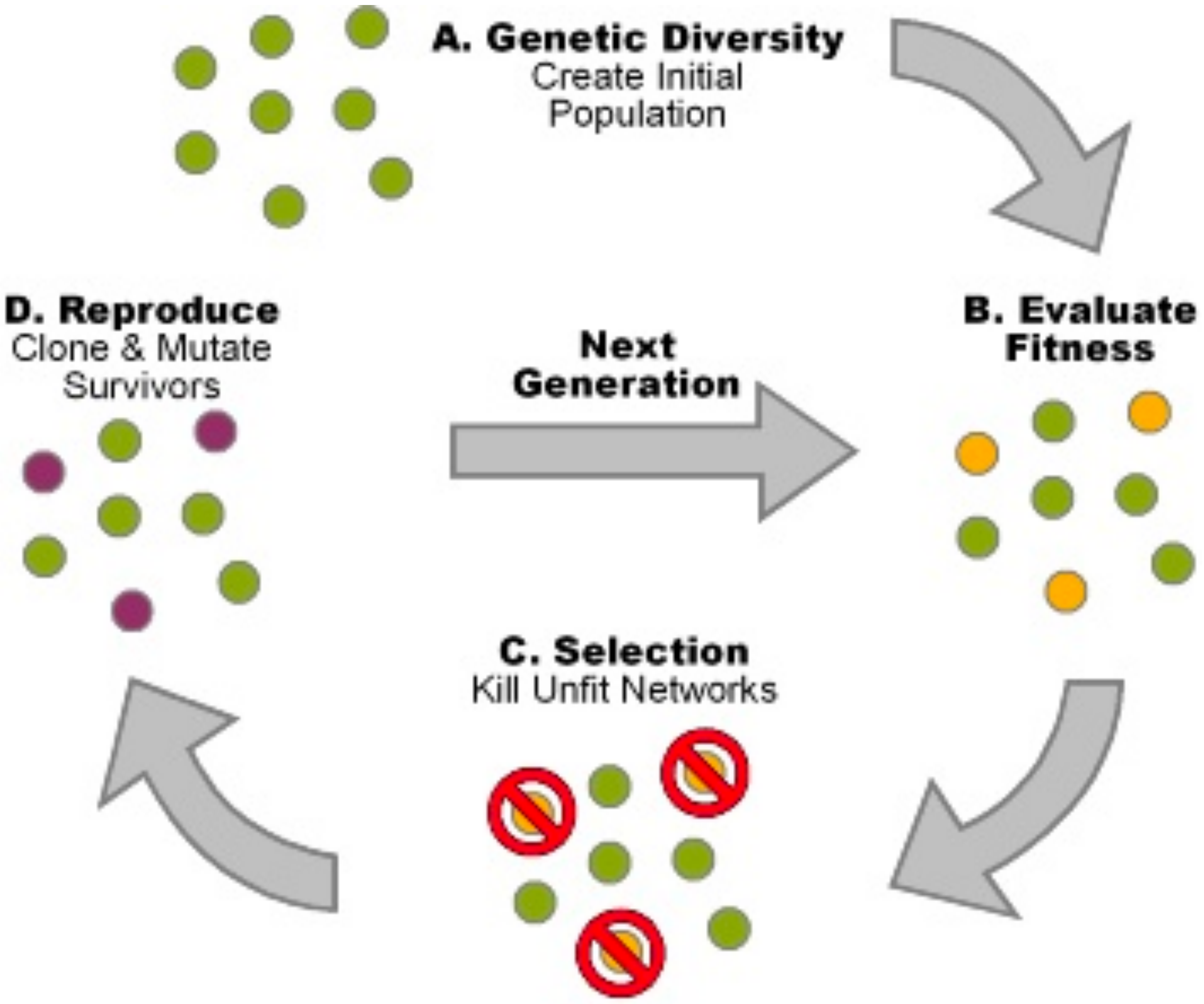

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- Millions of function evaluations
- Based on having cheap evaluations of the objective function

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Expensive problem:

