

# **Multi-objective optimization and Symbolic Regression**

## **Classical and meta-heuristic methods**

# Table of contents

Four lectures course: 4x2 hrs

## Lecture 1:

- Introduction to MOO framework and taxonomy
- Classical scalarization methods

## Lecture 3:

- Evaluation metrics
- Python packages

## Lecture 2:

- Meta-heuristic methods
- Simulated annealing
- Swarm Particle
- Genetic algorithms

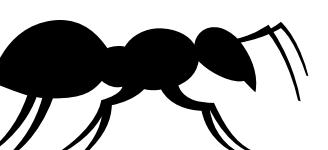
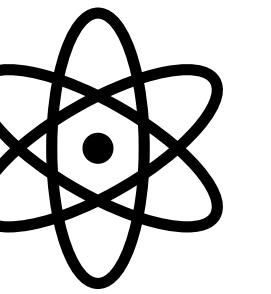
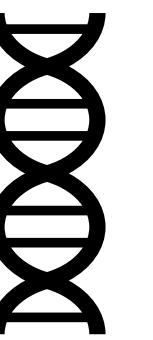
## Lecture 4:

- Symbolic regression
- Multi-objective symbolic regression
- Case studies

# Meta-heuristic methods

## Evolutionary algorithms

- Genetic algorithms
- Particle Swarm Optimization
- Simulated annealing
- Ant-Colony Optimization



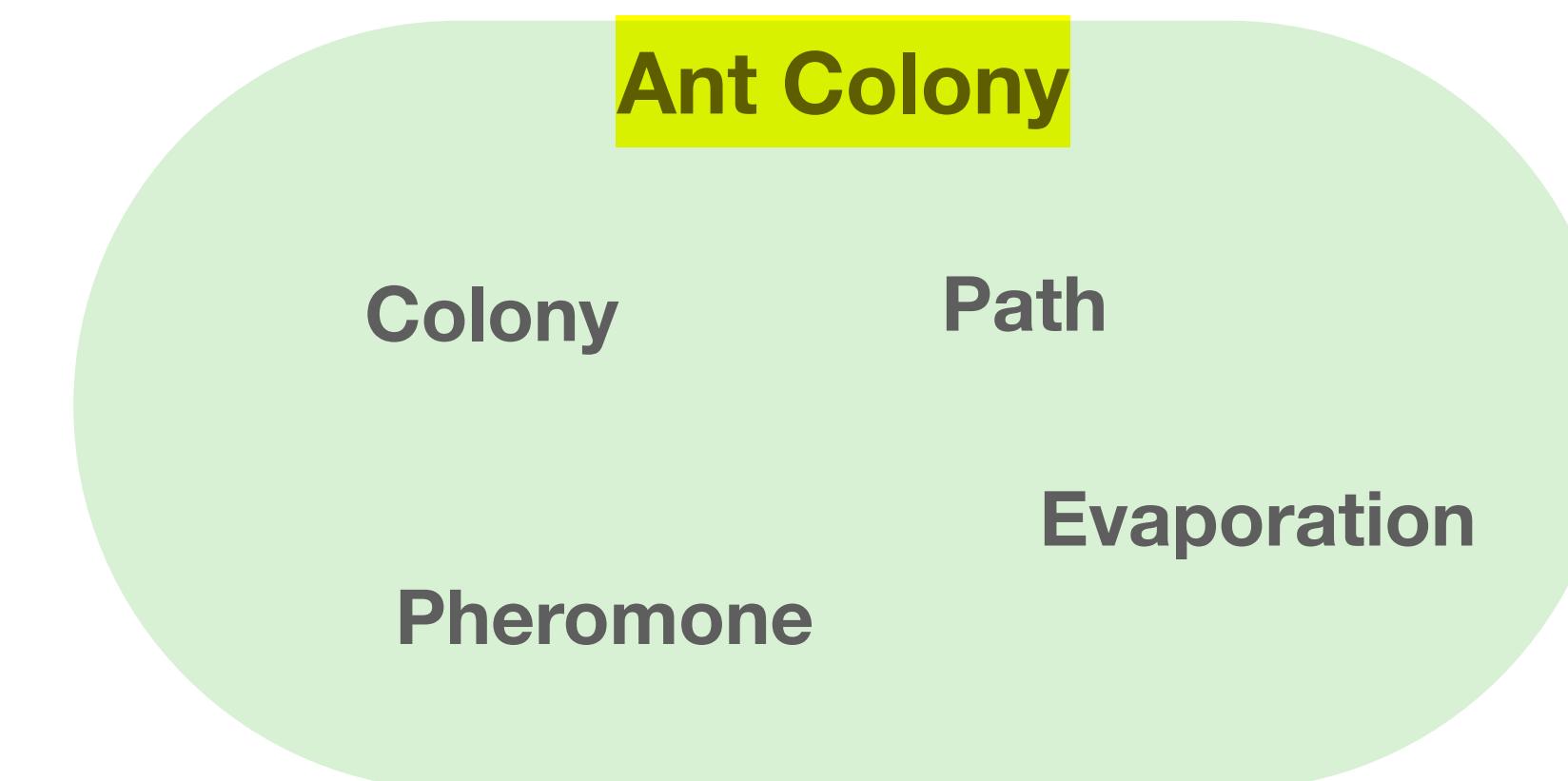
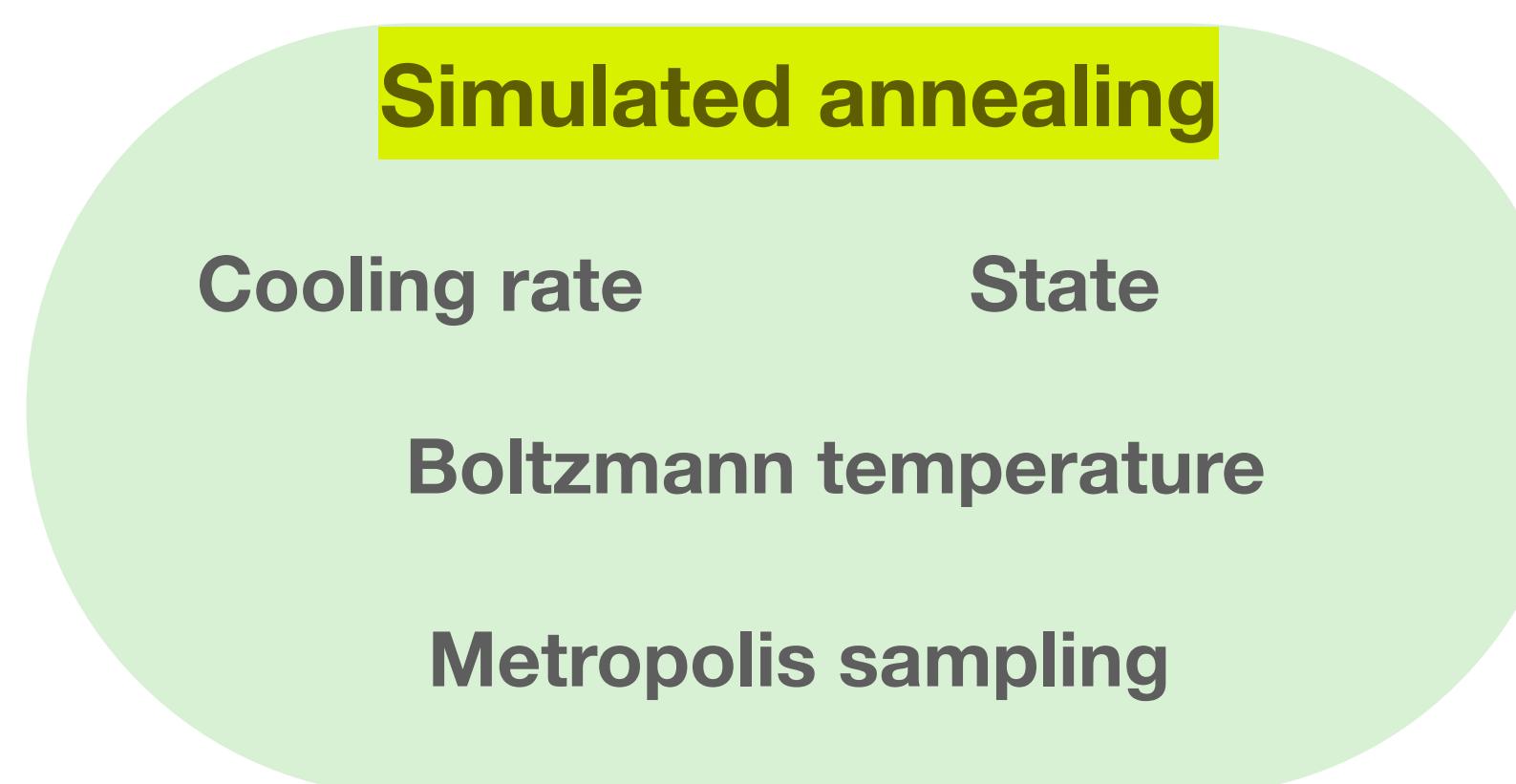
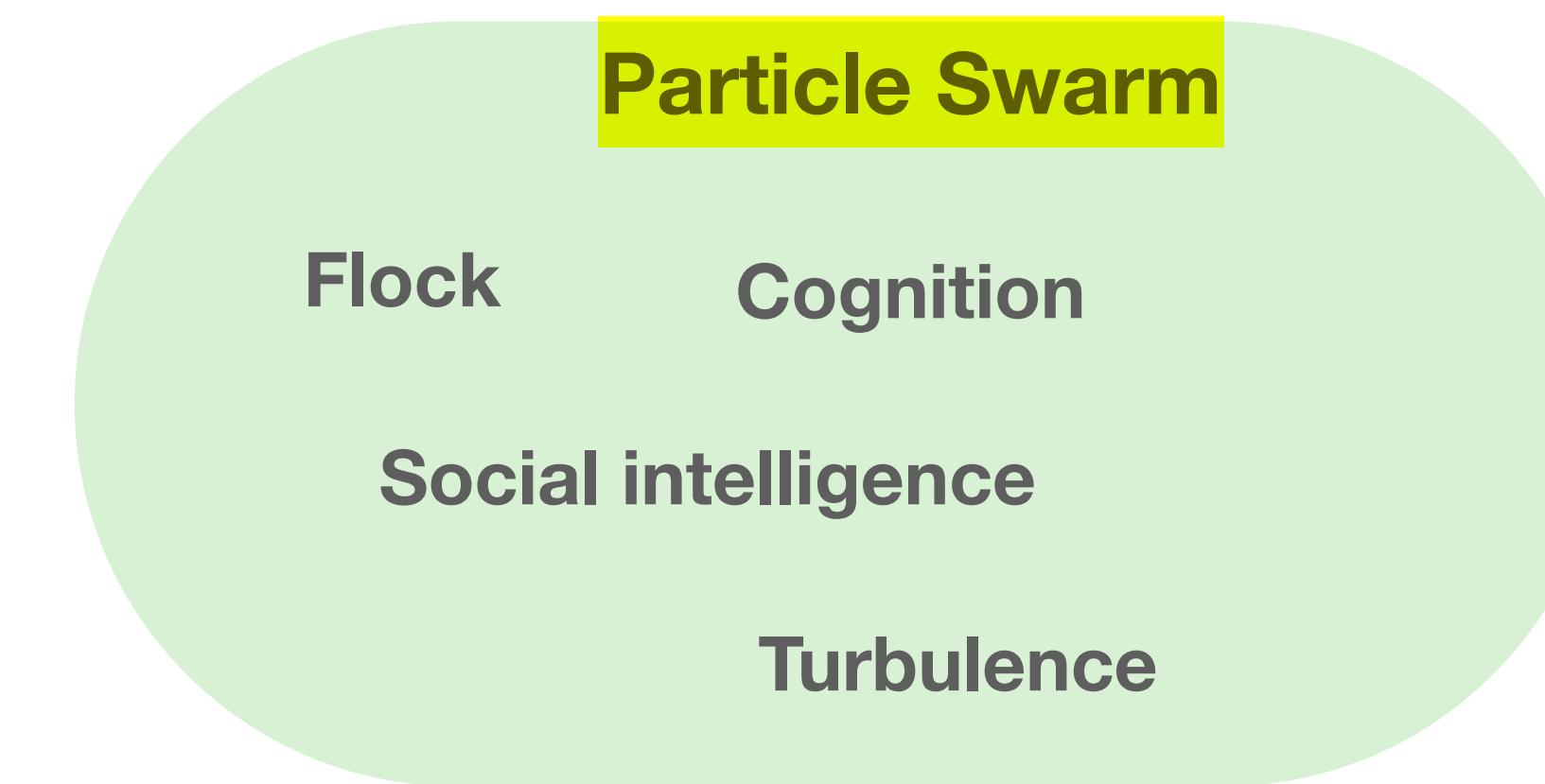
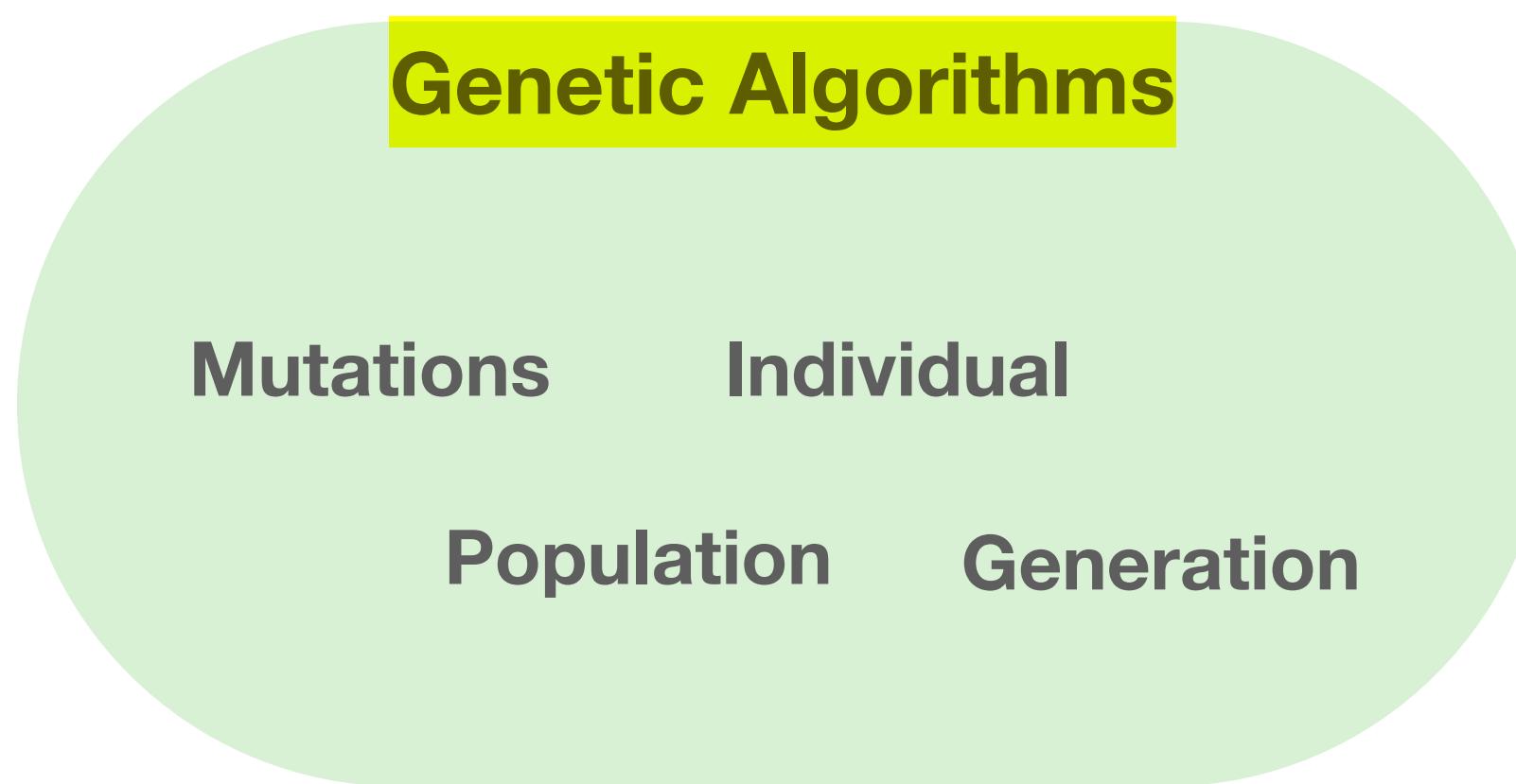
# **Meta-heuristic methods**

## **Benefits**

- Objectives: differentiable and NOT
- Pareto Set in one run
- Parallel computing

# Nomenclature

Method you use, dictionary you find



# Solution ranking

## Goldberg

Starting from a set of candidates S

- Non-dominated in S: rank 1
- Non-dominated in  $S/\text{PF1}$ : rank 2
- ...

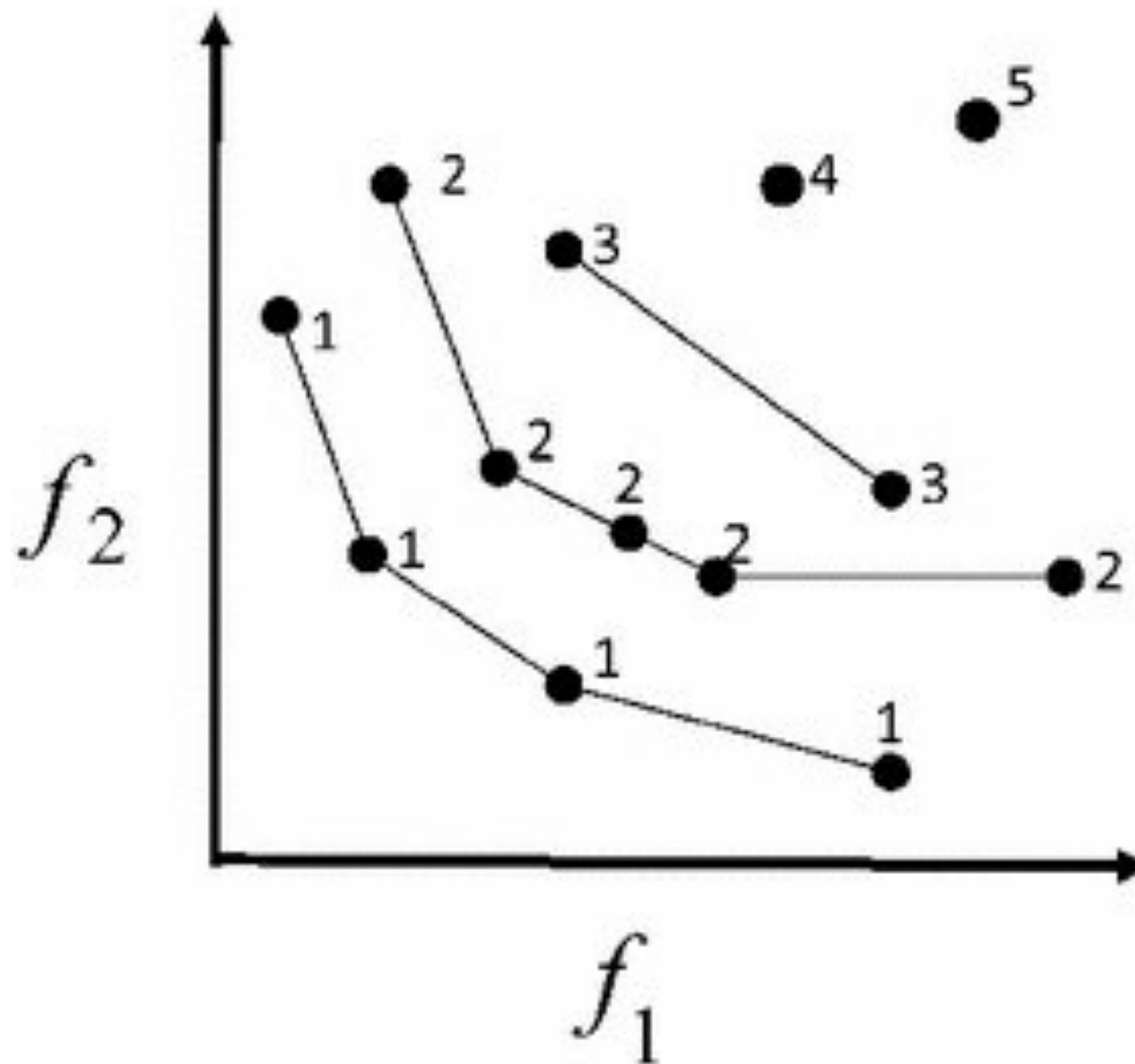
## Fonseca and Fleming

Starting from a set of candidates S

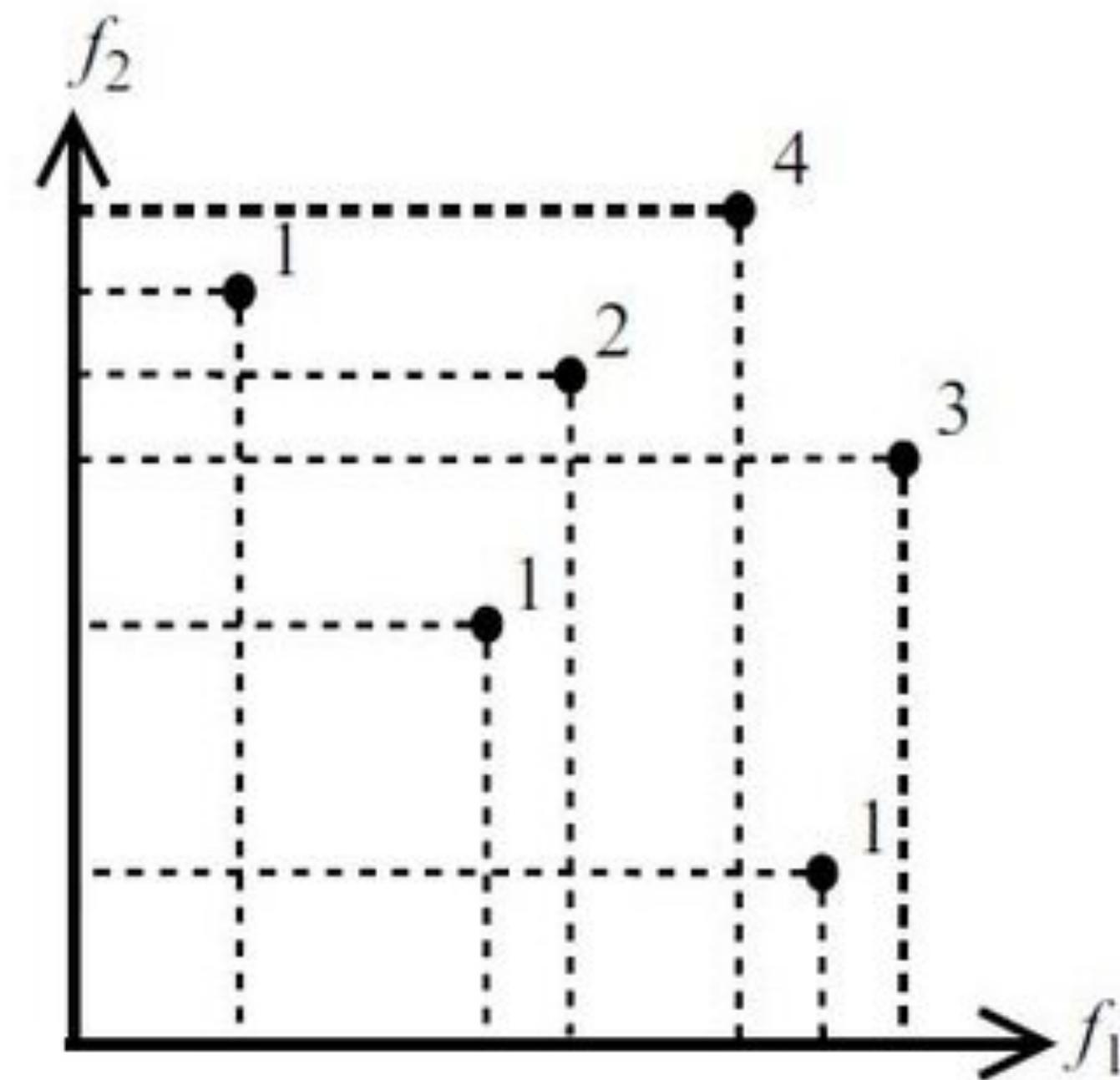
- Non-dominated in S: rank 1
- Rank = # dominating solutions  
+1