The fitness function f takes lot of time/money

We can evaluate it *few* times

Problem setting

- Find the permutation σ that minimizes the fitness function $f(\sigma)$ subject to
  - Black-box f: query the fitness function but not look at the instance
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- Bayesian optimization
    - CEGO is the state-of-the-art
    - Incremental sample
    - Gaussian process -> probability models for permutations

Notation

- $\sigma = (3,1,2,5,4)$
- Bijection of the set $[n]$ onto itself,
  Symmetric group, $\mathbb{S}_n$
  - $e = (1,2,3,4,5)$
  - Inverse $\sigma^{-1} : \sigma(i) = j \Leftrightarrow \sigma^{-1}(j) = i$
  - Composition, $\sigma \cdot \pi(i) = \sigma(\pi(i))$

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- Interpretation
  - Ranking $\sigma = (3,5,2,1,4)$
  - Ordering $\sigma^{-1} = (4,3,1,5,2)$

UMM, Unbalanced Mallows model

Big picture of our proposal

$S \leftarrow 10$ random permutations

for $i \in \ [1 \ldots evaluations]$:

$\forall \sigma \in S : w_\sigma \leftarrow \rho^{f(\sigma)}$

$\mu \leftarrow wmedian(S, \{w_\sigma\})$

$\sigma' \sim M(\mu, \theta_i)$

$S \leftarrow S \cup \{\sigma'\}$

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$$w_\sigma = \begin{cases} 0 & \arg\max_{\sigma \in S} f(\sigma) \\ 1 & \arg\min_{\sigma \in S} f(\sigma) \end{cases}$$

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When solving a problem of interest,
do not solve a more general problem
as an intermediate step

Borda is a *good* approximation of the median

	Item 1	Item 2	Item 3	Item 4
σ_1	1	2	4	3
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- It is a 5/11 approximation
- Unbiased estimator

Weighted Borda

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Mallows, probability distribution for permutation

Analogous to the Gaussian distribution

- $p(\sigma \mid \mu, \theta) \propto \exp(-\theta d(\sigma, \mu))$
- Easy to sample [1,4]
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Kendall's-τ distance

Median

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- $p(\sigma \mid \mu, \theta) \propto \exp(-\overset{\text{Variance}}{\theta}\,\overset{\text{Kendall's-}\tau\text{ distance}}{d}(\sigma, \overset{\text{Median}}{\mu}))$
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The uncertainty of the median decreases with iterations

Decreasing variance

- The variance is not intuitive
- For $\sigma \sim M(\mu, \theta)$
  - $$\mathbb{E}[d(\sigma, \mu)] = \frac{n \cdot \exp(-\theta)}{1 - \exp(-\theta)} - \sum_{j=1}^{n} \frac{j \cdot \exp(-j\theta)}{1 - \exp(-j\theta)}$$
  - $\mathbb{E}[d(\sigma, \mu)]$ is a function of θ
- The $\mathbb{E}[d(\sigma, \mu)]$ linearly decreases with iterations

Exploration - exploitation

Both the learning rate ρ and the model variance θ balance this ratio

$S \leftarrow 10$ random permutations

for $i \in [1 \ldots evaluations]$:

$\forall \sigma \in S : w_\sigma \leftarrow \rho^{f(\sigma)}$ The sample is more accurate