# Solution ranking

**Goldberg**

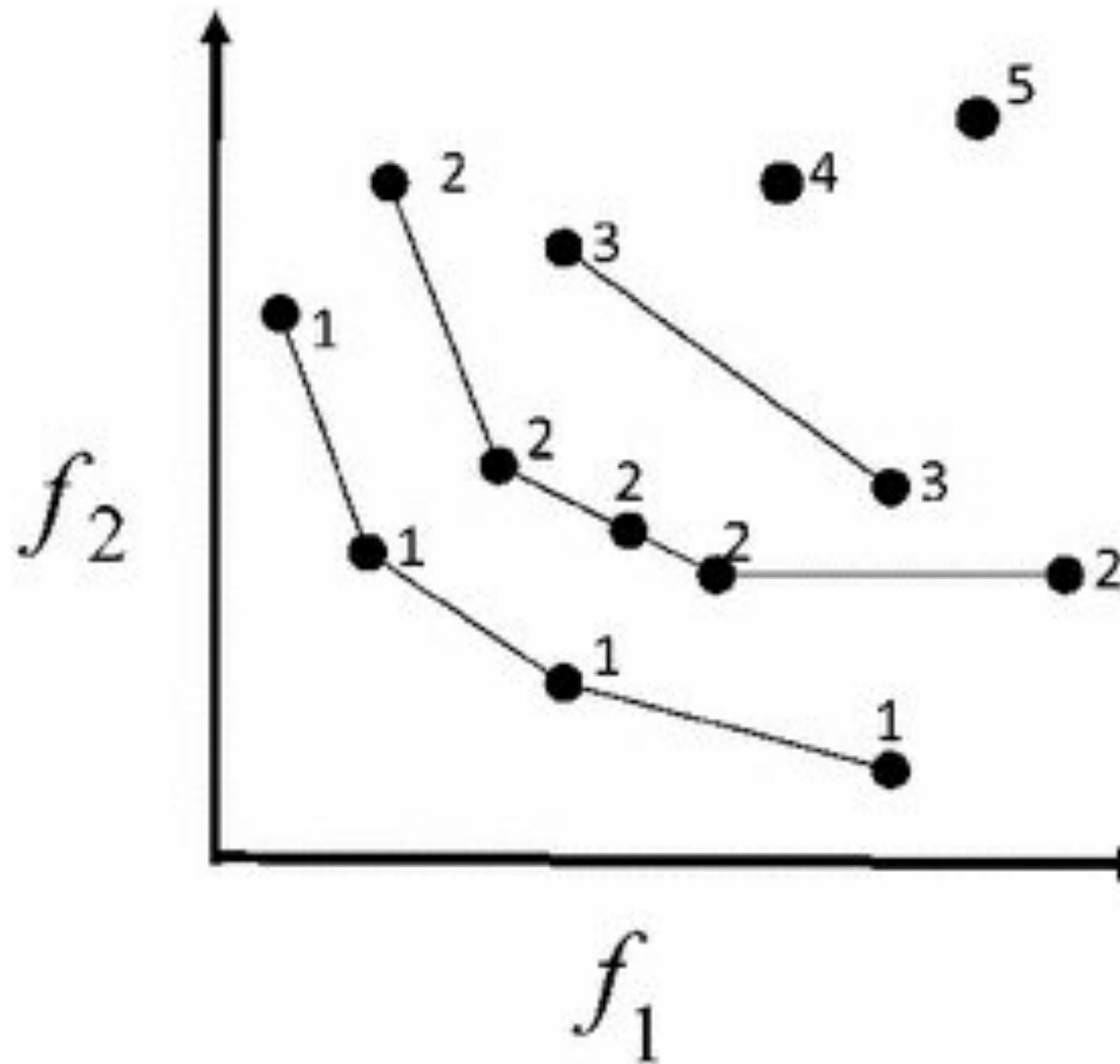


**Fonseca and Fleming**



# Solution ranking

## Goldberg



fast-non-dominated-sort( $P$ )

**(from Deb et al. 2002)**

for each  $p \in P$

$S_p = \emptyset$       <- individuals dominated by  $p$

$n_p = 0$       <- number of individuals dominating  $p$

for each  $q \in P$

if  $(p \prec q)$  then

$S_p = S_p \cup \{q\}$

else if  $(q \prec p)$  then

$n_p = n_p + 1$

if  $n_p = 0$  then

$p_{\text{rank}} = 1$

$\mathcal{F}_1 = \mathcal{F}_1 \cup \{p\}$

$i = 1$

while  $\mathcal{F}_i \neq \emptyset$

$Q = \emptyset$

for each  $p \in \mathcal{F}_i$

<- for each element belonging to the current Pareto front

for each  $q \in S_p$

<- for each element dominated by  $p$

$n_q = n_q - 1$

<- decrease its domination number

if  $n_q = 0$  then

$q_{\text{rank}} = i + 1$

$Q = Q \cup \{q\}$

$i = i + 1$

$\mathcal{F}_i = Q$

If  $p$  dominates  $q$

Add  $q$  to the set of solutions dominated by  $p$

Increment the domination counter of  $p$   
 $p$  belongs to the first front

Initialize the front counter

Used to store the members of the next front

<- for each element belonging to the current Pareto front

<- for each element dominated by  $p$

<- decrease its domination number

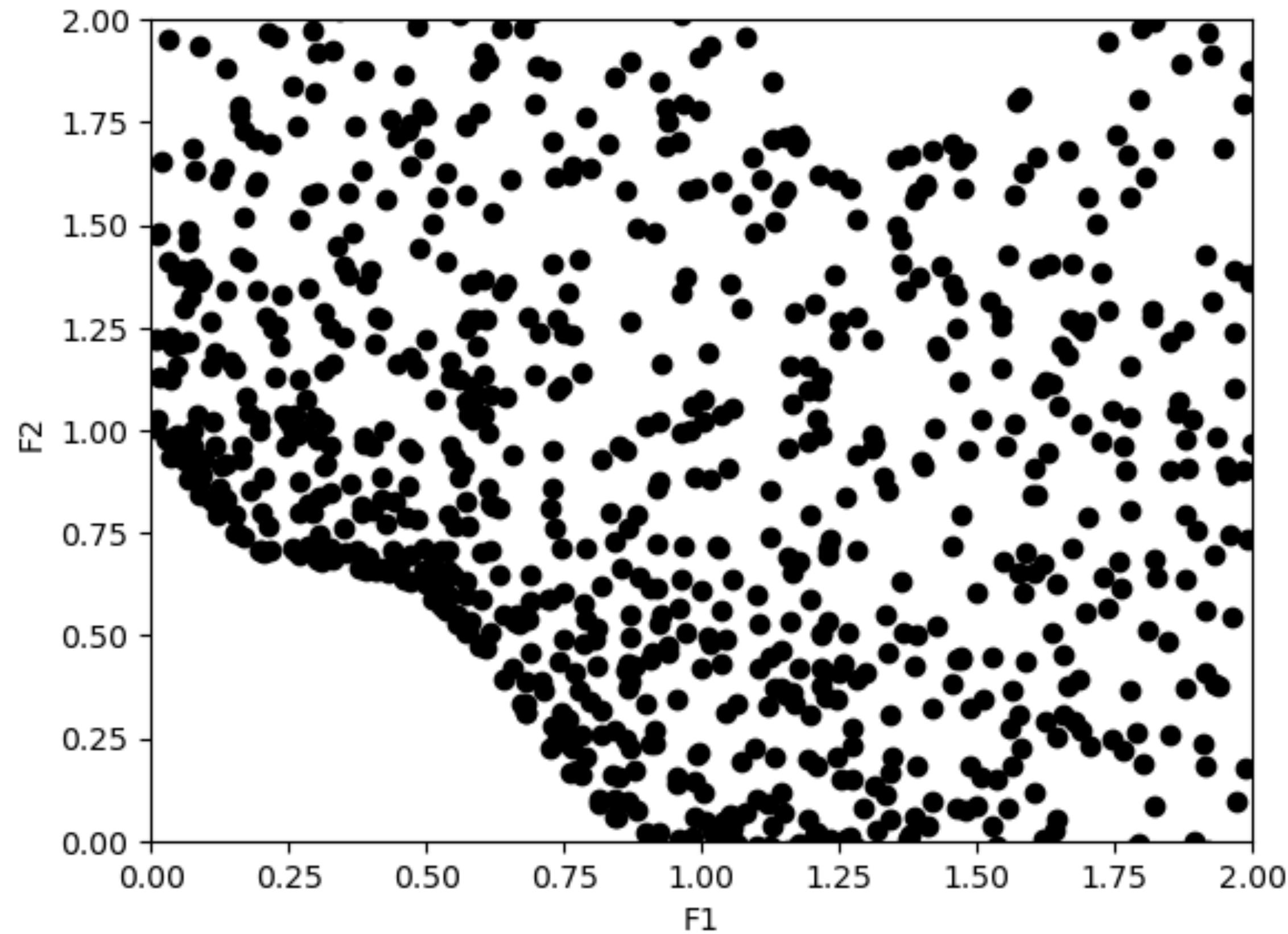
$q$  belongs to the next front

# Our good old concave task

$$f_1(x_1, x_2) = x_1$$

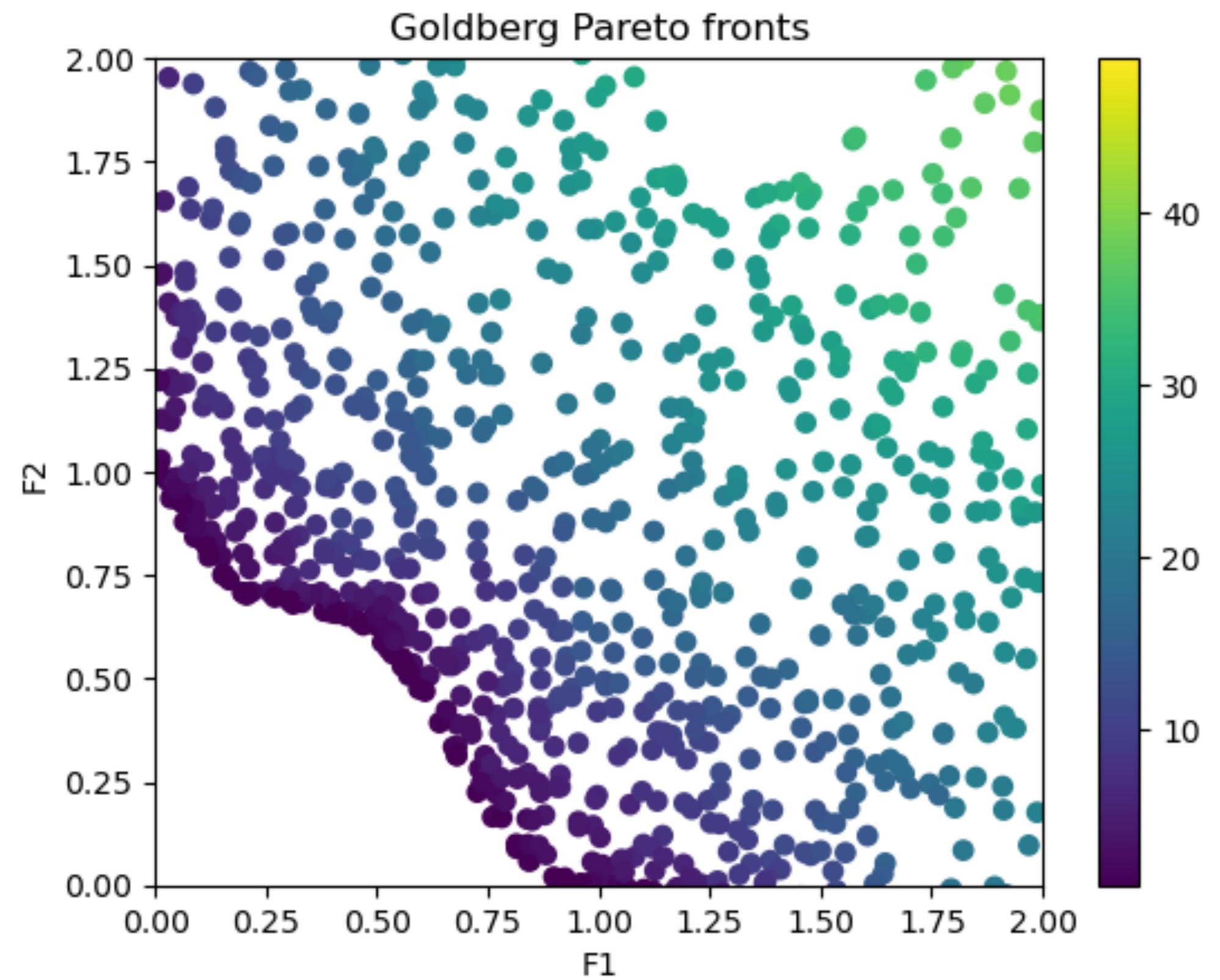
$$f_2(x_1, x_2) = 1 - x_1 - \alpha \sin(\beta \pi x_1) + x_2^2$$

$$\alpha = 1/10 \quad \beta = 3$$

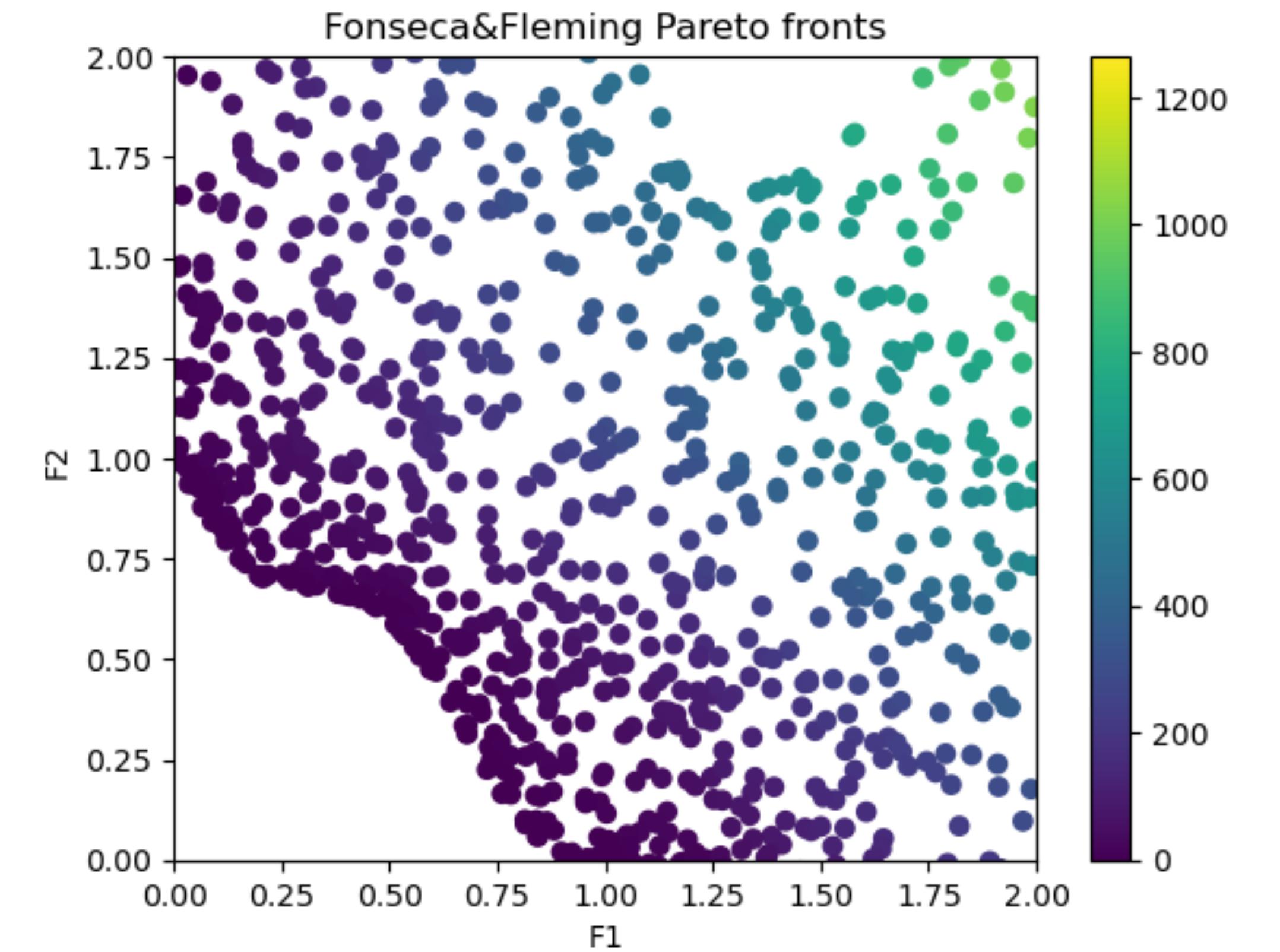


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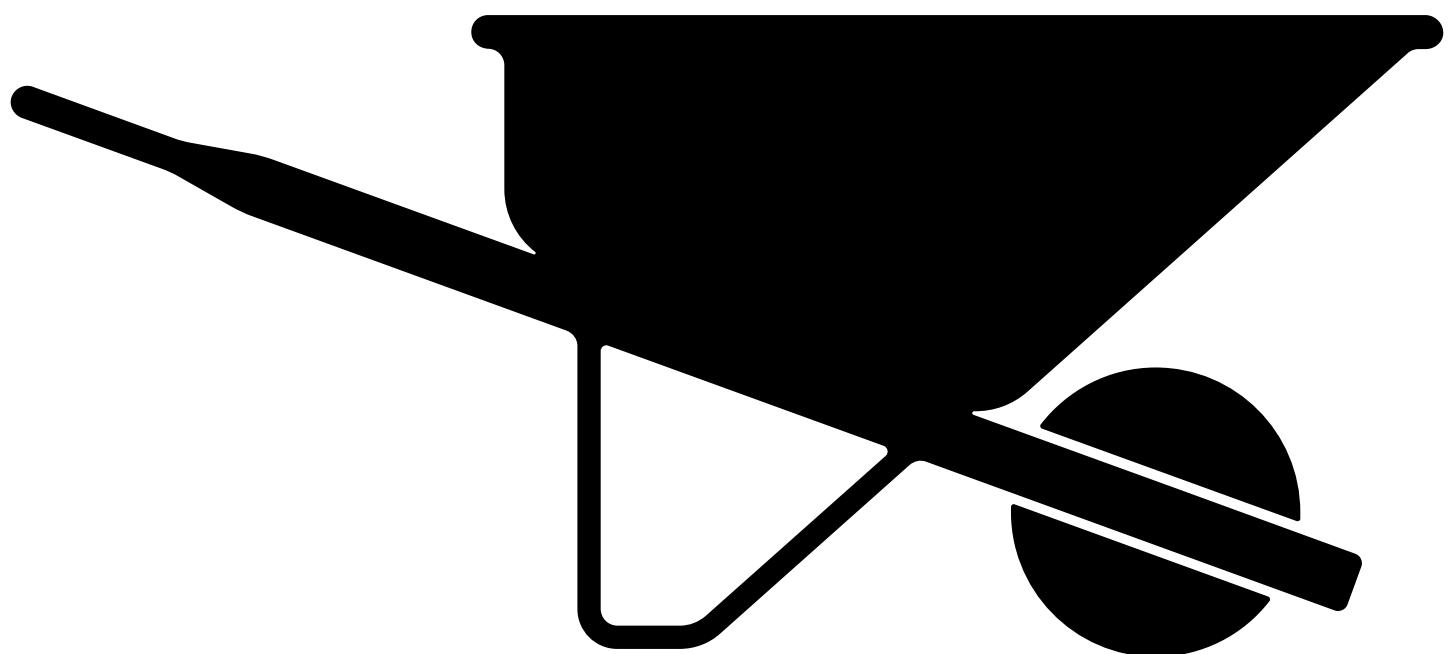
**Goldberg**



**Fonseca and Fleming**



# **Hands on**



# Simulated Annealing (*Kirkpatrick, Černy 1980s*)

## Physics-inspired algorithm

NP-hard problems can use the Metropolis's model for simulating the annealing of solids

Annealing: heat up a material up to the melting temperature, then slowly cool the material up to a stable crystalline state with minimum energy.

Molecular positions	→	decision variables
Temperature	→	control parameter
Energy of the system	→	objective functions
System state	→	possible solution
Metastable state	→	local minimum
Ground state	→	global minimum

# **Simulated Annealing** (*Kirkpatrick, Černy 1980s*)

## Physics-inspired algorithm

*Ising model*

<https://www.youtube.com/watch?v=g1h71X55hyw>

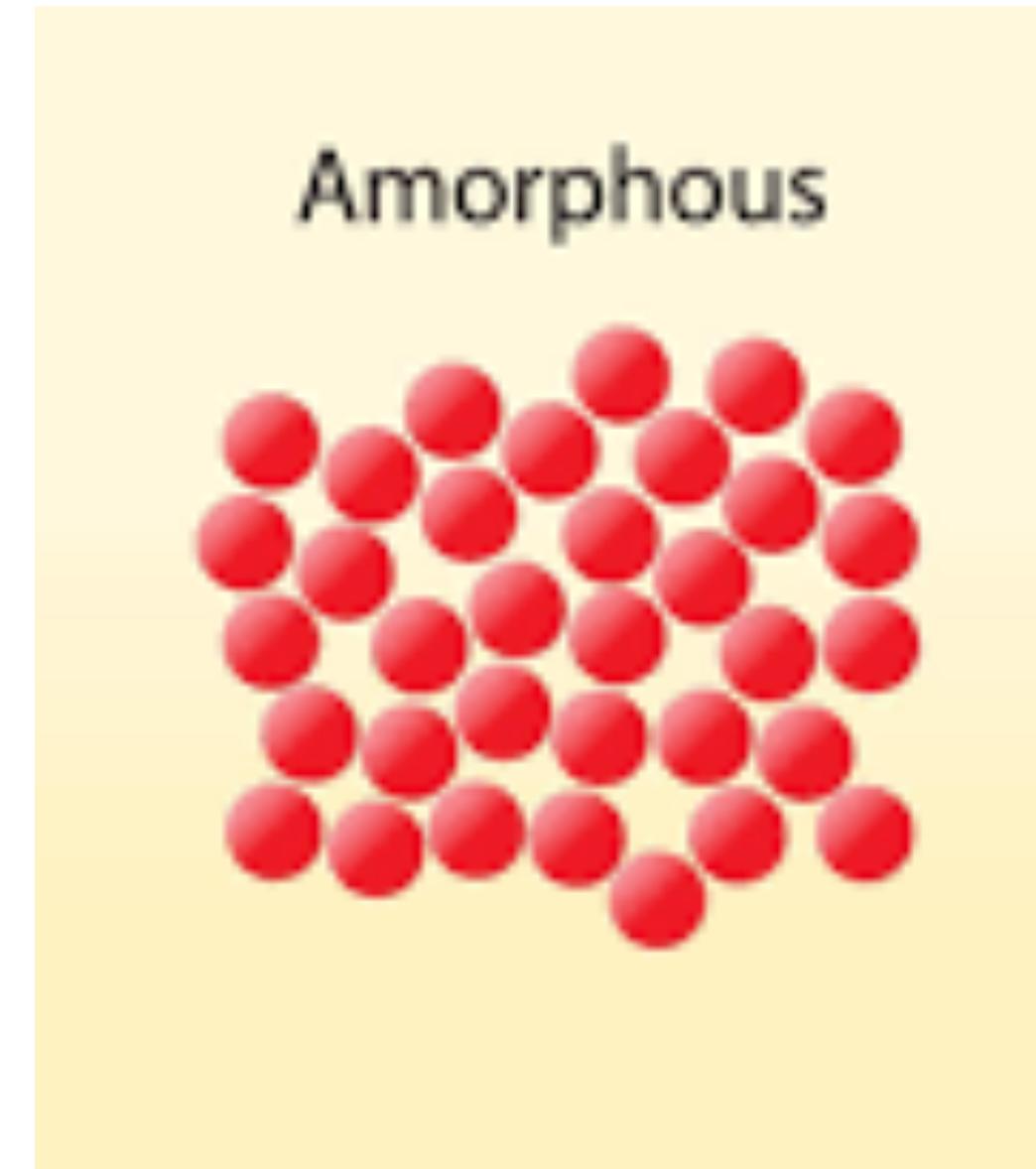
*Traveling salesman problem*

[https://www.youtube.com/watch?v=W-aAjd8\\_bUc](https://www.youtube.com/watch?v=W-aAjd8_bUc)

# Simulated Annealing (*Kirkpatrick, Černy 1980s*)

Why does this work in Nature?

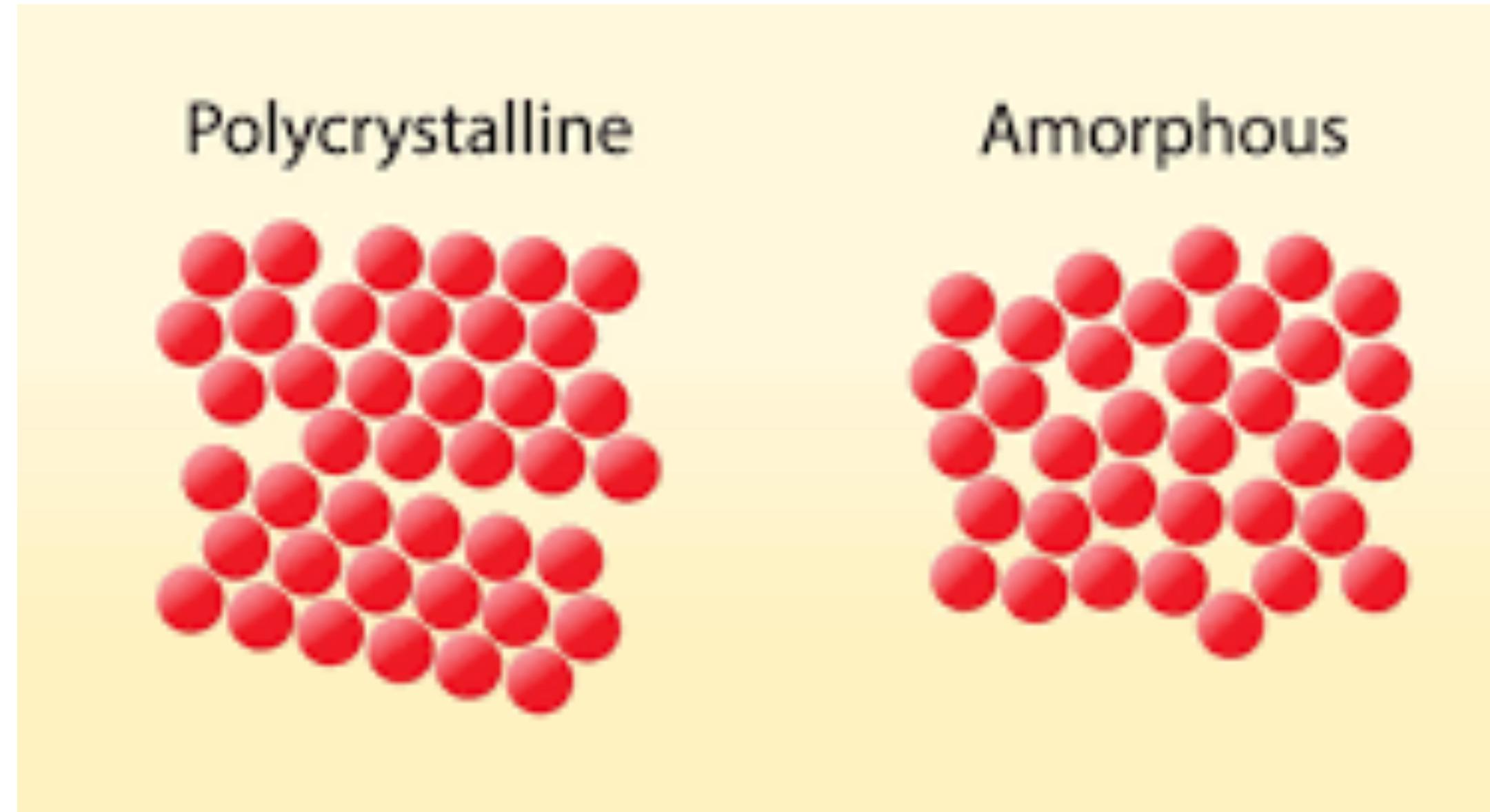
- Melt a solid and then cool it **fast**



# Simulated Annealing (*Kirkpatrick, Černy 1980s*)

## Why does this work in Nature?

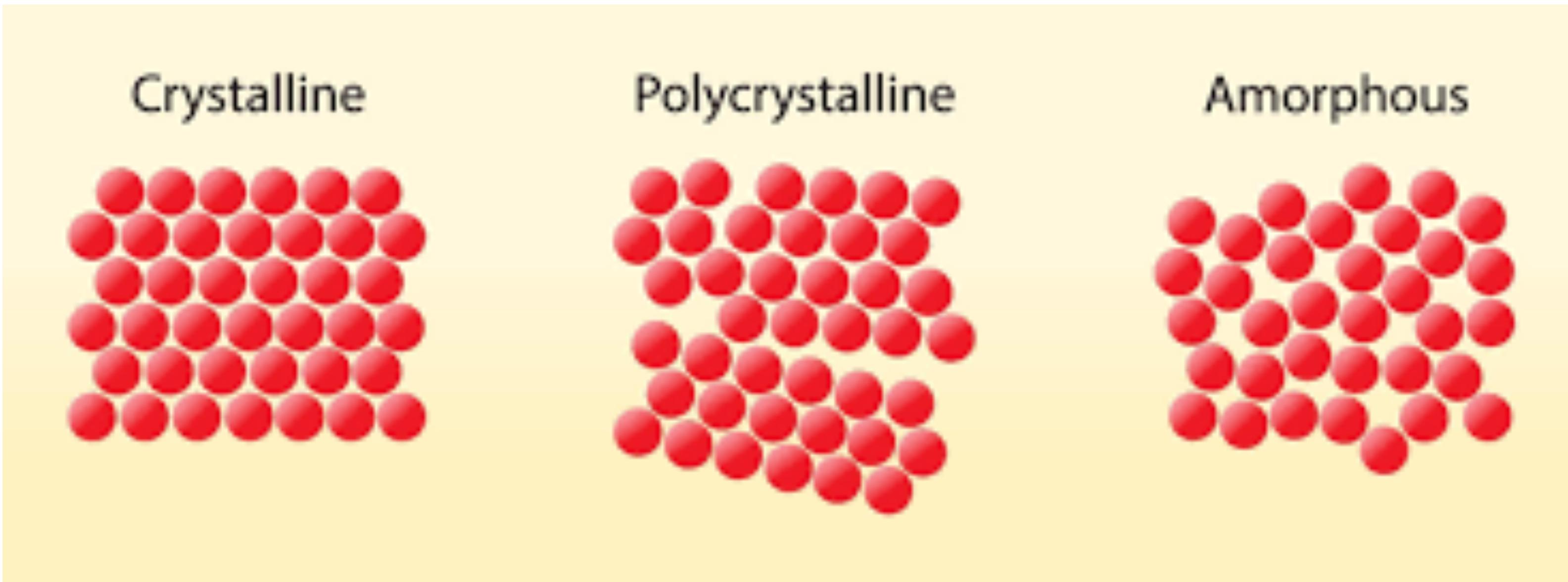
- Melt a solid and then cool it **slowly**



# Simulated Annealing (*Kirkpatrick, Černy 1980s*)

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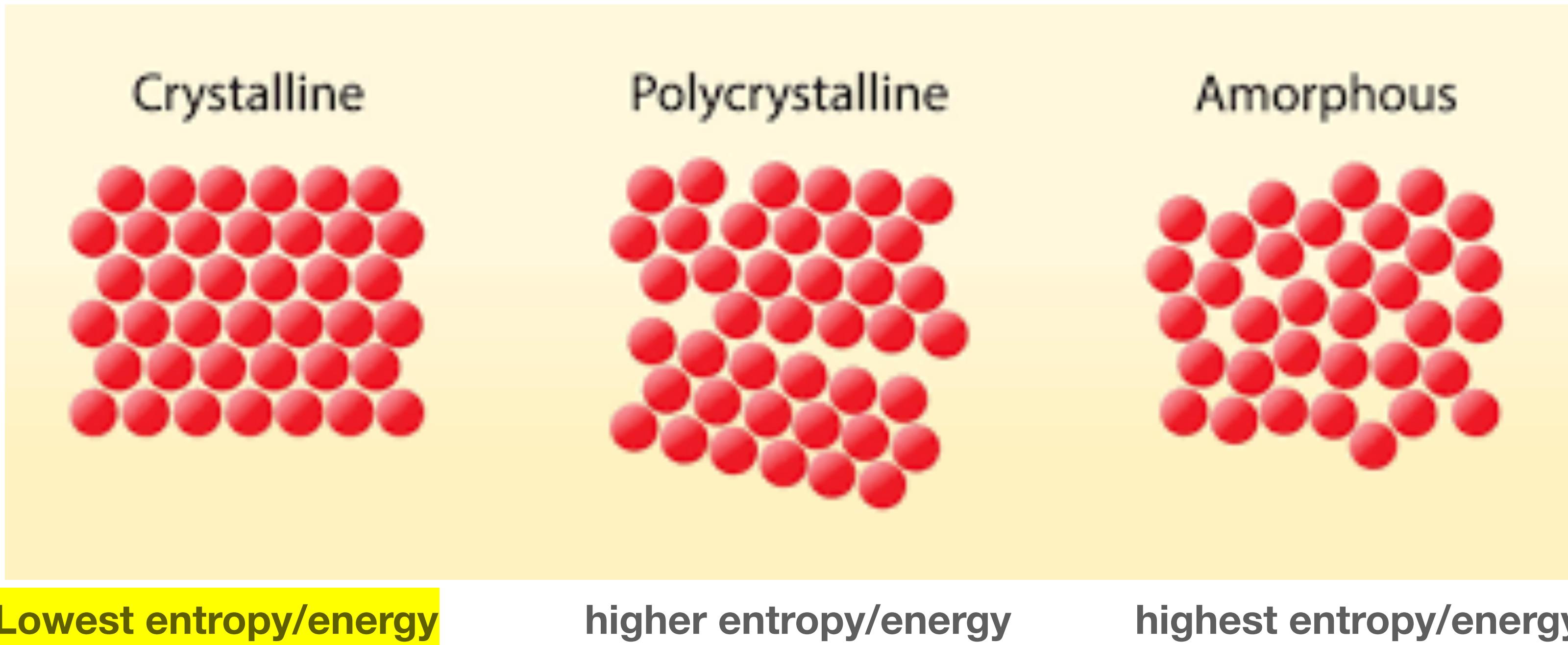
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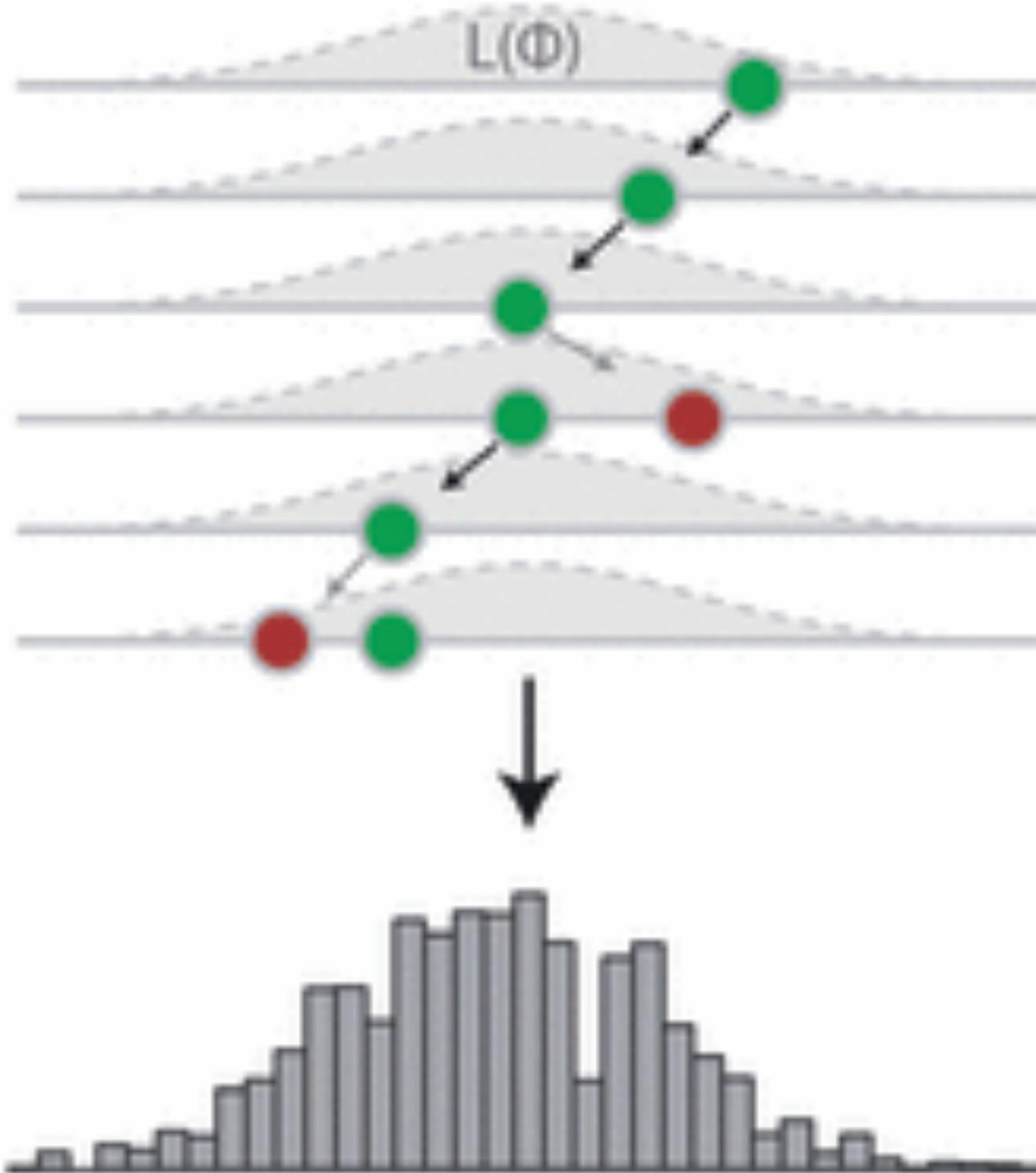


# Simulated Annealing (*Kirkpatrick, Černy 1980s*)

## Physics-inspired algorithm

Probabilistic evolution:

$$P\{x \rightarrow x' : x(t) = x\} = \frac{1}{Z} \exp \left\{ -\frac{1}{T} \max(0, f(x') - f(x)) \right\}$$



# Simulated Annealing (*Kirkpatrick, Černy 1980s*)

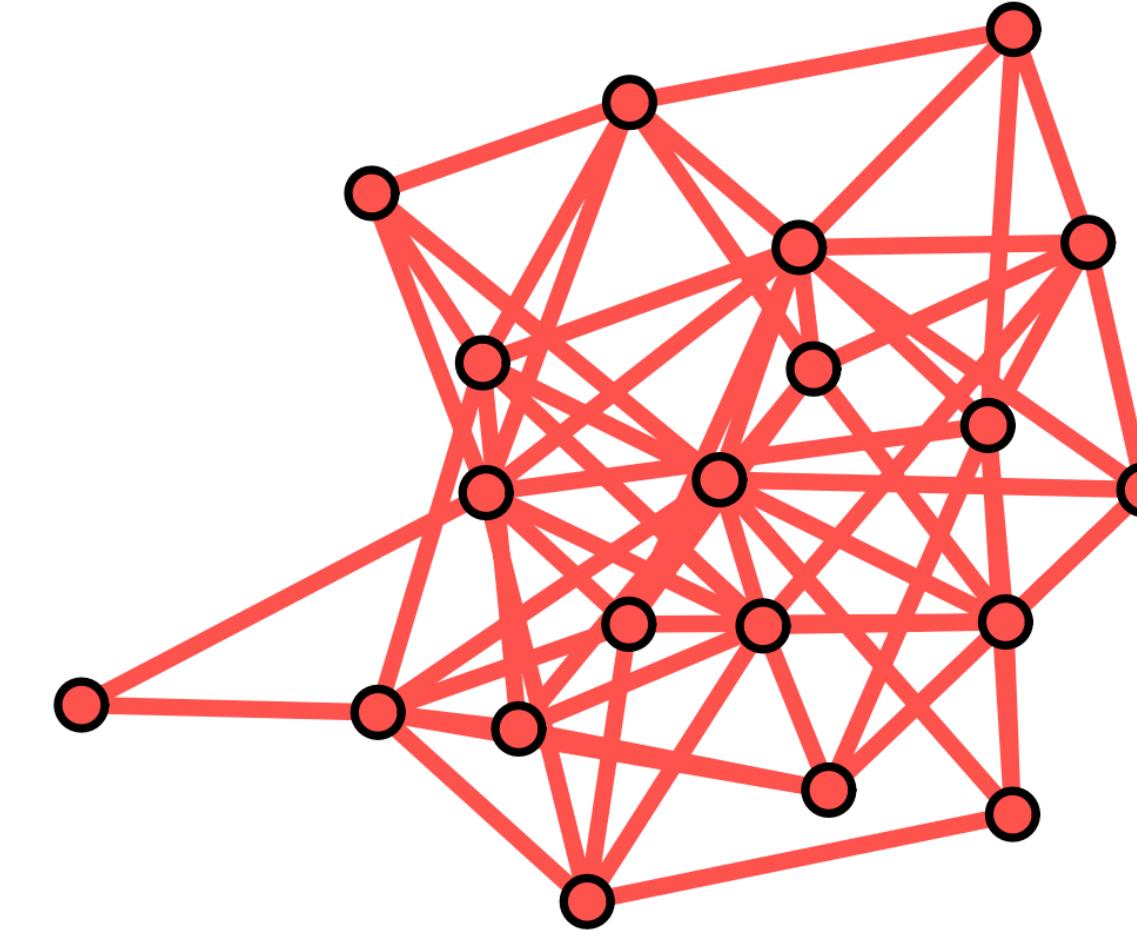
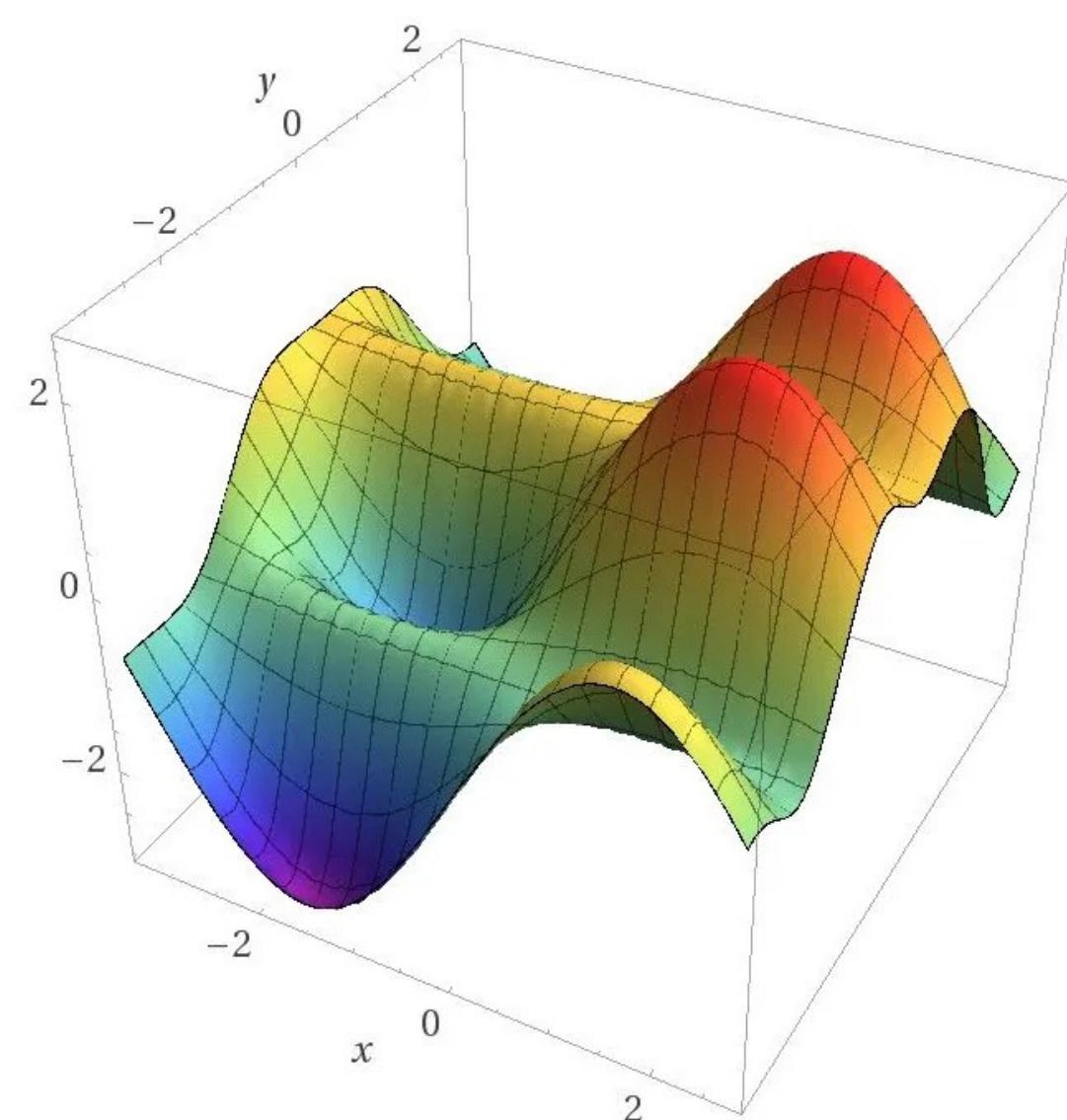
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Need to specify:

- Problem representation: define solution space and cost function



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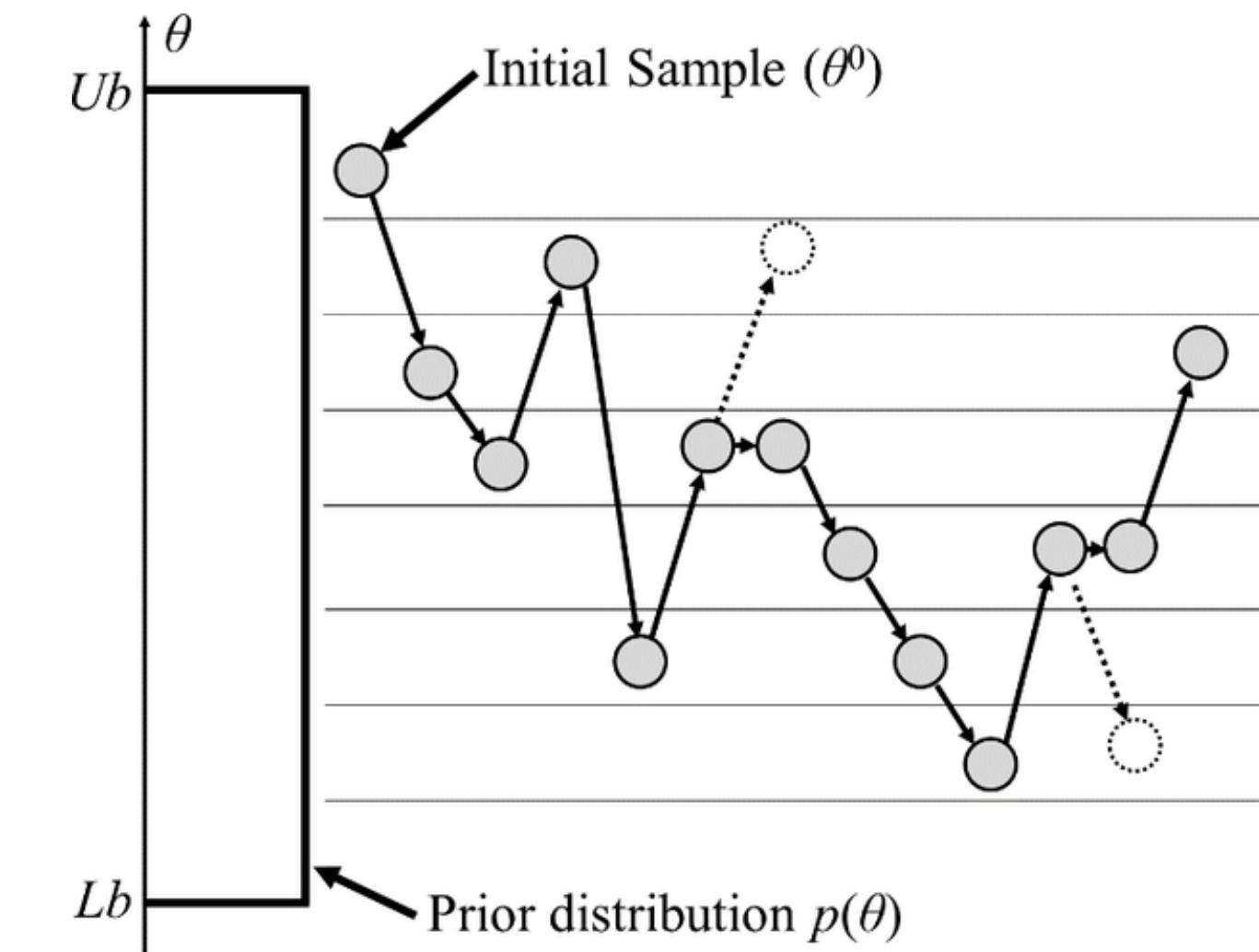
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- Cooling procedure: how to decrease  $T$  at each step

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- Cooling procedure: how to decrease  $T$  at each step
- Handling constraint:  $Obj(x, \alpha) = f(x) + \sum_{j=1}^m \alpha_j (g_j(x))^2$

# Simulated Annealing (*Kirkpatrick, Černy 1980s*)

## Cooling methods

- Linear cooling

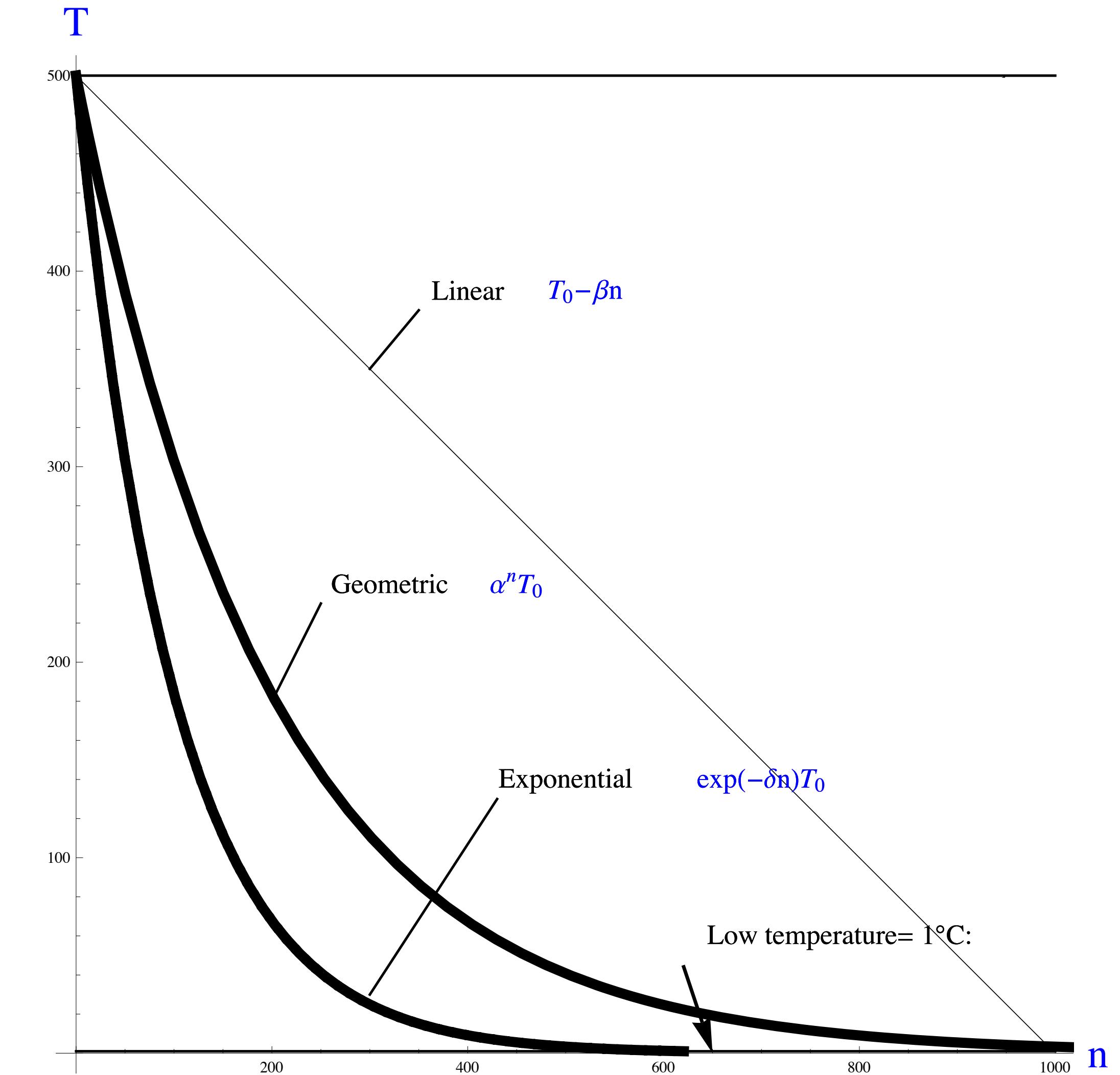
$$T[n] = T[n - 1] - \Delta_0$$

- Geometric cooling

$$T[n] = \alpha T[n - 1] \quad \alpha \in [0, 1] \quad \alpha = 0.995$$

- Exponential cooling

$$T[n] = e^{-\beta} T[n - 1] \quad \beta \in [0, 1] \quad \beta = 0.01$$



# Simulated Annealing (*Kirkpatrick, Černy 1980s*)

## Pseudo-algorithm

$T=T_0$  set initial temperature

$X = X_0$  random initial solution

$E = \text{Energy}(X)$  compute the initial energy

While  $T > 0$  or not (termination\_criterion):

$X' = \text{generate\_solution}(x, N(x))$

$E' = \text{Energy}(X')$

$\Delta = E' - E$

    If  $\Delta < 0$ :

$X = X'$

$E = E'$

    Else:

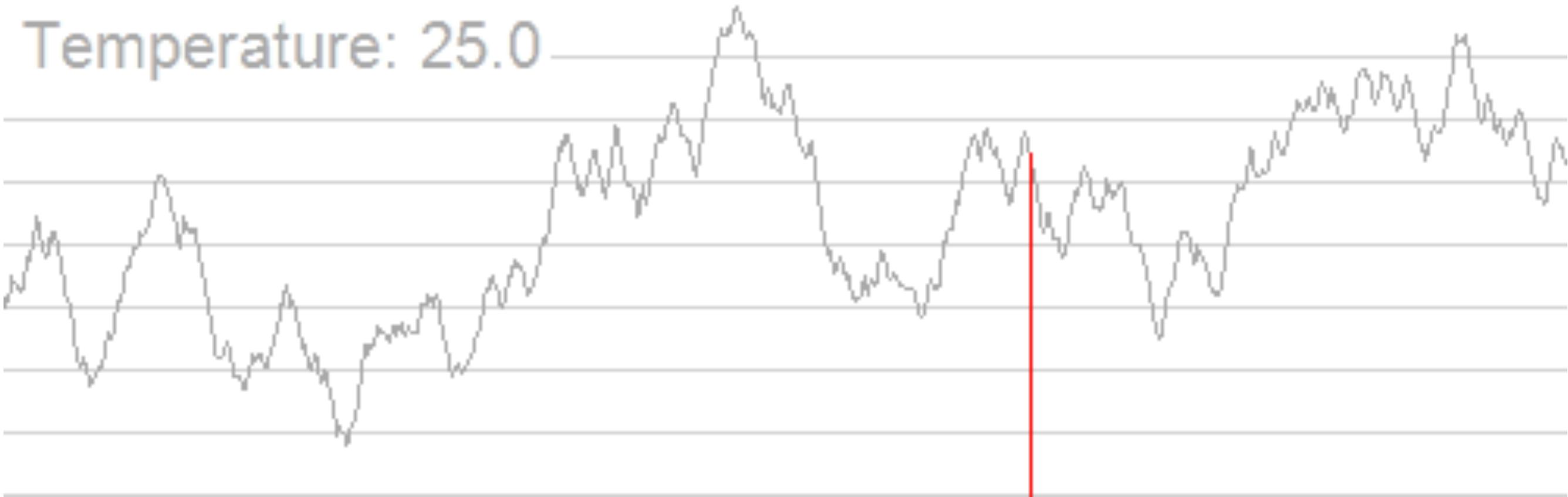
$p = \exp(-\Delta / (kT))$

        If  $p \leq \text{random}(0,1)$ :

$X = X'$

$E = E'$

$T = \text{cooling}(T)$



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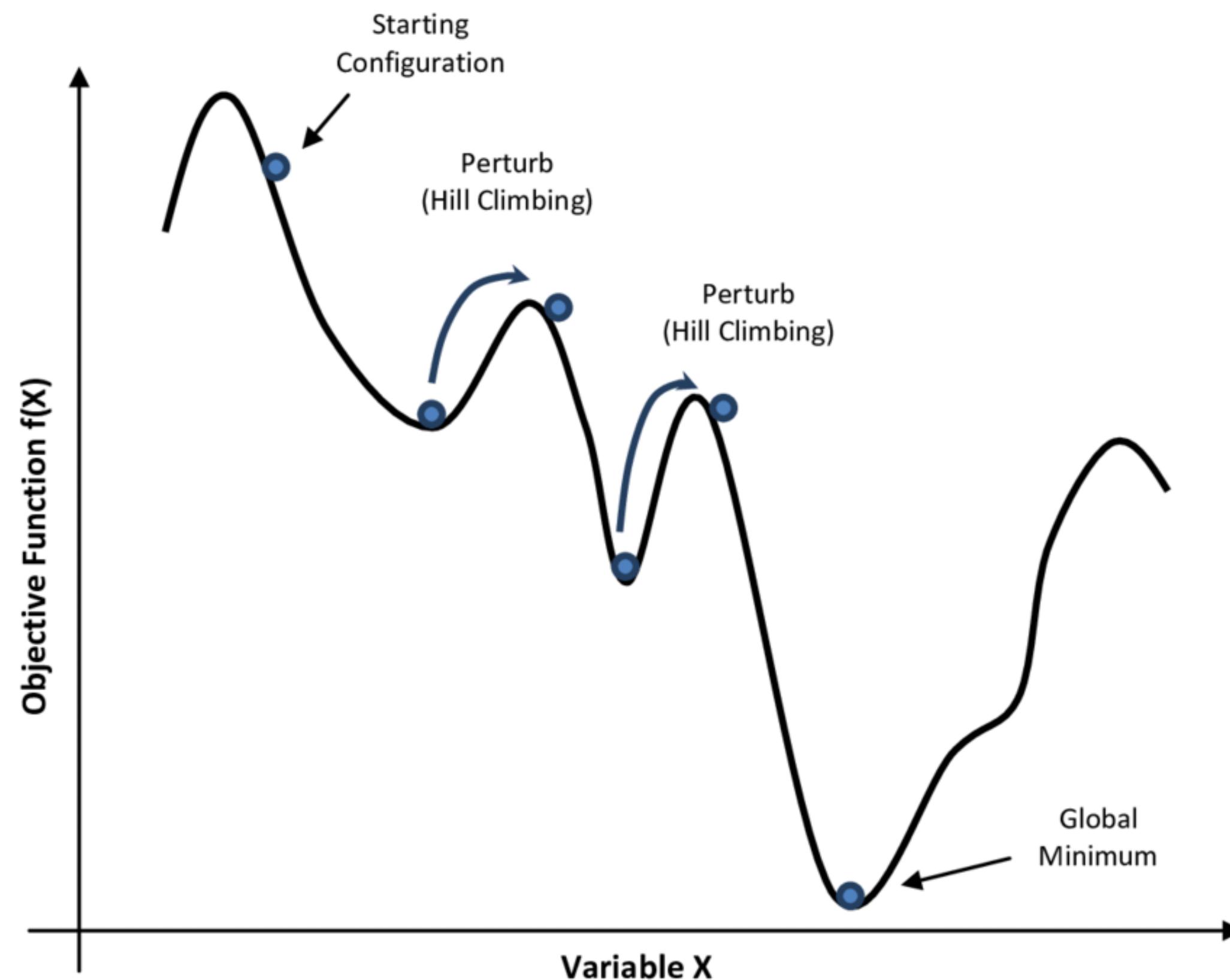
$p = \exp(-\Delta / (kT))$

        If  $p \leq \text{random}(0,1)$ :

$X = X'$

$E = E'$

$T = \text{cooling}(T)$



# MO Simulated Annealing (*Ulungu et al. 1999*)

## What changes?

Transition probability  $x \rightarrow x'$  should adapt to multiple objectives.

- If  $x'$  dominates  $x$  (case A):

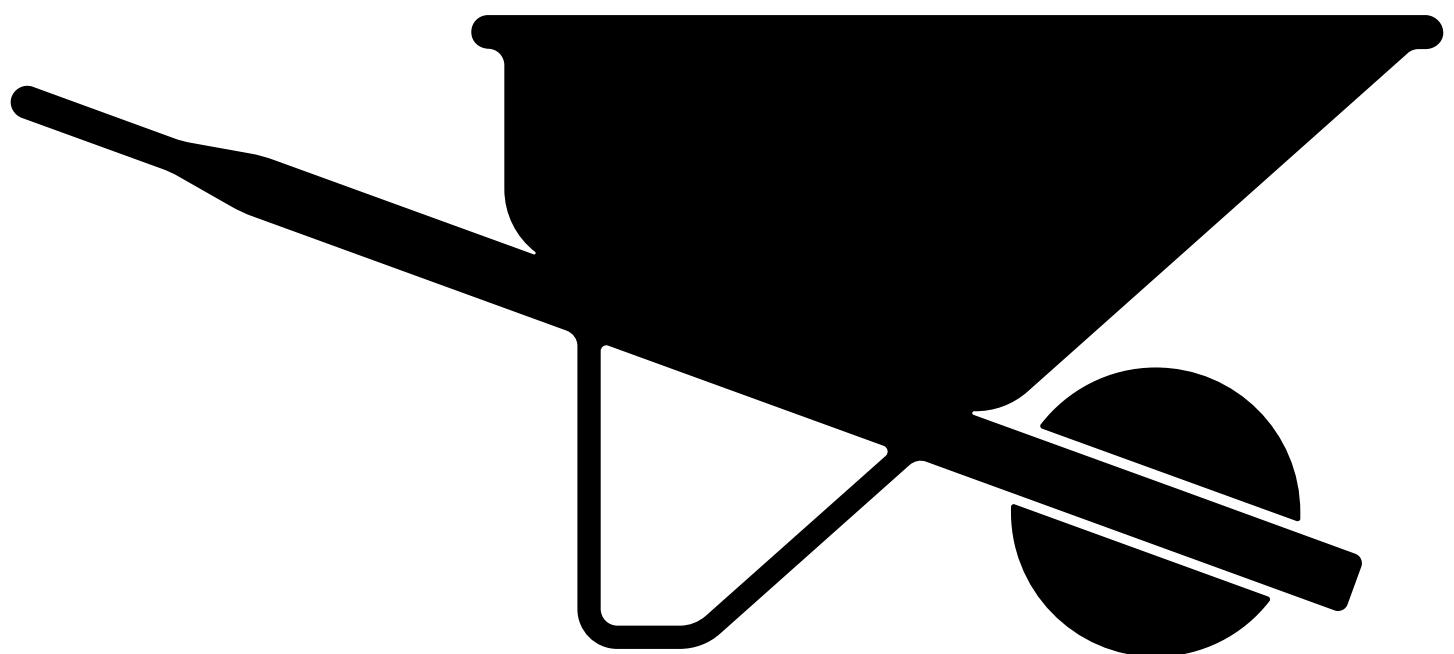
$$P\{x \rightarrow x' : x(t) = x\} = 1$$

- If  $x'$  is dominated by  $x$  (case C) or if there is no clear dominance relation

$$P\{x \rightarrow x' : x(t) = x\} = \prod_{i=1}^{n_{obj}} \exp \left\{ -\frac{\Delta f_i}{T(t)} \right\}$$

	$\Delta f_1 \leq 0$	$\Delta f_1 > 0$
$\Delta f_2 \leq 0$	A	B
$\Delta f_2 > 0$	B	C

# **Hands on**



# Particle Swarm Optimization (*Kennedy, Eberhart 1995*)

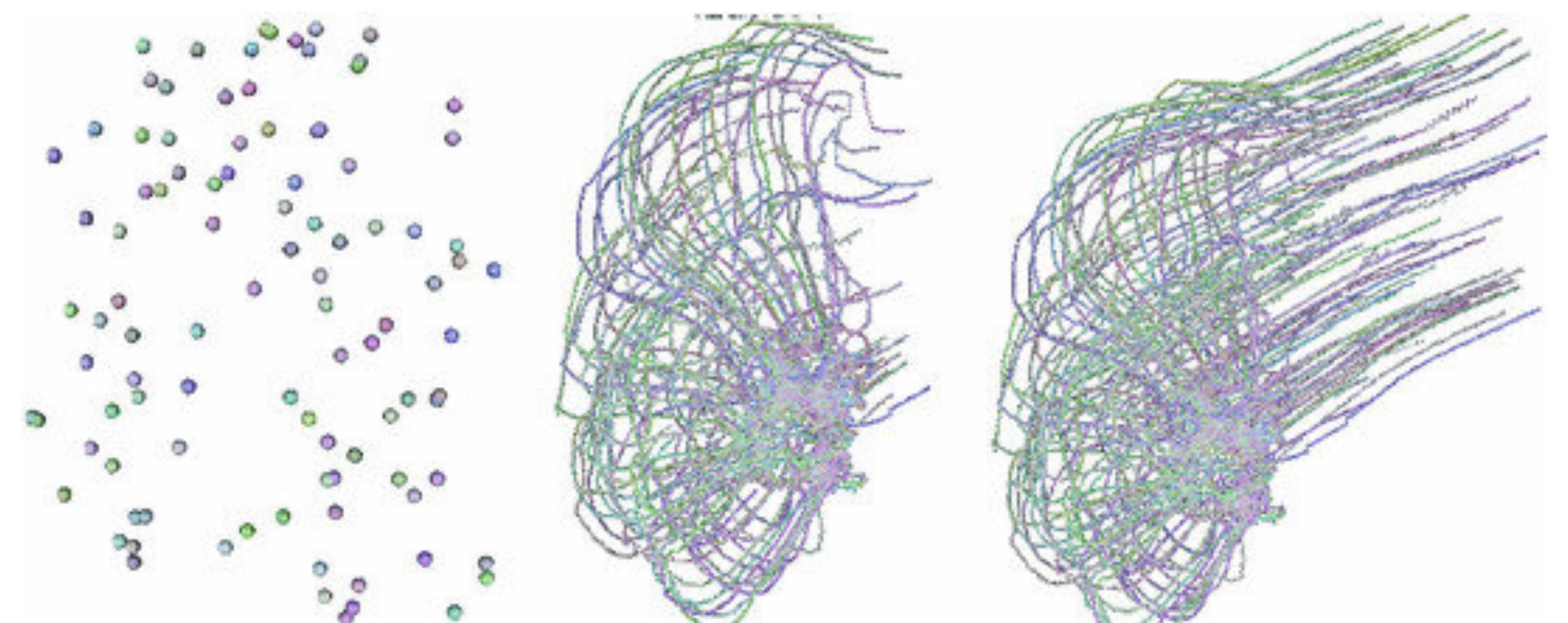
## Nature-inspired social behavior

The swarm/population is the set of current solutions

A particle is a single solution

Social behavior is sketched using:

- Memory/Cognition
- Social interaction and communication



# Particle Swarm Optimization (*Kennedy, Eberhart 1995*)

## Nature-inspired social behavior

We need to track

- Position  $\vec{x}(t) = (x_1(t), \dots, x_D(t))^T$
- Velocity  $\vec{v}(t) = (v_1(t), \dots, v_D(t))^T$
- Personal best  $\vec{x}_b(t) = (x_{b1}(t), \dots, x_{bD}(t))^T$
- Leader's best (global or local)  $\vec{x}_n(t) = (x_{n1}(t), \dots, x_{nD}(t))^T$

**Leader:** particle guiding another particle in the search space

# Particle Swarm Optimization (*Kennedy, Eberhart 1995*)

## Visual inspection

Each iteration requires updating the particles' velocity and position

$$\vec{v}_i(t+1) = \omega \vec{v}_i(t) + c_1 r_1 (\vec{x}_{bi} - \vec{x}_i(t)) + c_2 r_2 (\vec{x}_{ni} - \vec{x}_i(t))$$

$$\vec{x}_i(t+1) = \vec{x}_i(t) + \vec{v}_i(t+1)$$

Velocity is given by:

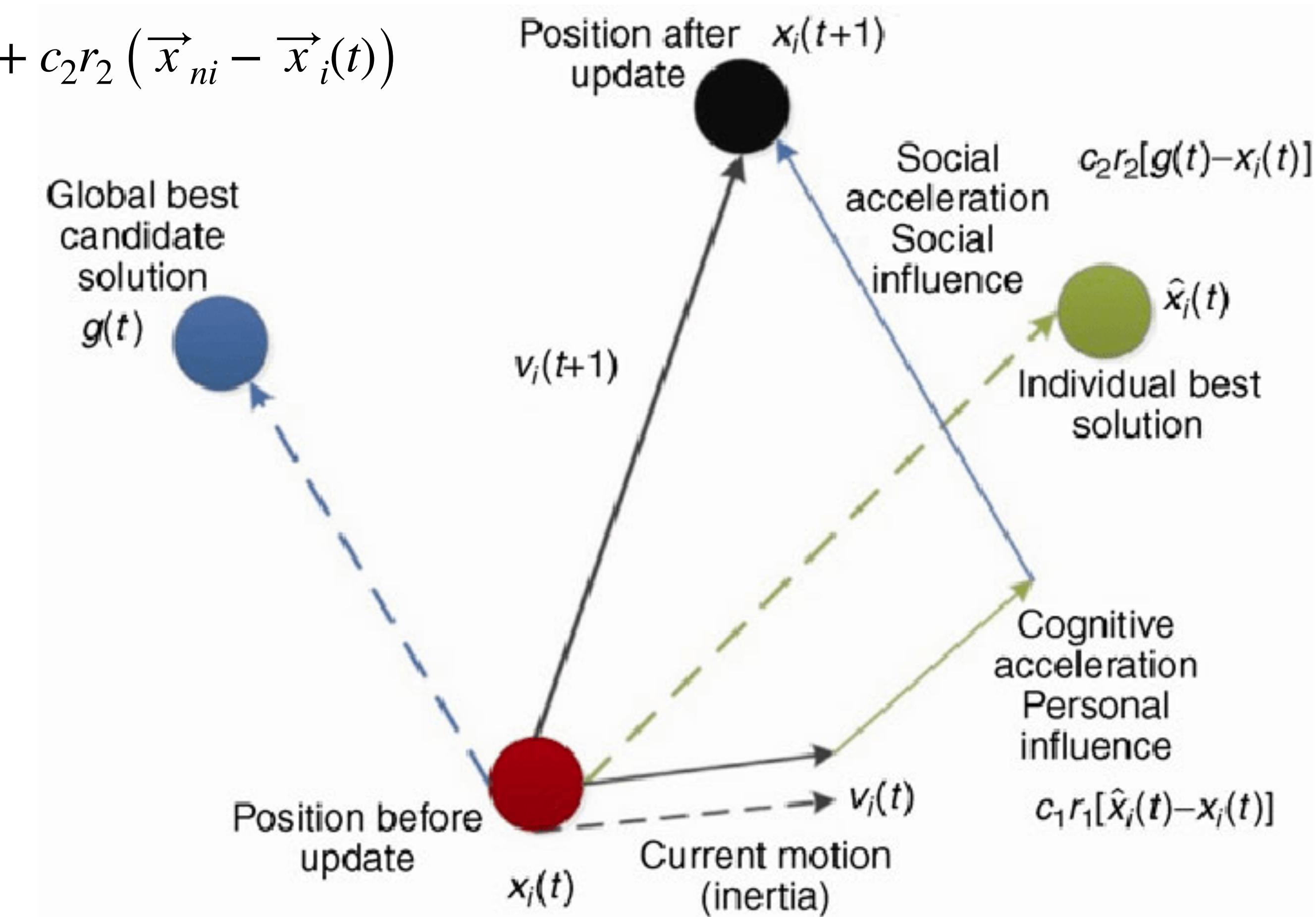
- Current flight direction  $\rightarrow \omega$  inertia
- Cognitive component  $\rightarrow c_1$  cognitive learning factor
- Social component  $\rightarrow c_2$  social learning factor
- Randomness  $\rightarrow r_1, r_2 \in \text{Random}[0,1]$

# Particle Swarm Optimization (*Kennedy, Eberhart 1995*)

## Dynamic equations

$$\vec{v}_i(t+1) = \omega \vec{v}_i(t) + c_1 r_1 (\vec{x}_{bi} - \vec{x}_i(t)) + c_2 r_2 (\vec{x}_{ni} - \vec{x}_i(t))$$

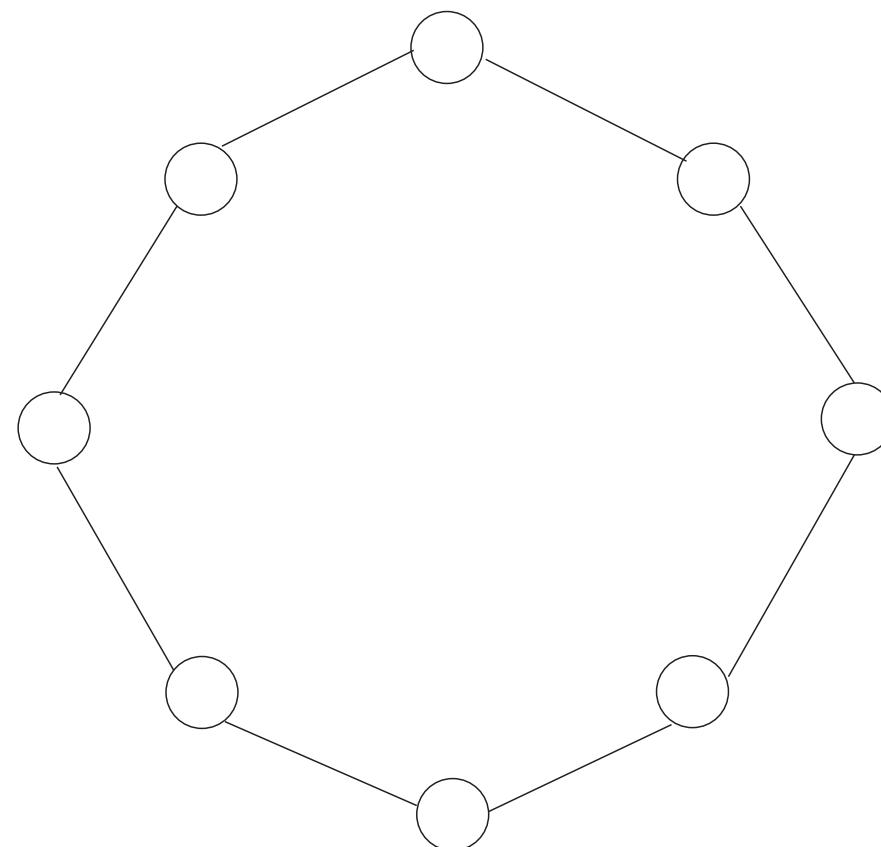
$$\vec{x}_i(t+1) = \vec{x}_i(t) + \vec{v}_i(t+1)$$



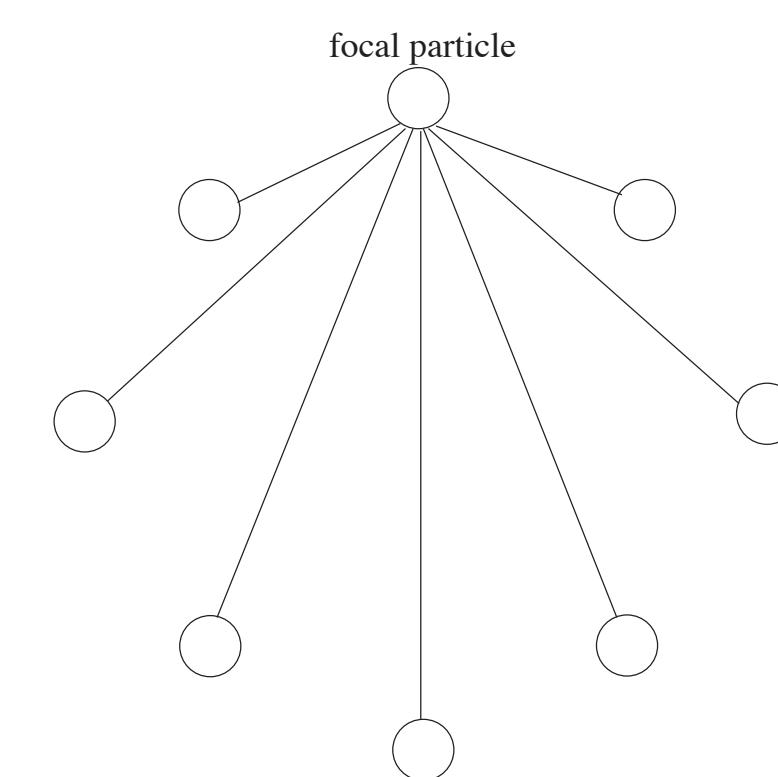
# Particle Swarm Optimization (*Kennedy, Eberhart 1995*)

## Neighborhood definitions

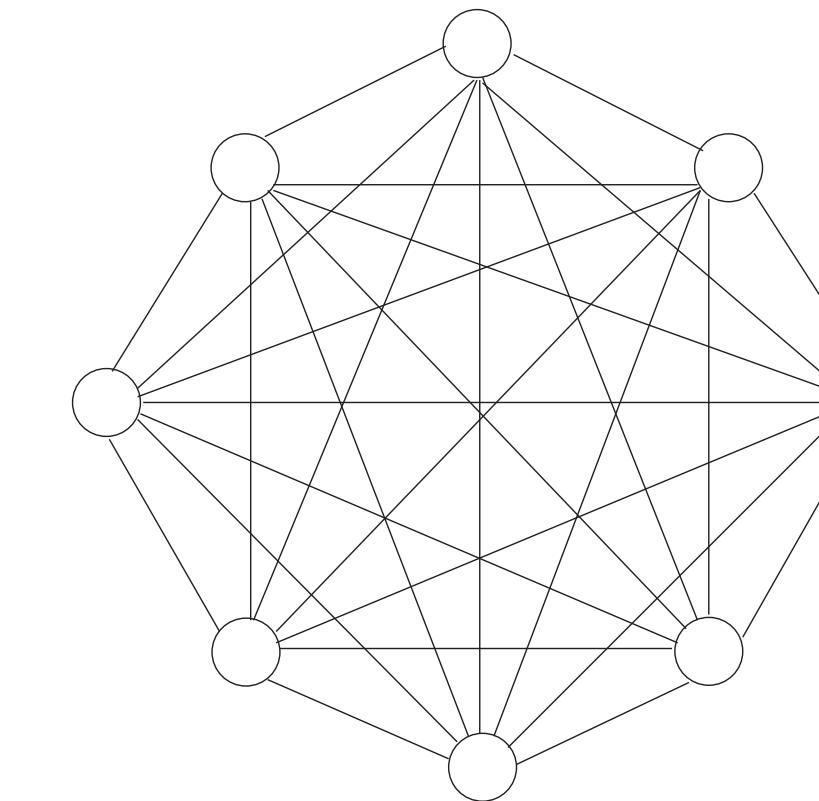
Social interaction can be represented as a graph:



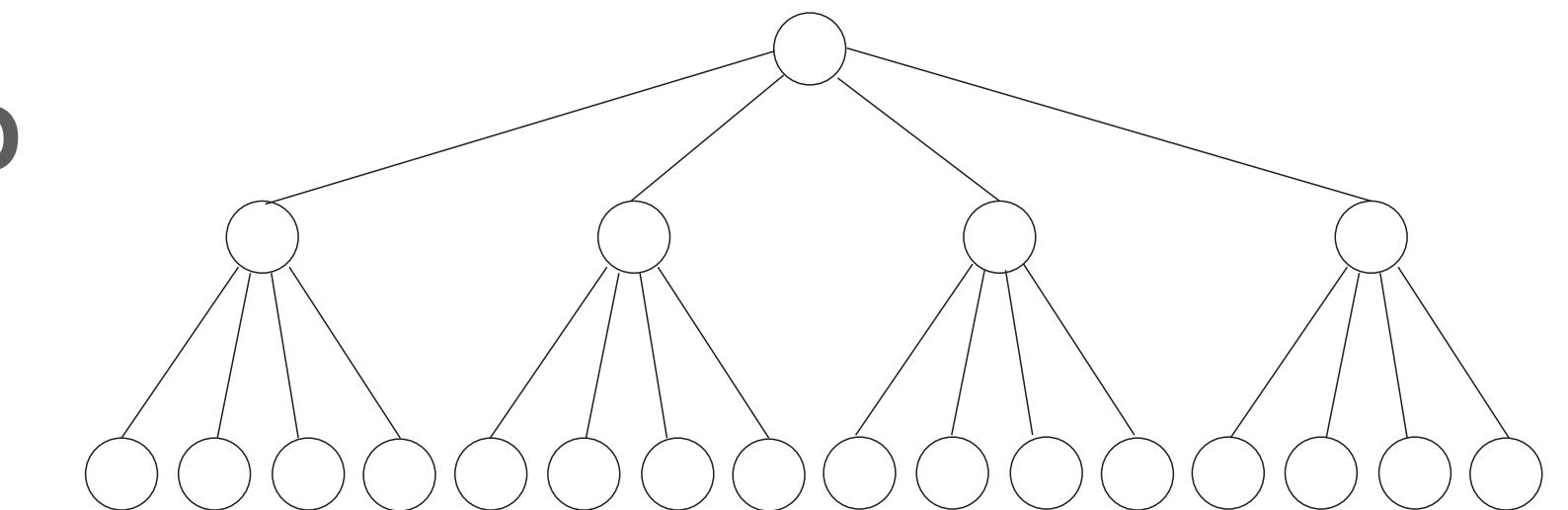
RING KNN=2



STAR NETWORK



FULLY CONNECTED



TREE HIERARCHICAL

Particles are influenced by the success of anyone they are connected to!

# PSO

## Pseudocode

```
Begin
    Initialize swarm
    Locate leader
     $g = 0$ 
    While  $g < g_{max}$ 
        For each particle
            Update Position (Flight)
            Evaluation
            Update  $p_{best}$ 
        EndFor
        Update leader
         $g++$ 
    EndWhile
End
```

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The outcome is strongly influenced by:

- Hyperparameters
- Social topology

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```

The outcome is strongly influenced by:

- Hyperparameters
- Social topology

$\omega : 0 \rightarrow 1$  min-to-max momentum

$c_1 : 0 \rightarrow 1$  min-to-max impact of memories

$c_2 : 0 \rightarrow 1$  min-to-max social pressure

In particular  $c_2 = 0 \cap c_1 > 0$  leads to an “everyone for himself” situation, and the system does not converge.

*No particle is an island!*

# **Multi-Objective PSO (MOPSO)**

## **What changes?**

Need to:

- Find as many optimal solutions as possible
  - The notion of best is not unique anymore
  - Need to initialize  $P$  archives for personal best (non-dominated) solutions
  - Need to initialize an archive for global best solutions
- Maximize their spread/search space

But:

- How to select among potential leaders/personal best?
- How to update the internal archive?
- How to maintain diversity in the archive?

# **Multi-Objective PSO (MOPSO)**

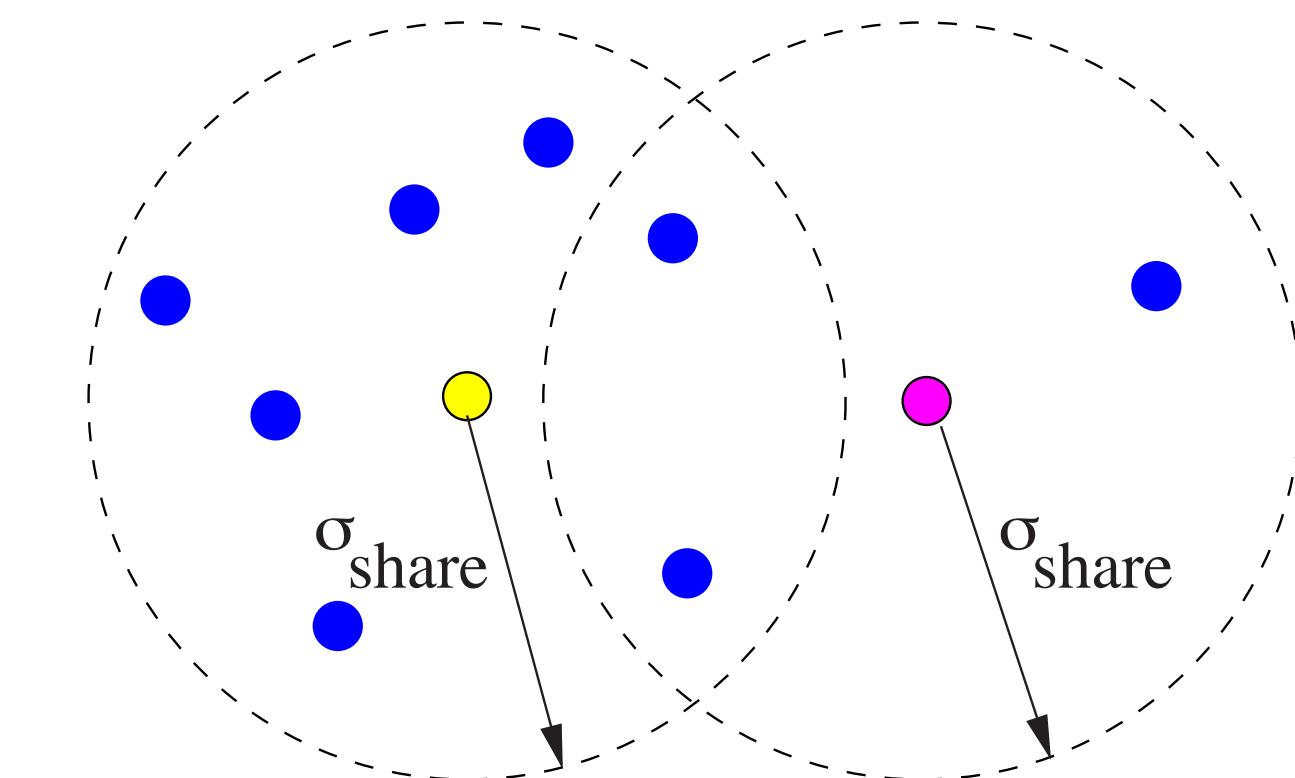
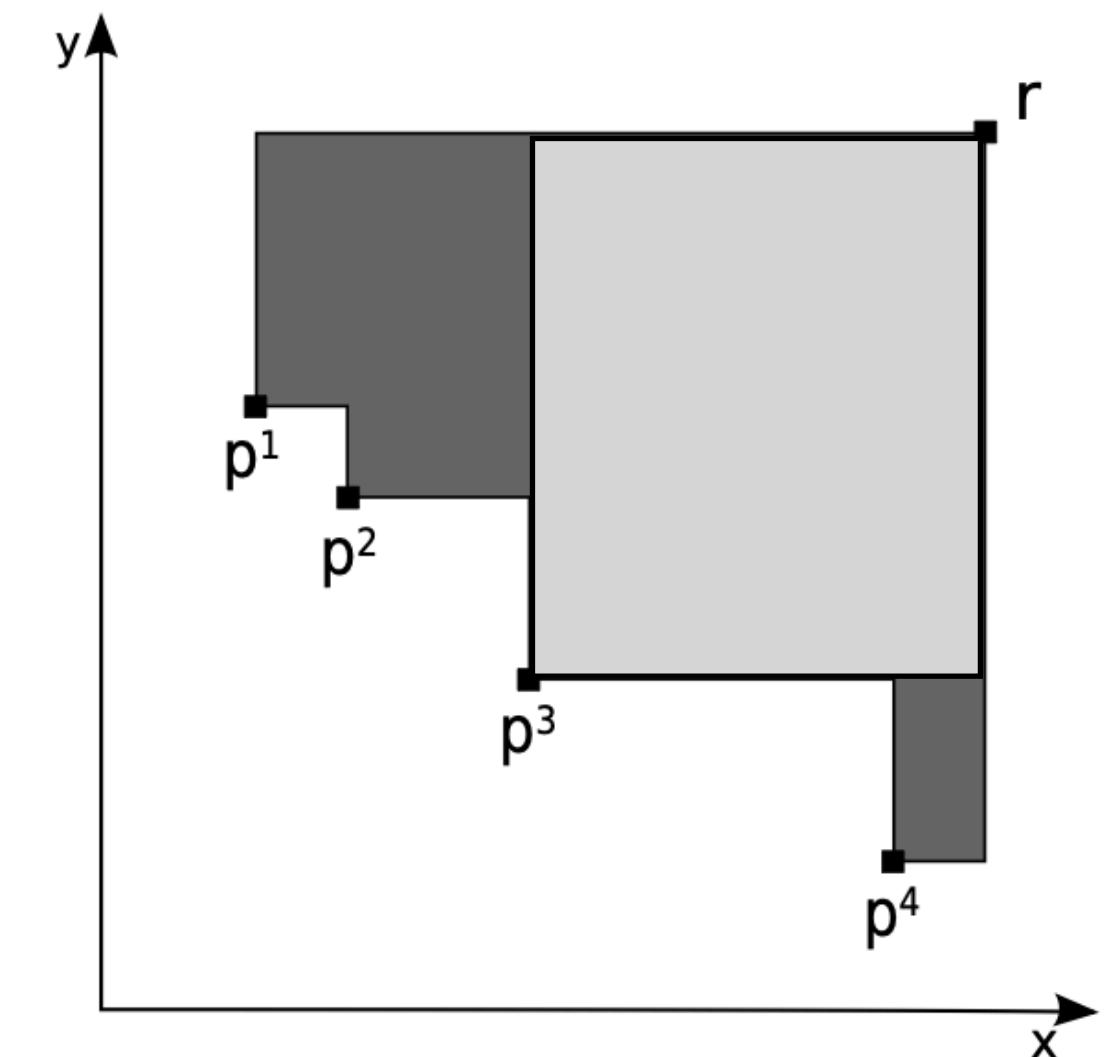
## **What changes?**