$\mu \leftarrow wmedian(S, \{w_\sigma\})$

$\sigma' \sim M(\mu, \theta_i)$ The estimator is more accurate

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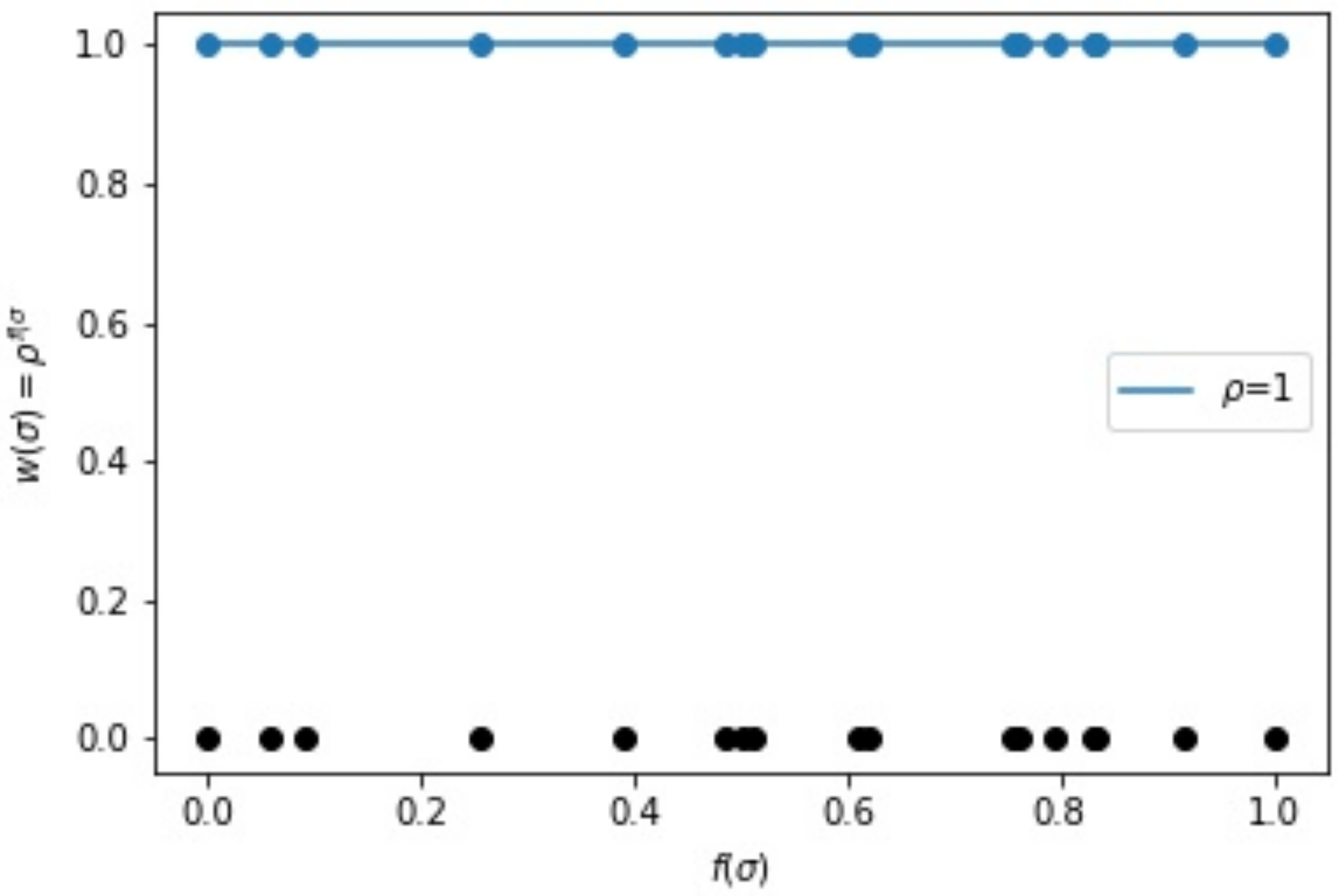
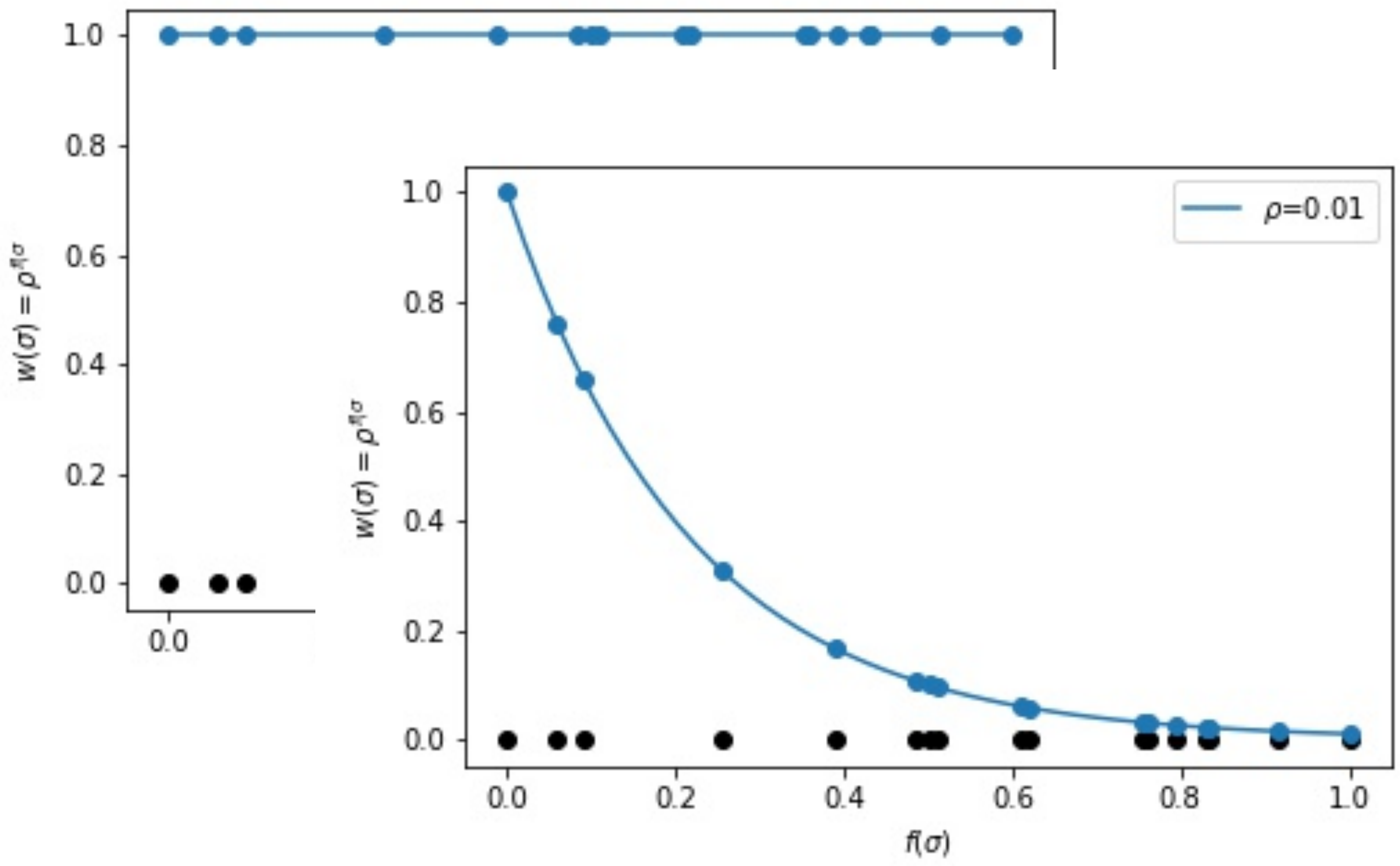