- How to select among potential leaders/personal best?
  - Random selection

# Multi-Objective PSO (MOPSO)

## What changes?

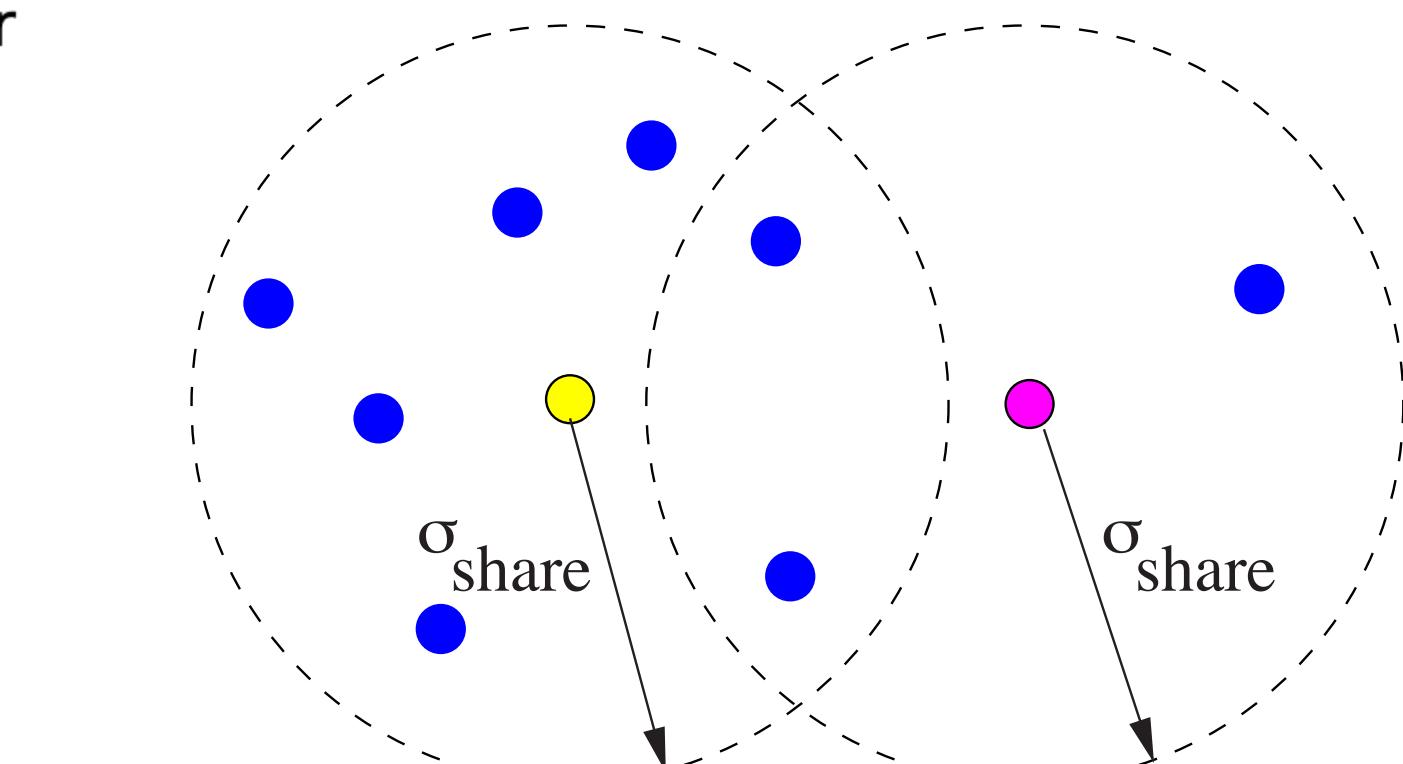
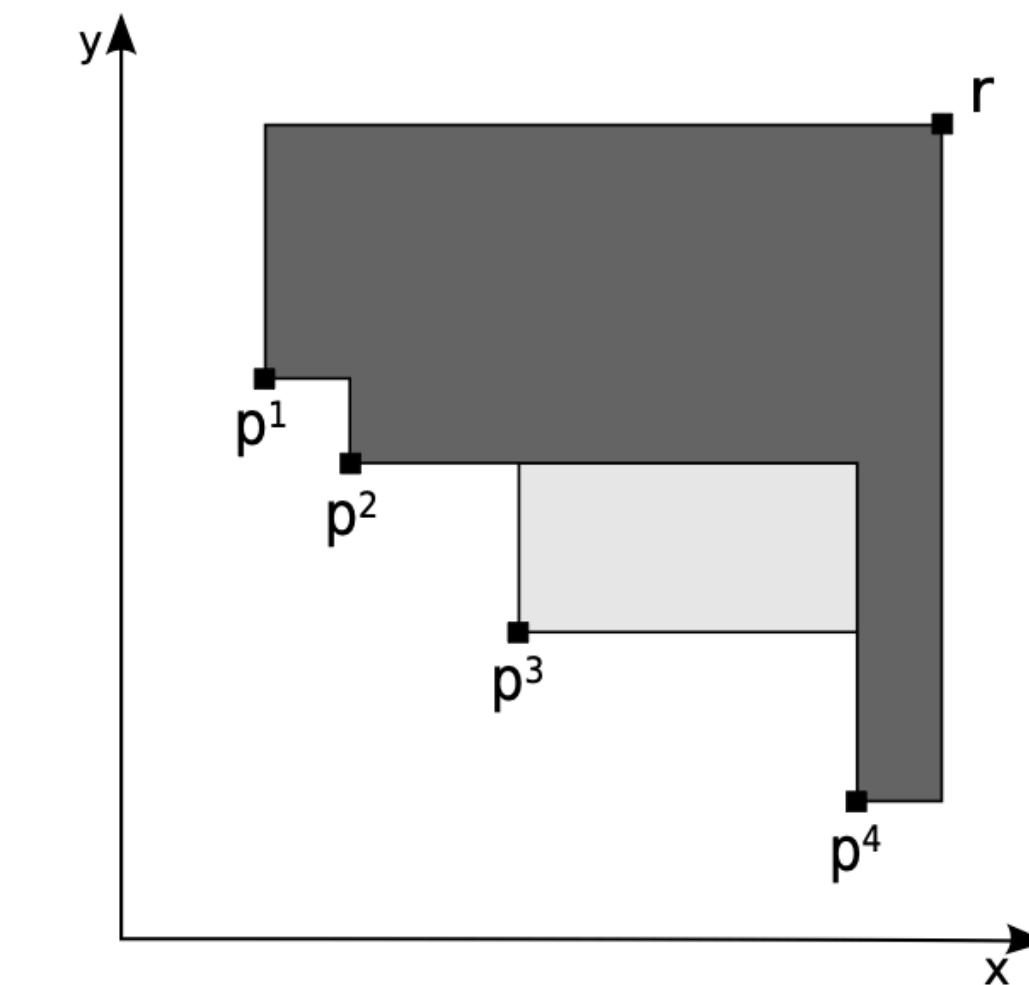
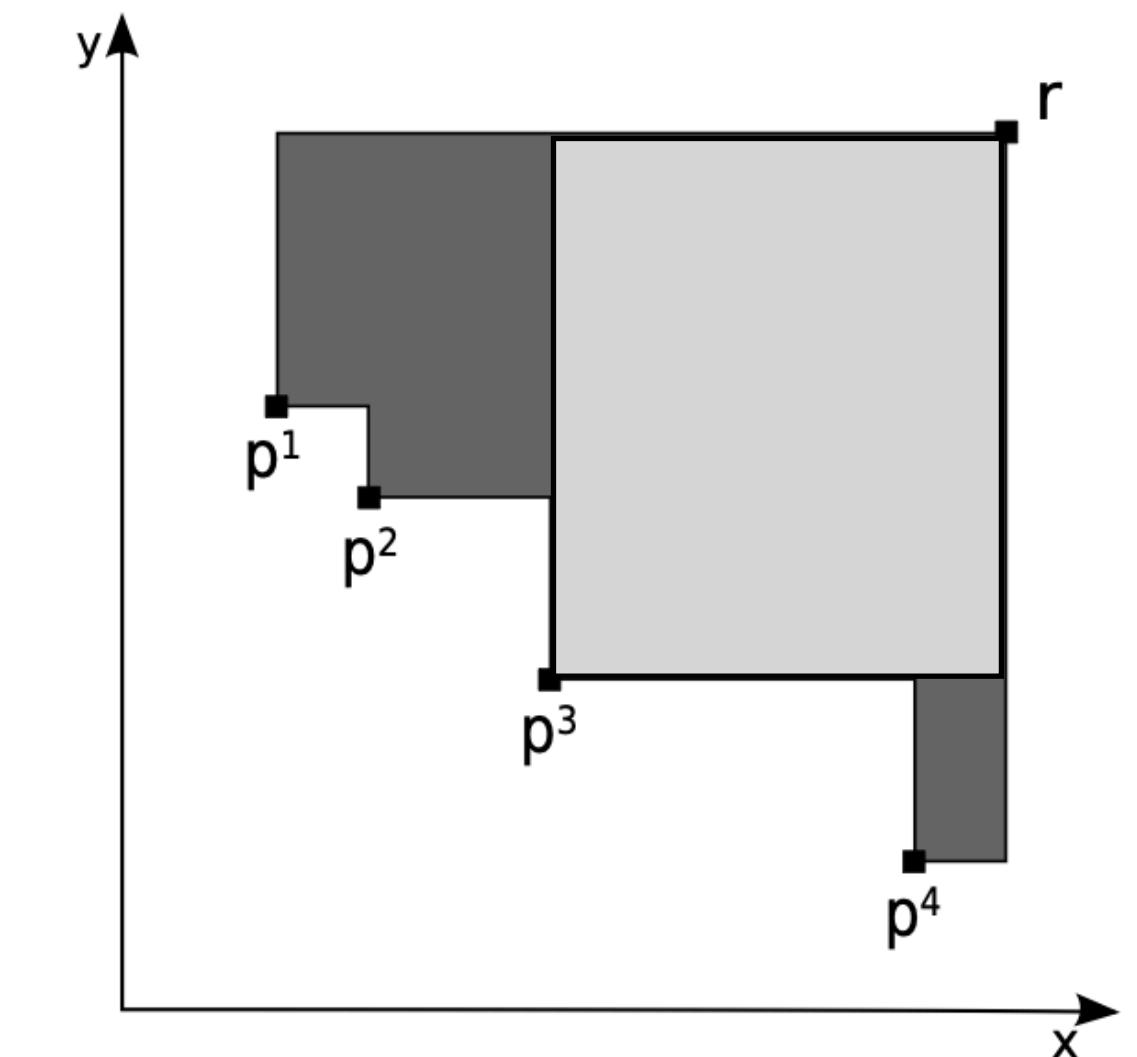
- How to select among potential leaders/personal best?
  - Random selection
  - Selection based on performance indicators



# Multi-Objective PSO (MOPSO)

## What changes?

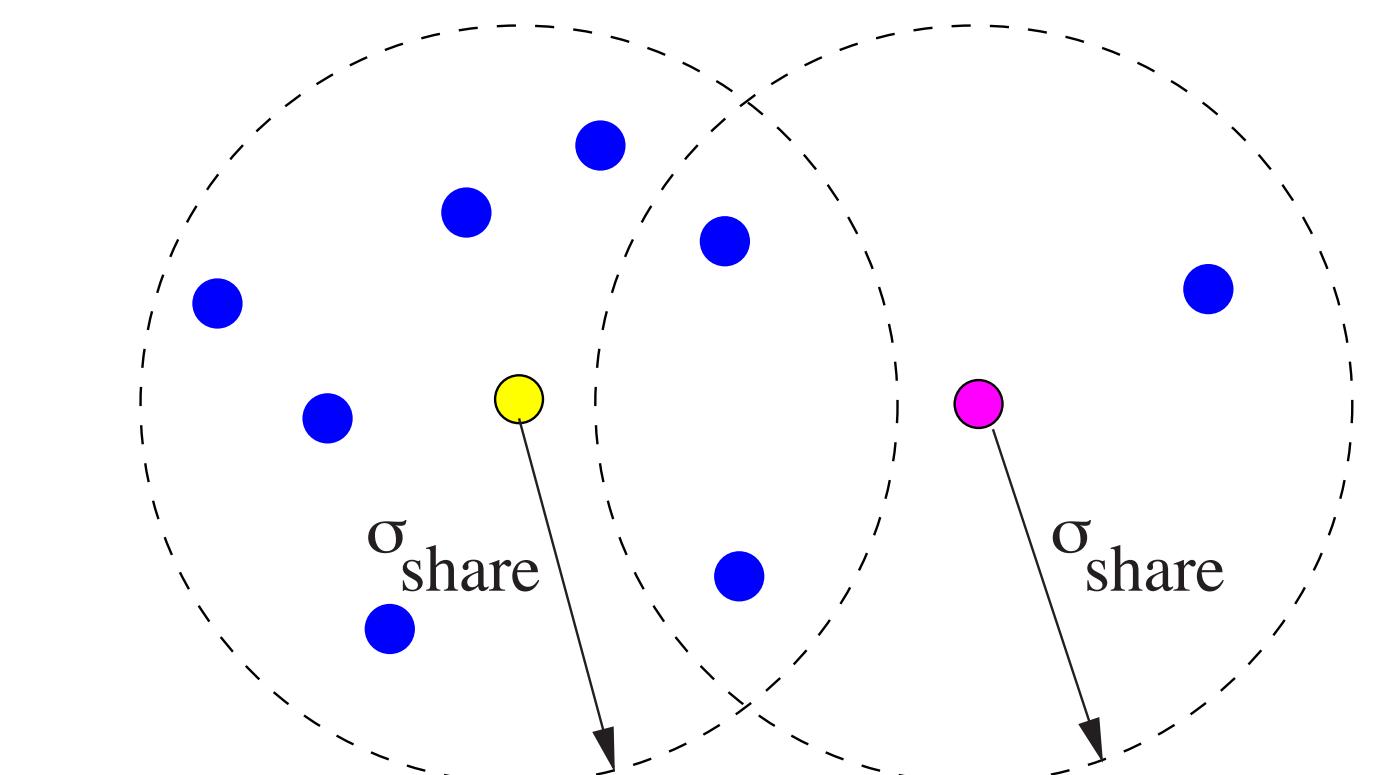
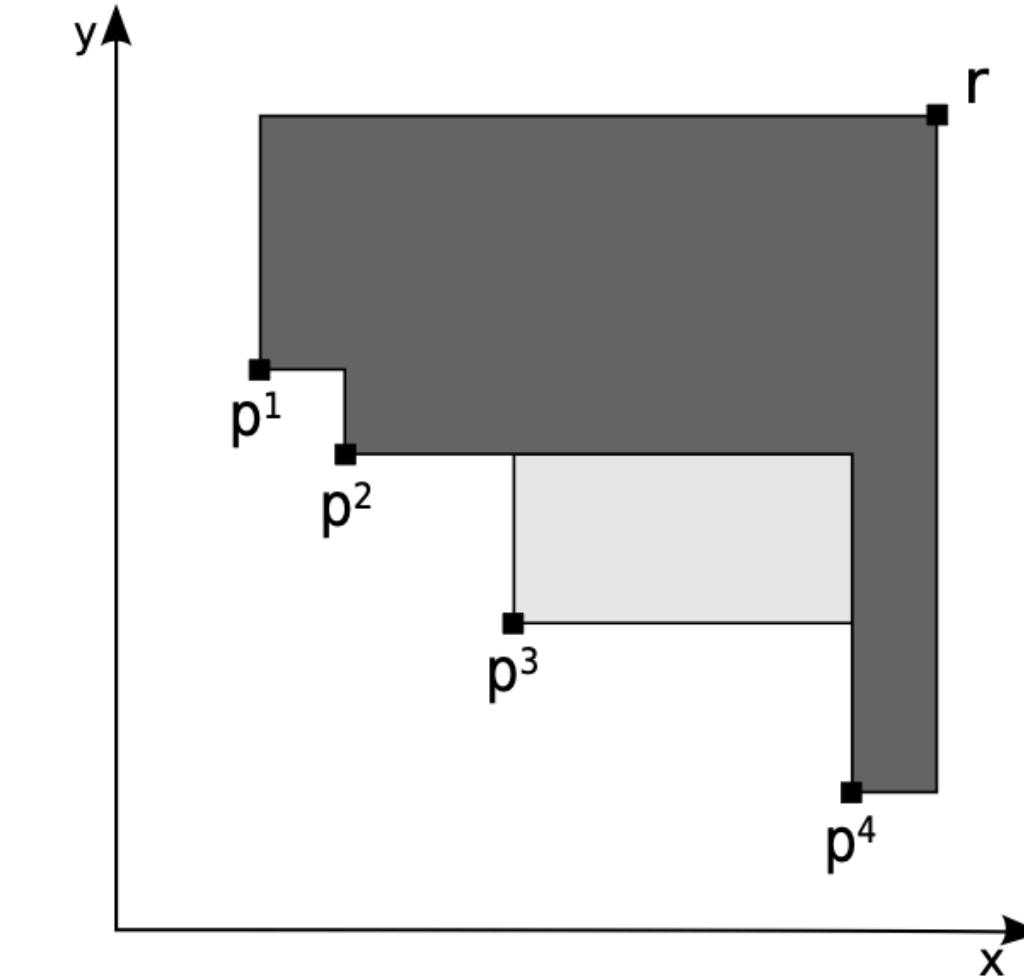
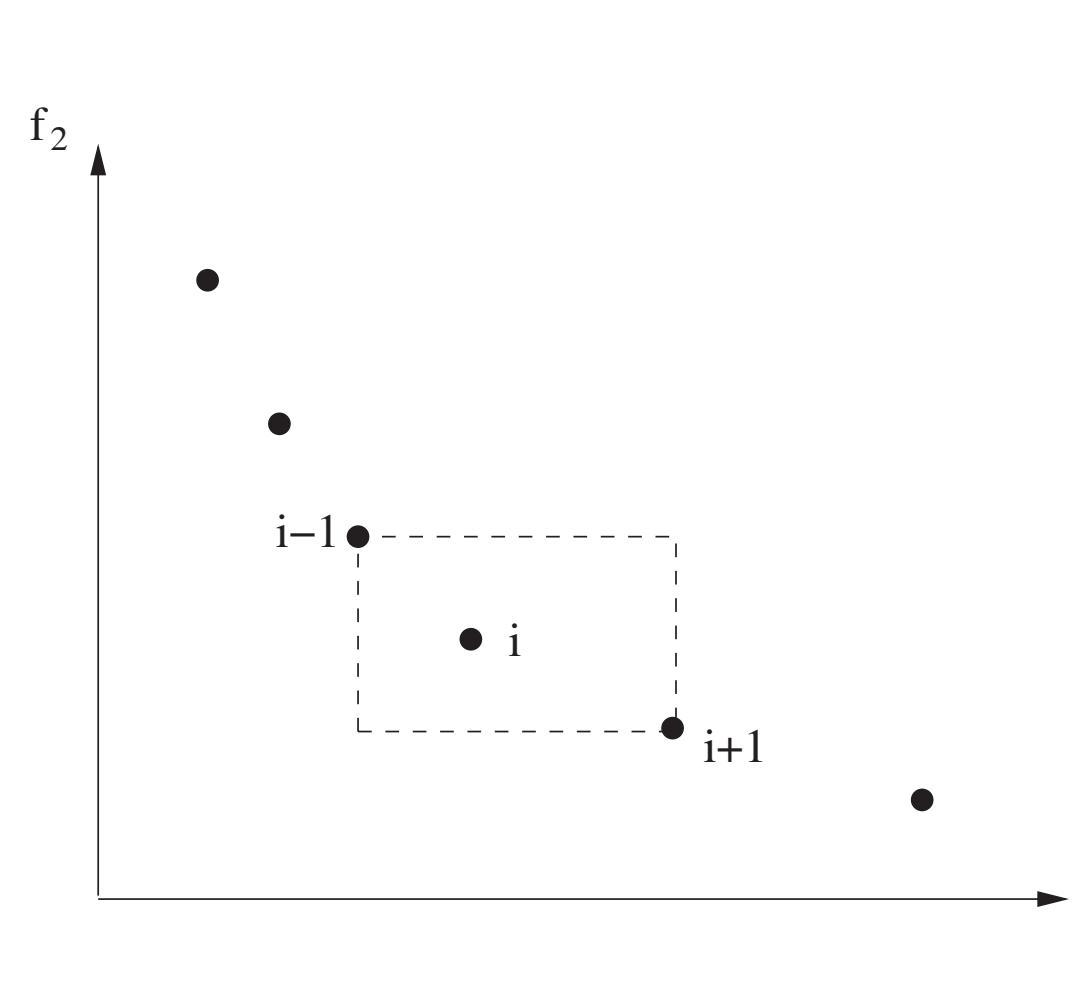
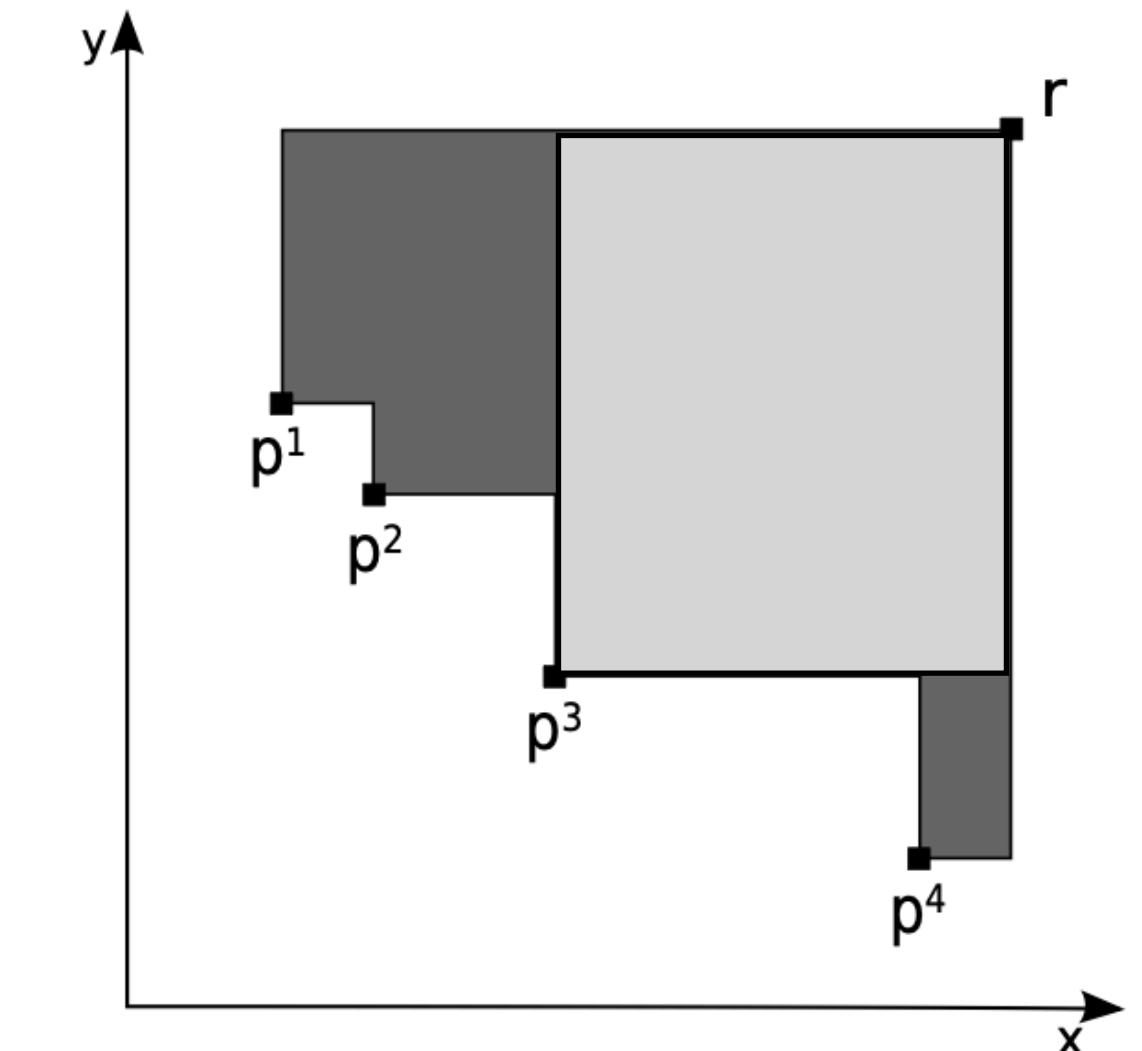
- How to select among potential leaders/personal best?
  - Random selection
  - Selection based on performance indicator
  - Selection based on exclusive dominance hypervolume



# Multi-Objective PSO (MOPSO)

## What changes?

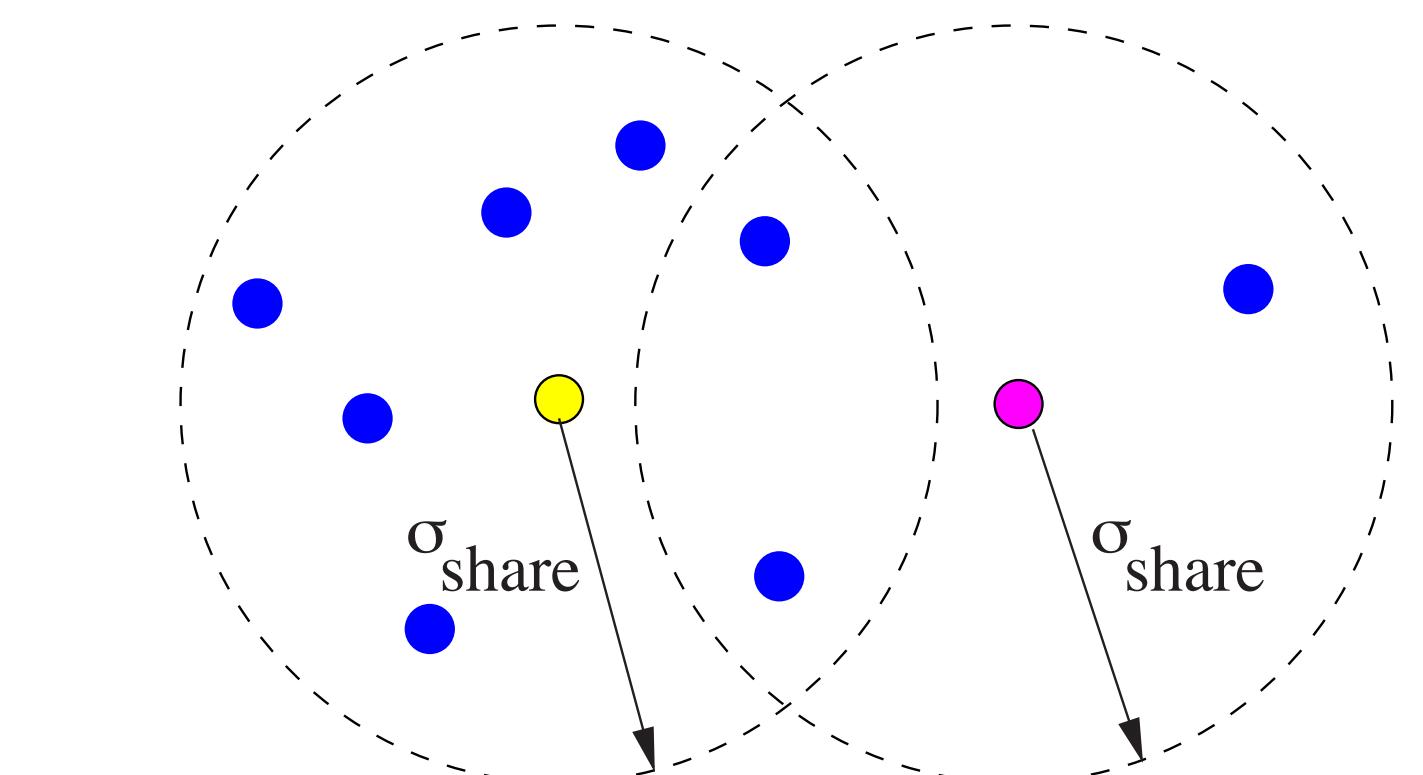
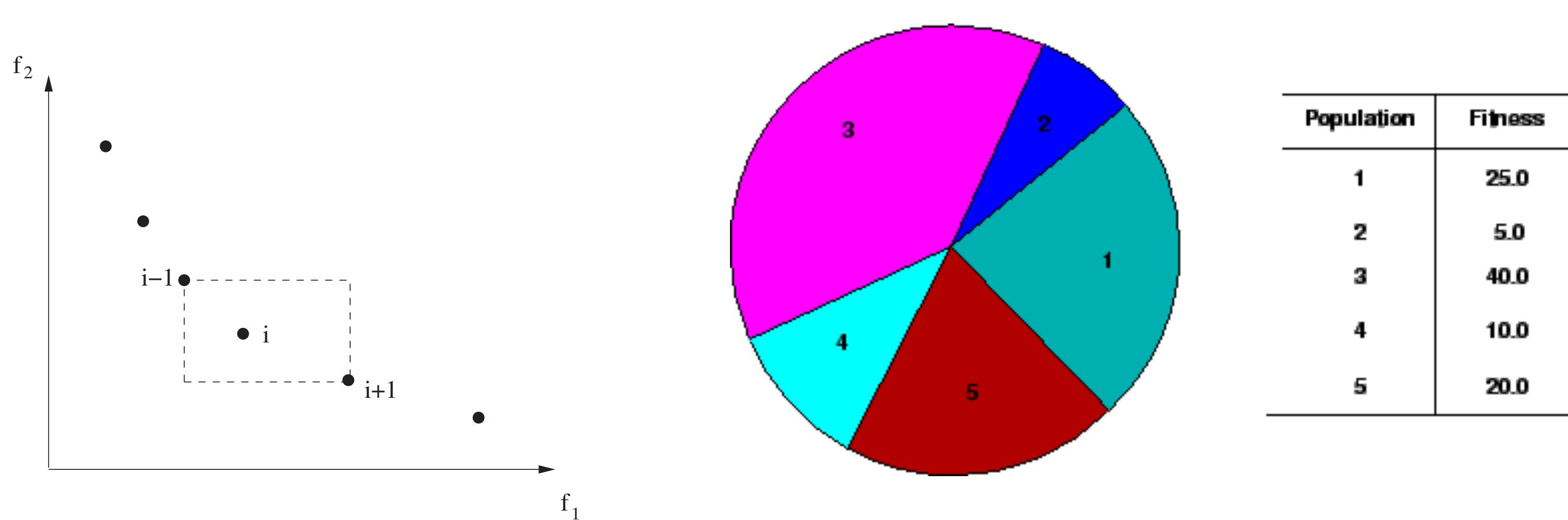
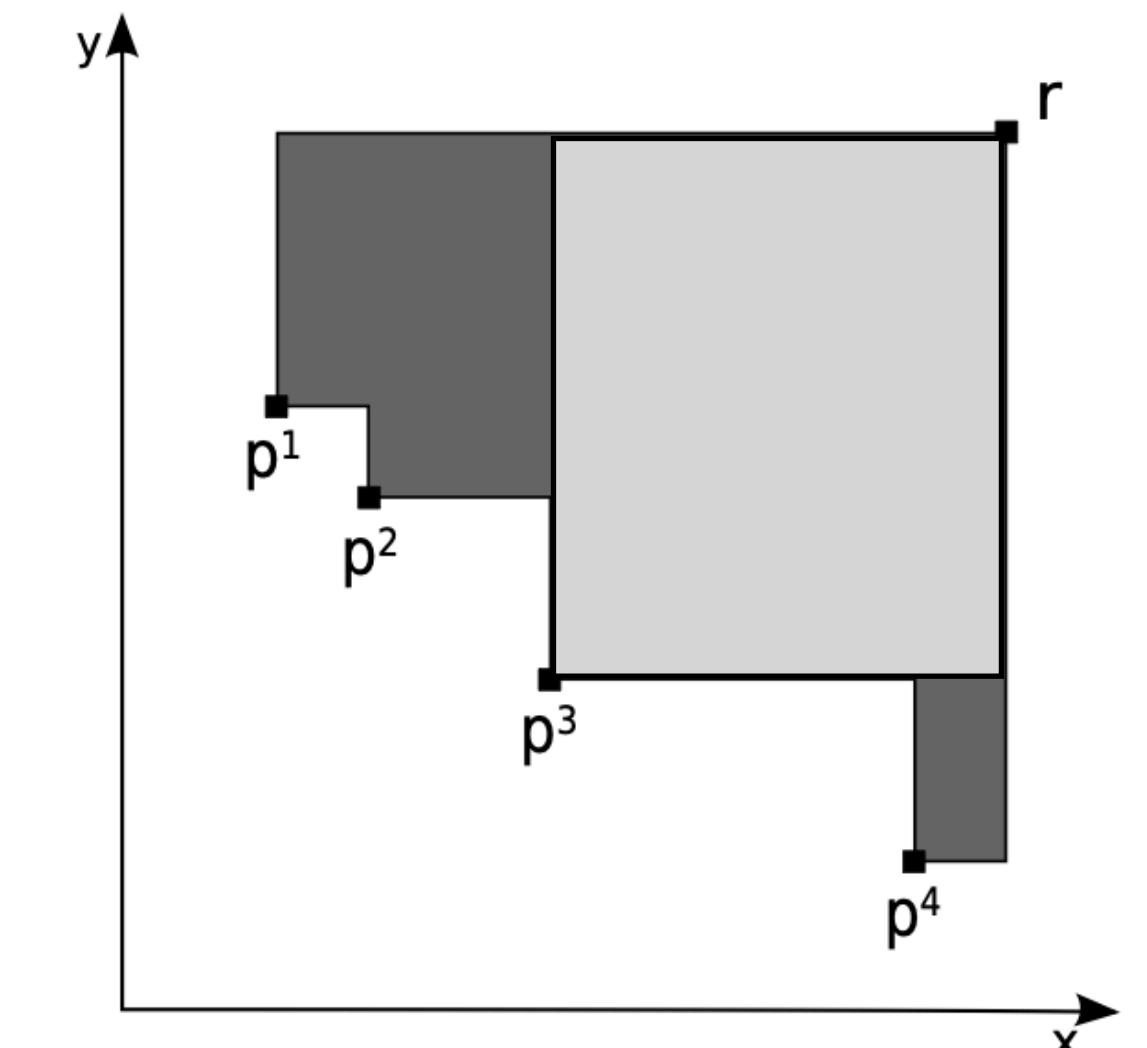
- How to select among potential leaders/personal best?
  - Random selection
  - Selection based on performance indicator
  - Selection based on exclusive dominance hypervolume
  - Selection based on NN density estimate



# Multi-Objective PSO (MOPSO)

## What changes?

- How to select among potential leaders/personal best?
  - Random selection
  - Selection based on performance indicator
  - Selection based on exclusive dominance hypervolume
  - Selection based on NN density estimate
  - ...  
(best or roulette selection)



# **Multi-Objective PSO (MOPSO)**

## **What changes?**

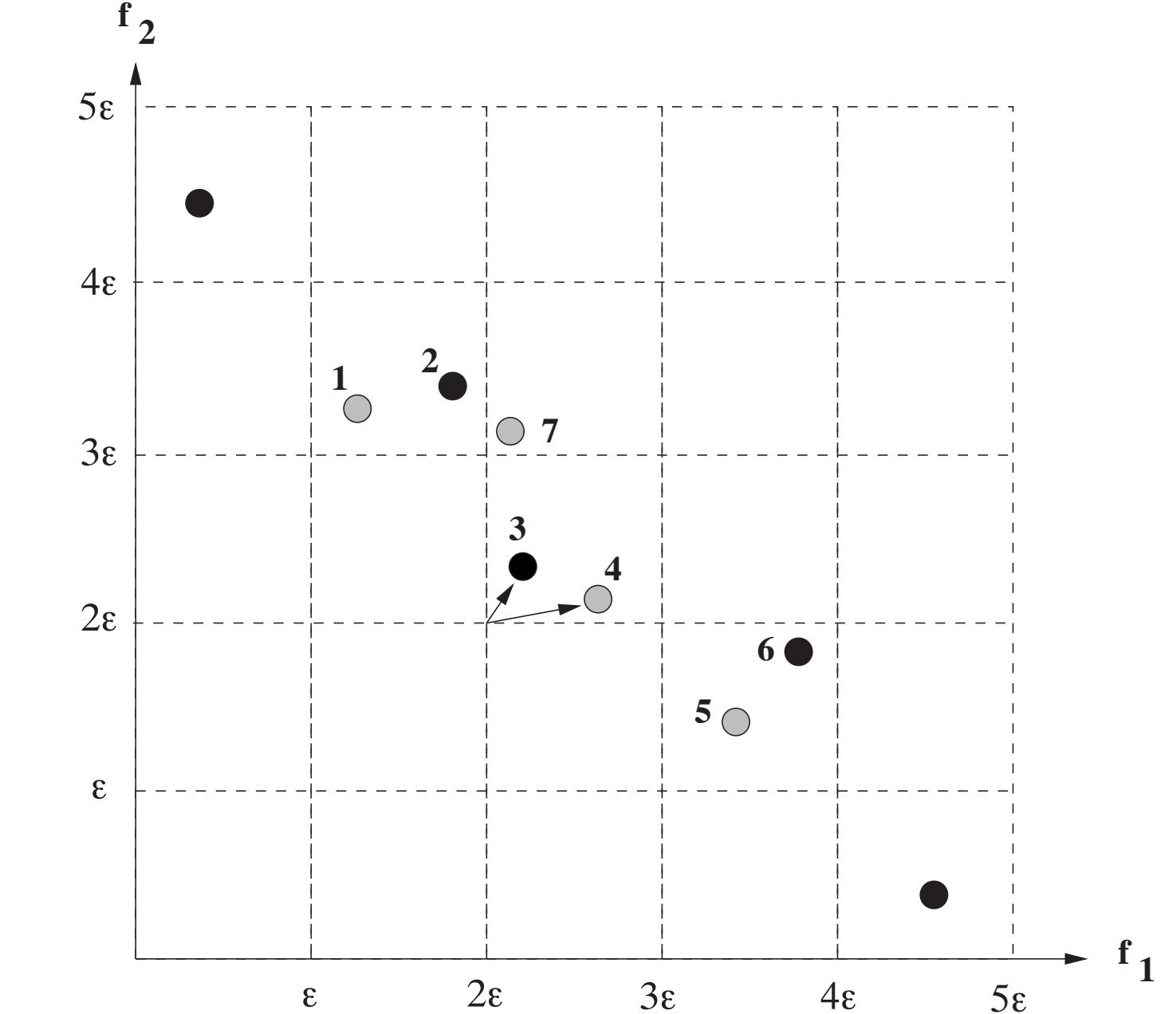
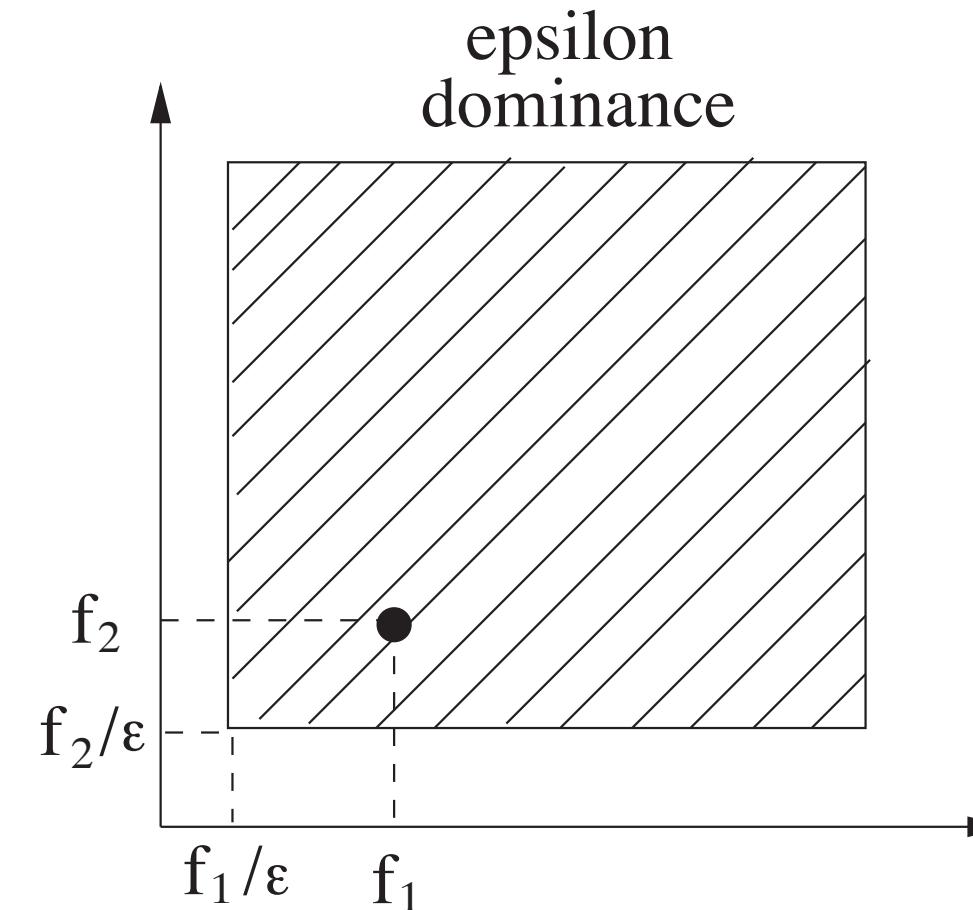
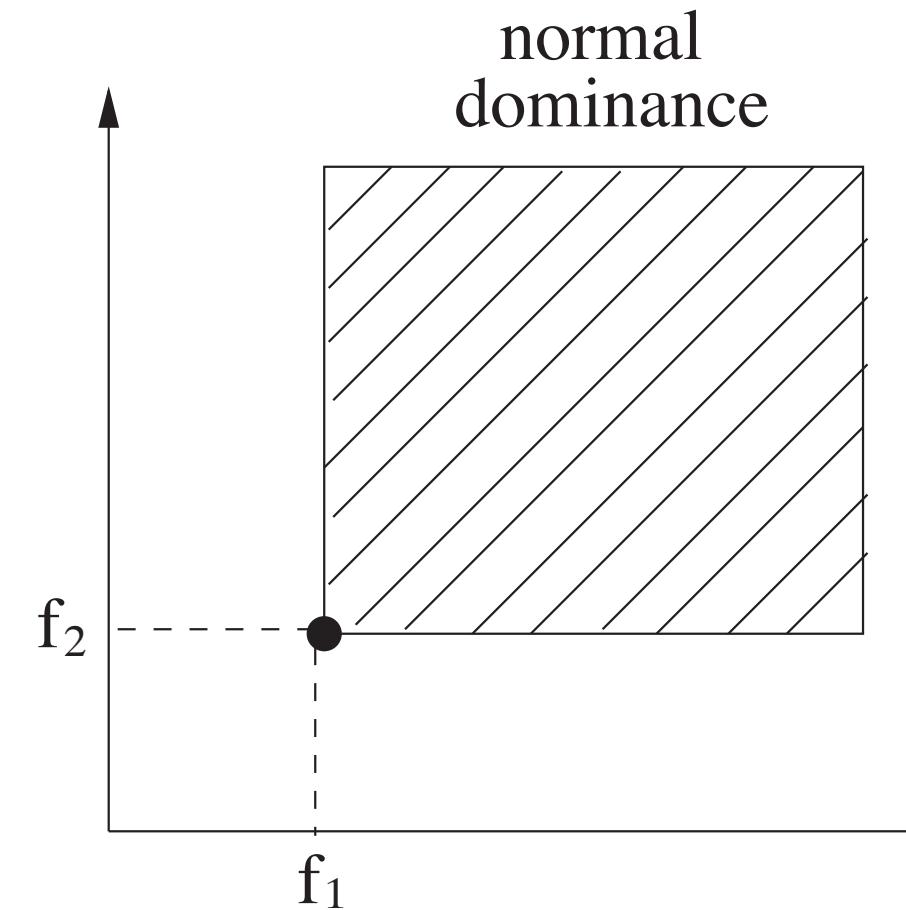
- How to update the internal archive?
  - If no clear dominance relation between the archive and the new solution
    - > add position and scores to the archive list
  - If new solution dominates those archived
    - > re-initialize the archive with the new position and scores

This is true for both the personal archives and the global archive

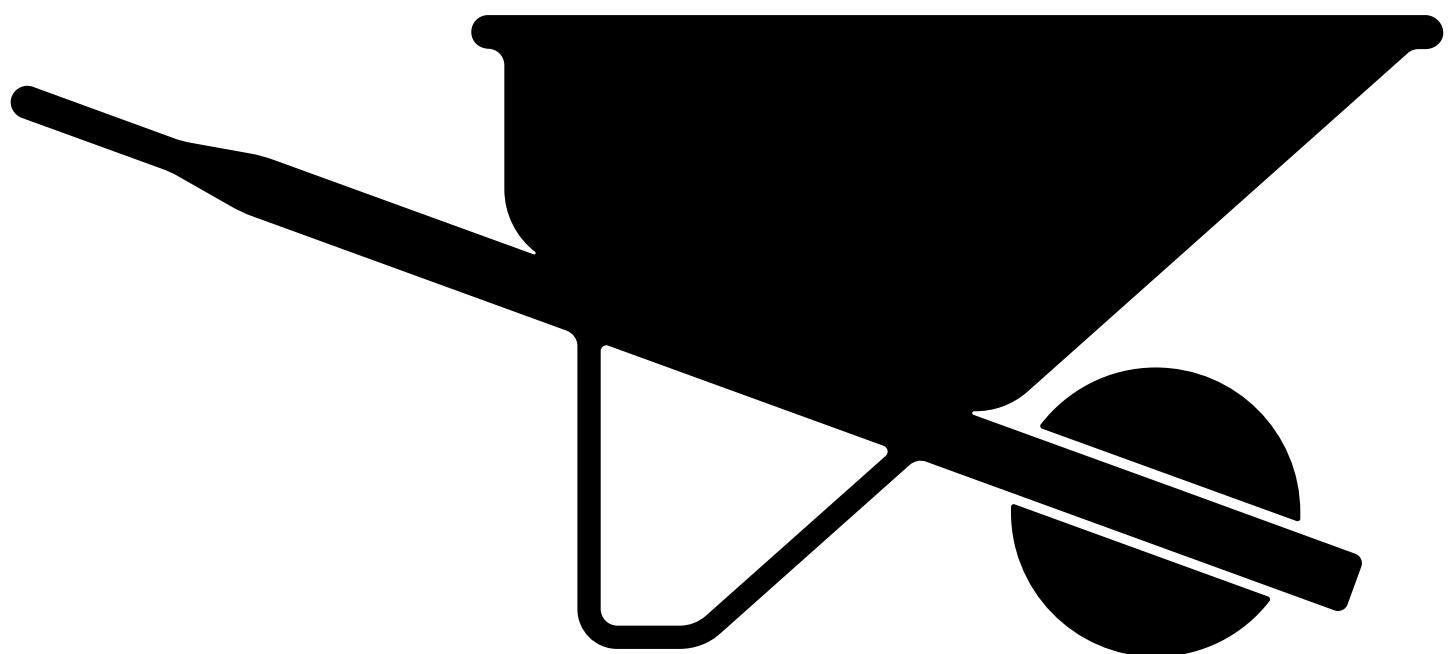
# Multi-Objective PSO (MOPSO)

## What changes?

- How to maintain diversity in the archive? When the archive limit is reached...
  - Use clustering technique
  - Use niche count to drop solutions ( cutoff + roulette? )
  - Use epsilon-dominance
  - ...