1.0
0.8
0.6
0.4
0.2
0.0
0.0
0.2
0.4
0.6
0.8
1.0
$w(\sigma) = \rho^{f(\sigma)}$
$f(\sigma)$
ρ=1



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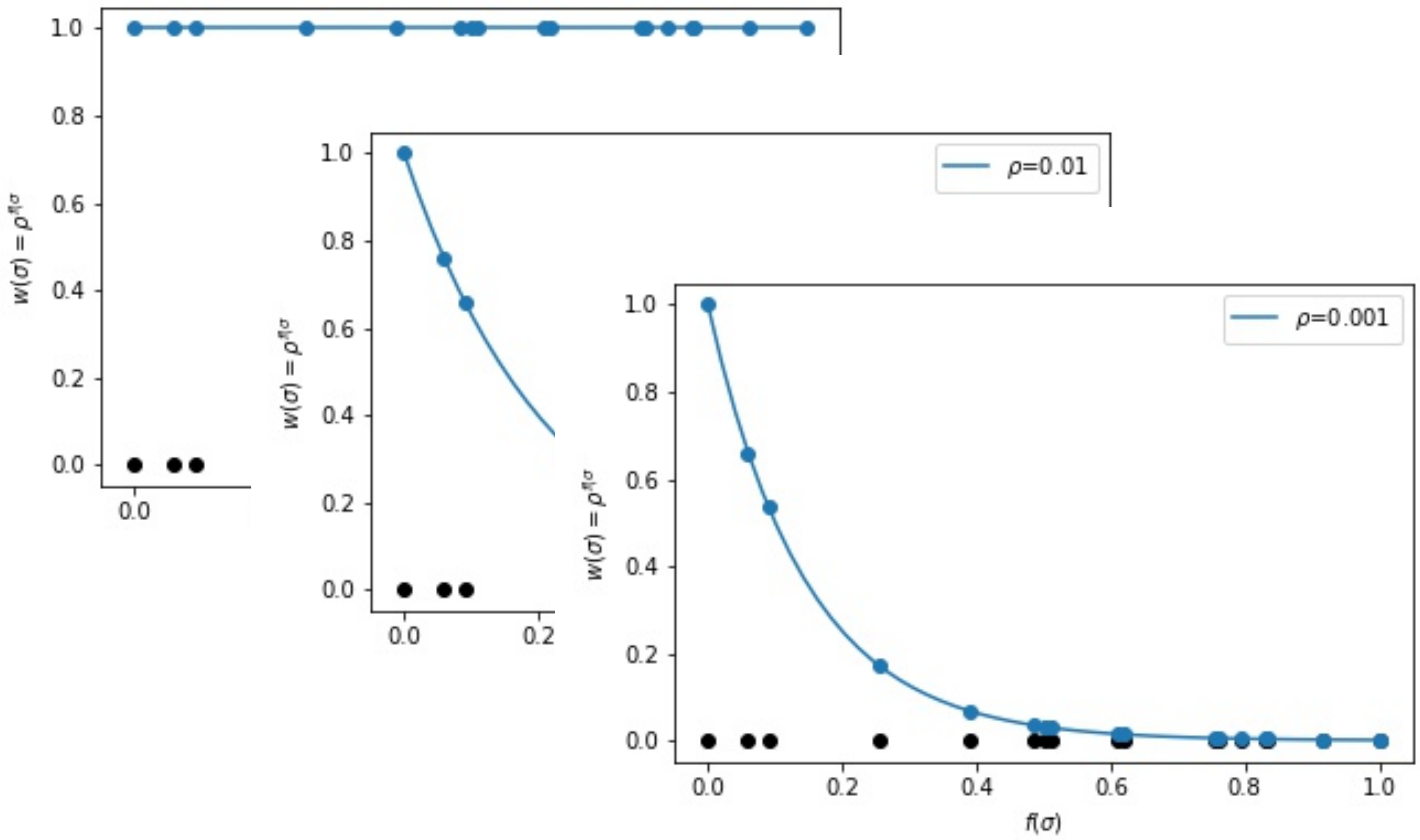
ρ=0.01



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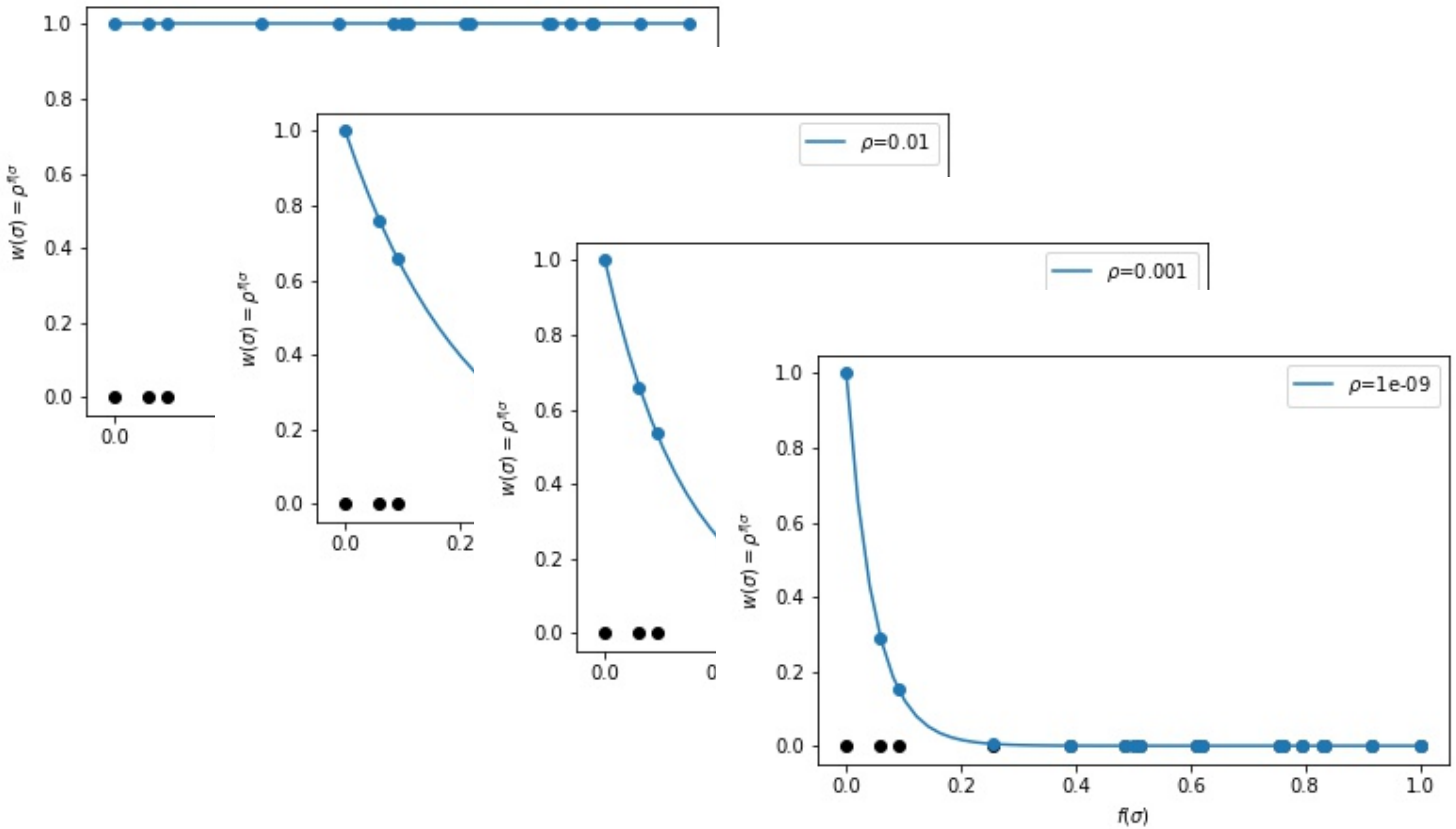

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$f(\sigma)$

Choose the learning rate ρ dynamically

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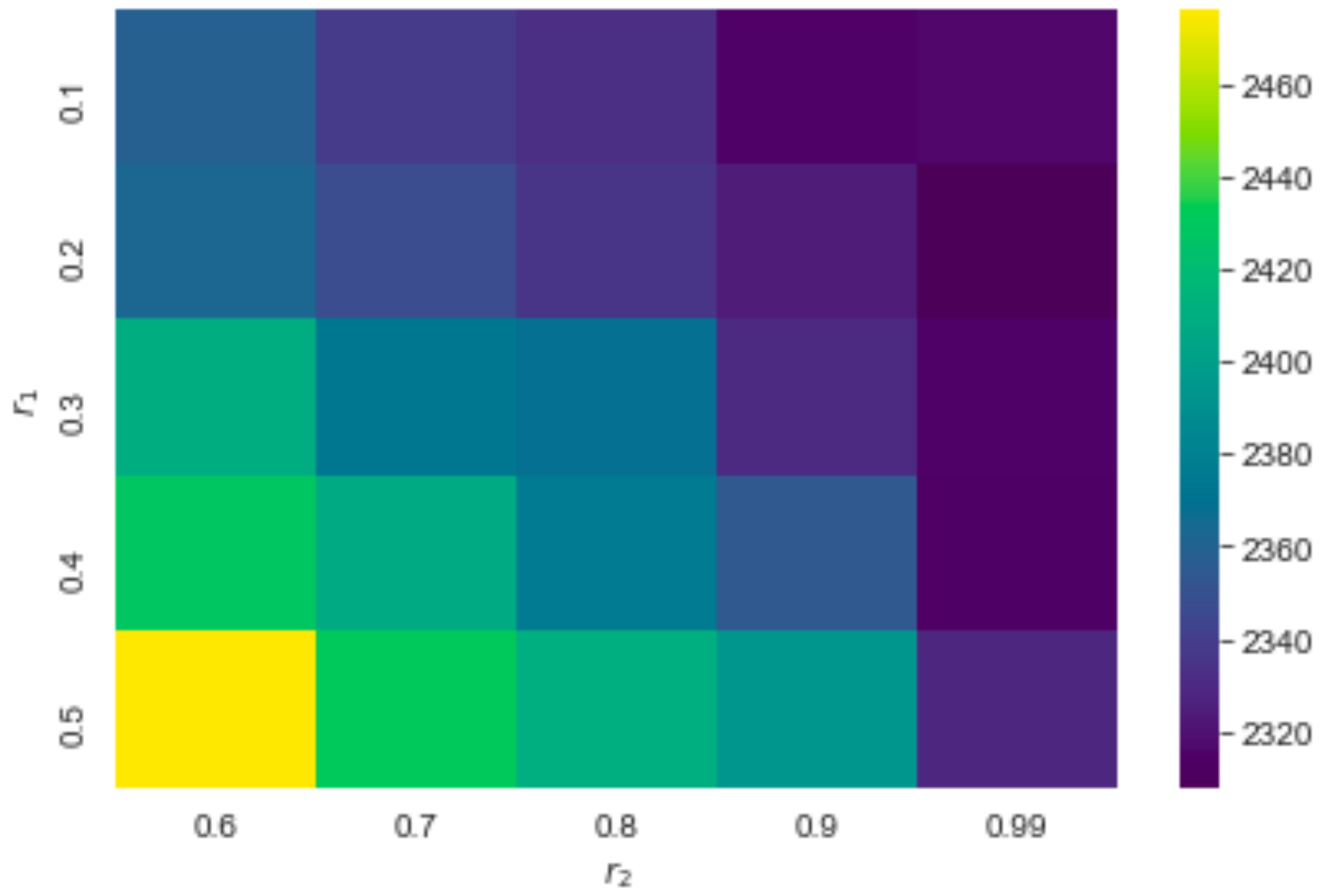
The ratios are obtained experimentally



Linear ordering problem

Usually consider orderings

- Find the permutation of rows and columns that minimizes the sum of the lower triangle
- $$\min_{\sigma \in S_n} f(\sigma) = \sum_{i=1}^{n} \sum_{j=1}^{i-1} a_{\sigma^{-1}(i),\sigma^{-1}(j)}$$

Permutation Flowshop Scheduling Problem, PFSP

- Minimize the *makespan*, the completion time of the last job on the last machine

- $\min_{\sigma \in S_n} \quad f(\sigma) = C_{n,M}$

  - $C_{1,j} = 0 \quad j \in [M], \qquad C_{i,1} = 0 \quad i \in [n]$

  - $C_{i,j} = p_{\sigma^{-1}(i),j} + \max\{C_{i-1,j}, C_{i,j-1}\} \quad i \in \{2,\ldots,n\}, j \in \{2,\ldots,M\}$

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State-of-the-art algorithm

- EGO/CEGO use Gaussian processes as a surrogate for the function
- CEGO is the state-of-the-art for expensive black-box permutation problems
  - Incremental sample
  - Maximize the E.I. criterion to predict the new point to evaluate
  - The surrogate model is explored with a GA

CEGO, the state-of-the-art

Minimization problem

CEGO, the state-of-the-art

Minimization problem

The variance of the model decreases linearly

CEGO_orig
UMM_100
UMM_200
200000
180000
160000
140000
120000
100000
Fitness
0
50
100
150
200
250
300
350
400
Function evaluations

CEGO_orig
UMM_100
UMM_200
UMM_400
Converged
Smooth
Fitness
Function evaluations
200000
180000
160000
140000
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400

Rankings and orderings

Not just an implementation detail

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4.5 minutes

Rankings and orderings

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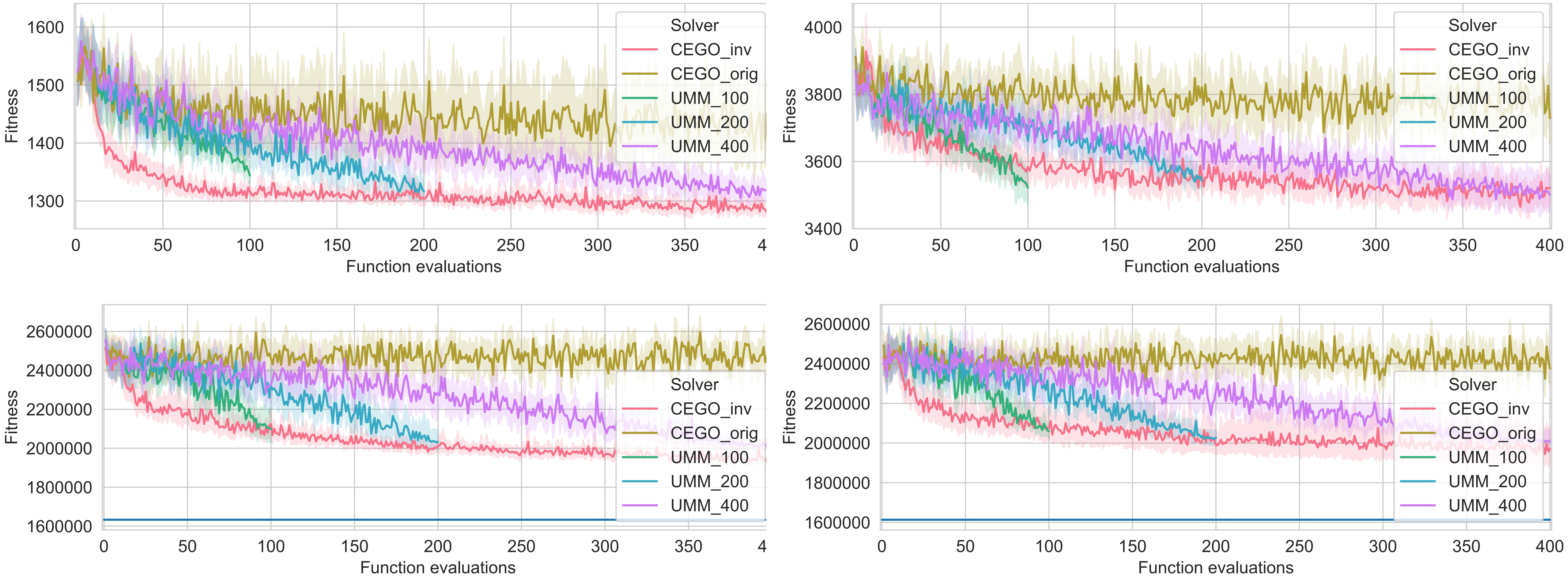
UMM outperforms the original CEGO
It is competitive with the modified version



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https://github.com/ekhiru

Conclusions

We present UMM

- A new framework for black-box expensive optimization
- Probabilistic, incremental sample
- Fast, efficient
  - Outperforms the state-of-the-art
  - Competitive with the modified version of the state state-of-the-art
- Permutations are not just ordered vectors
- Ad-hoc strategies for permutations often outperform the adaptations