# **Hands on**



# Ant Colony Optimization (Dorigo, 1992)

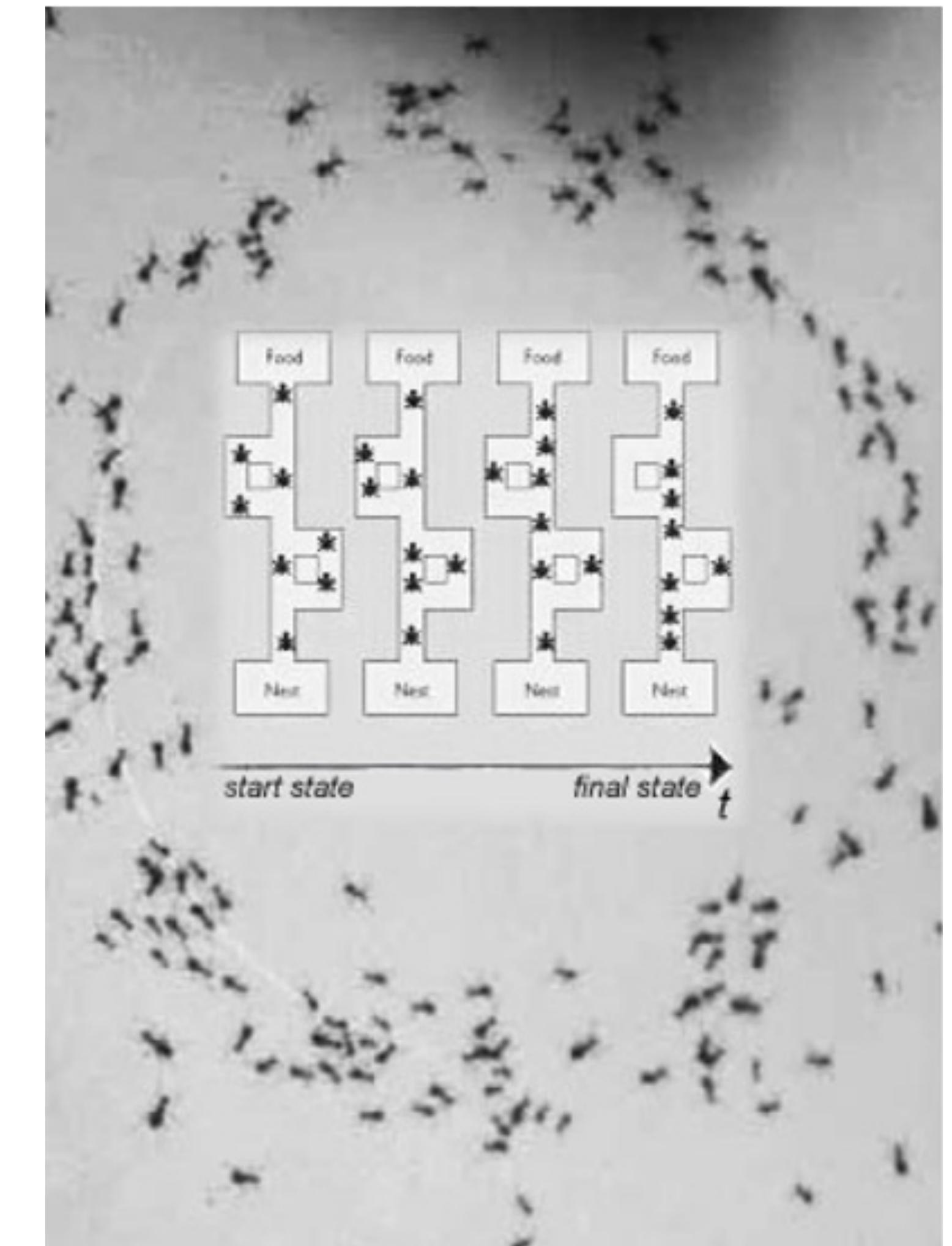
**Multi-agent method inspired by ant behavior**

Some ant species are able to communicate without physical interaction.

Once moved to a new place, ants move at random (initially)

After they find some food source, ants leave pheromone on their way back to the nest

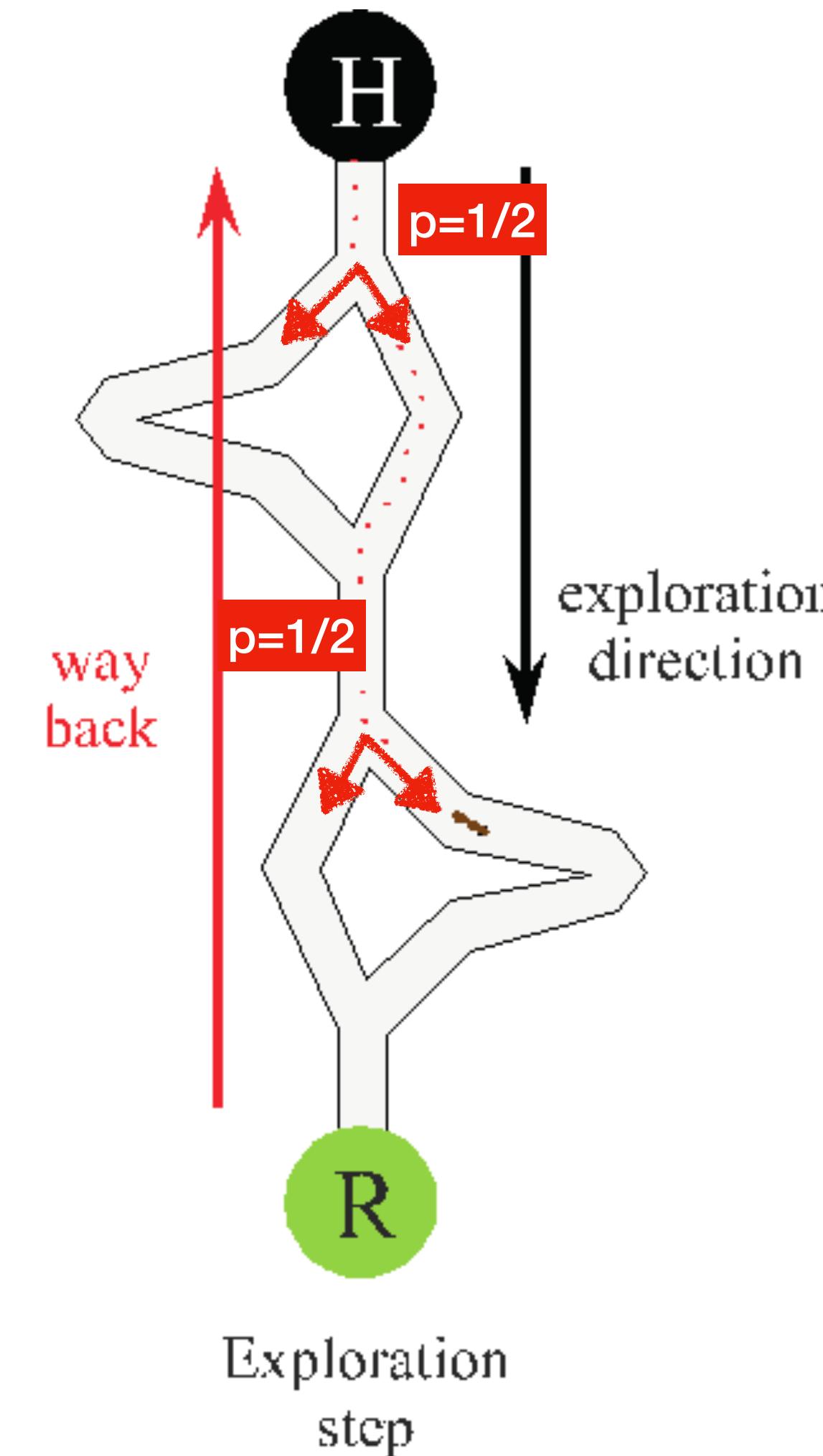
Pheromone evaporates in time



# Ant Colony Optimization (Dorigo, 1992)

## Warm-up

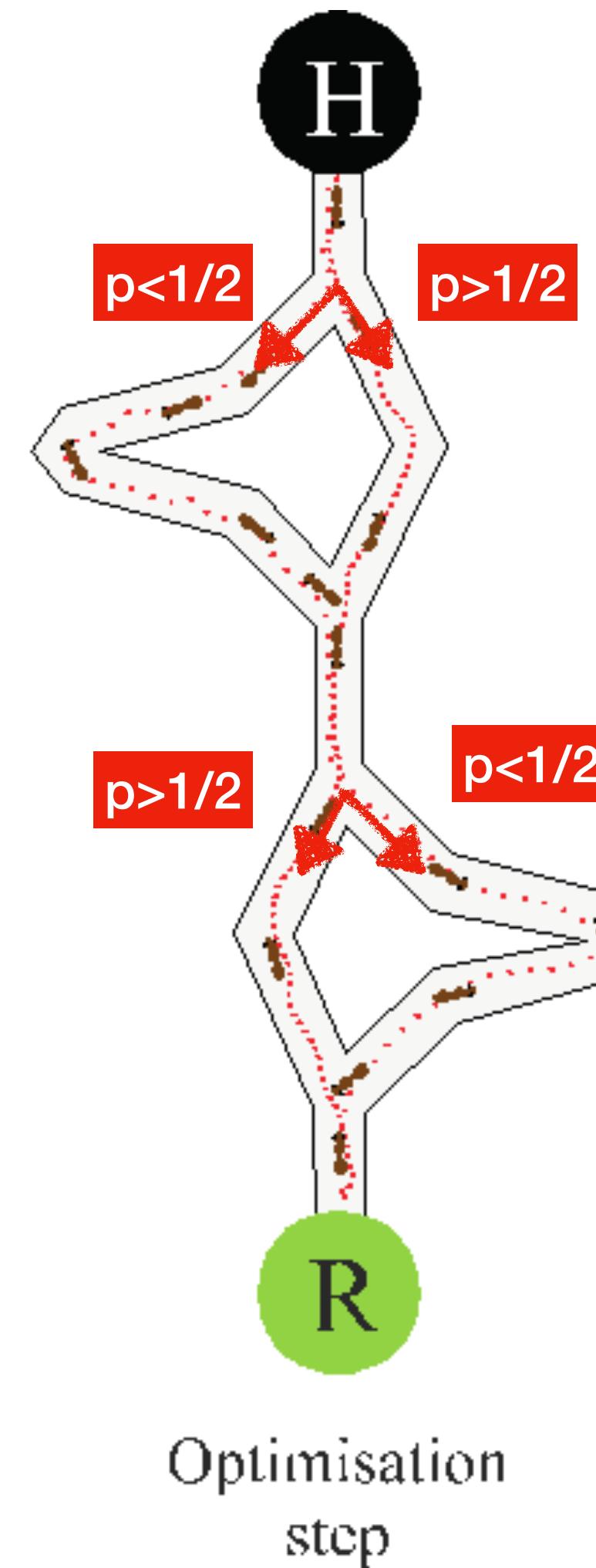
Probabilistic evolution



# Ant Colony Optimization (Dorigo, 1992)

## Warm-up

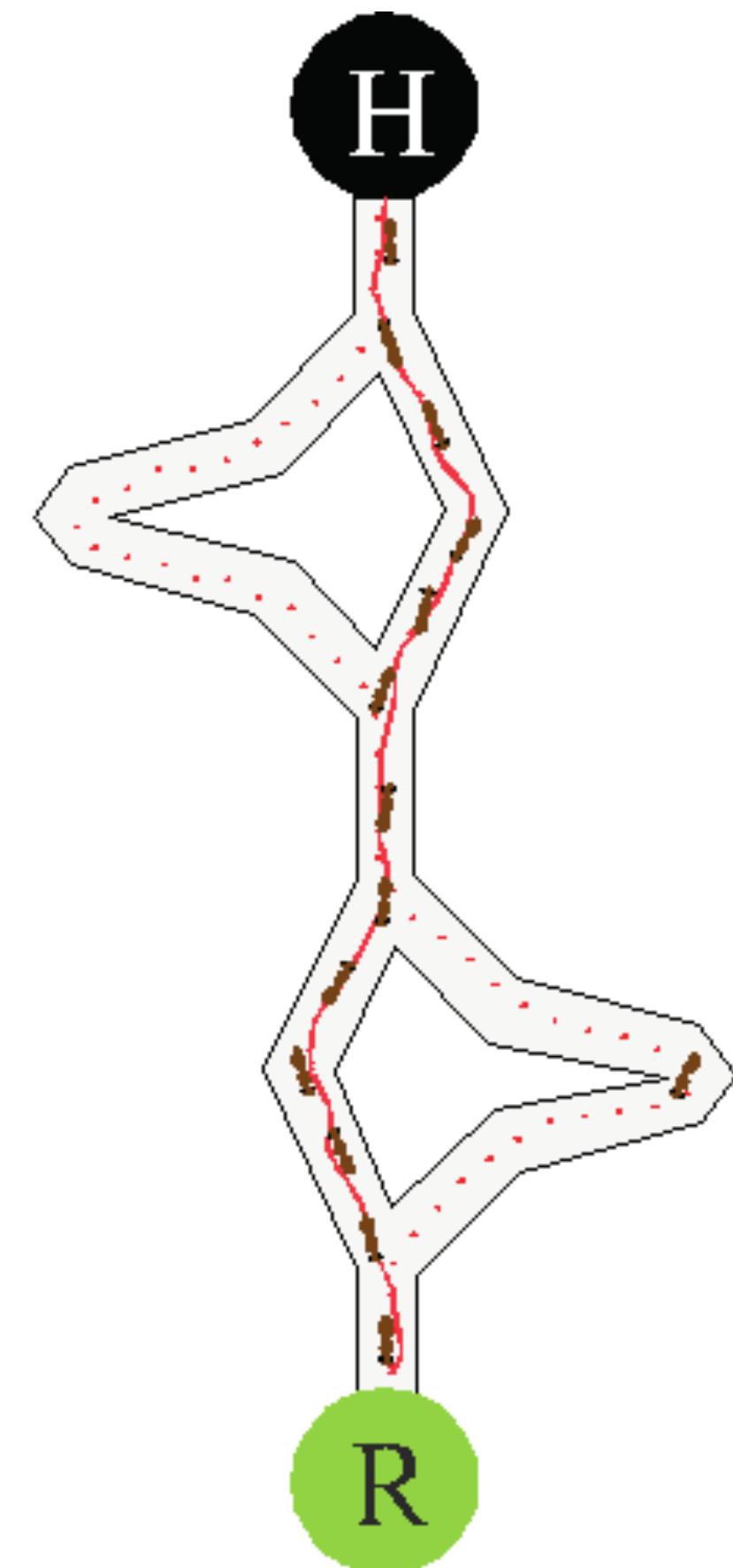
Probabilistic evolution



# Ant Colony Optimization (Dorigo, 1992)

## Warm-up

Probabilistic  
evolution

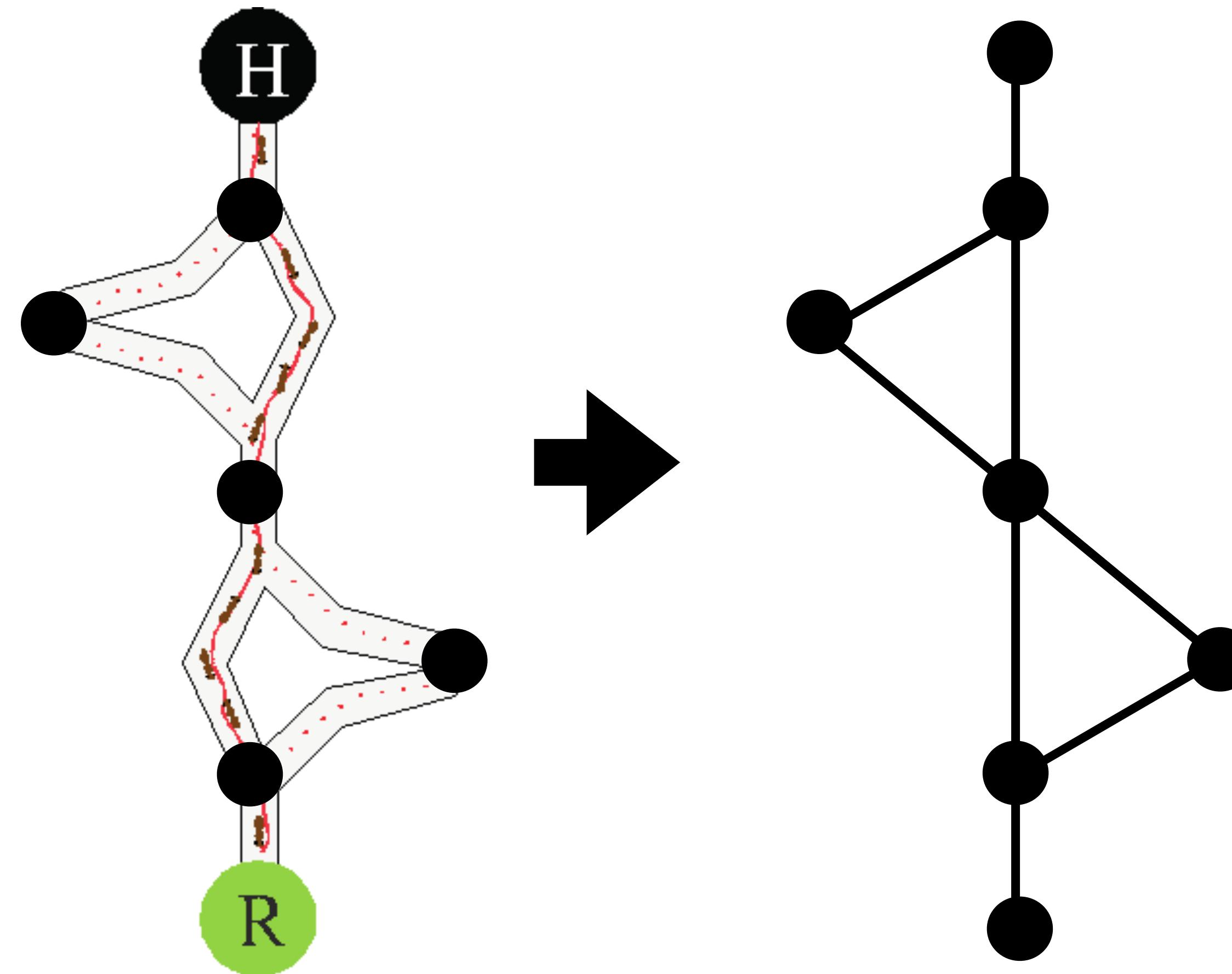


Research extraction  
step

# Ant Colony Optimization (Dorigo, 1992)

## Warm-up

Probabilistic evolution



Research extraction  
step

# Ant Colony Optimization (Dorigo, 1992)

## The algorithm

Introduce a heuristic (benefit/cost) matrix:  $\eta_{ij}$

$$\eta_{ij} = 1/d_{ij}$$

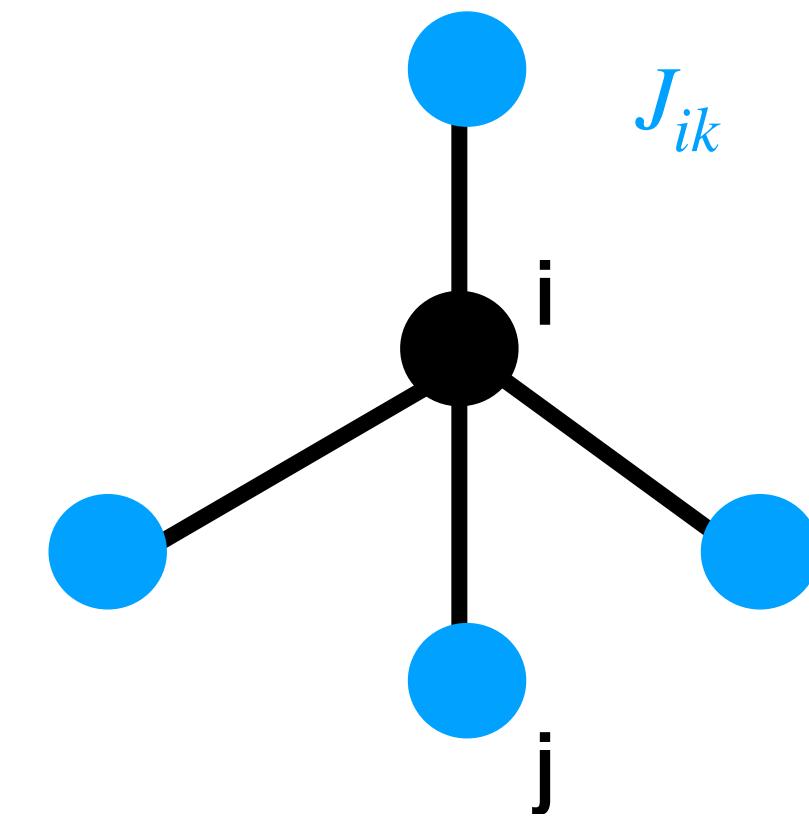
Reciprocal of the distance, proximity, between nodes i and j

Initialize a pheromone matrix:  $\tau_{ij}$

Pheromone between nodes i and j

Probability of a path:

$$p_{ij,k}(t) = \begin{cases} \frac{(\tau_{ij}(t))^\alpha (\eta_{ij}(t))^\beta}{\sum_{l \in J_{ik}} (\tau_{il}(t))^\alpha (\eta_{il}(t))^\beta} & \text{if } j \in J_{ik} \\ 0 & \text{if } j \notin J_{ik} \end{cases}$$



# Ant Colony Optimization (Dorigo, 1992)

## The algorithm

Introduce a heuristic (cost) matrix:  $\eta_{ij}$

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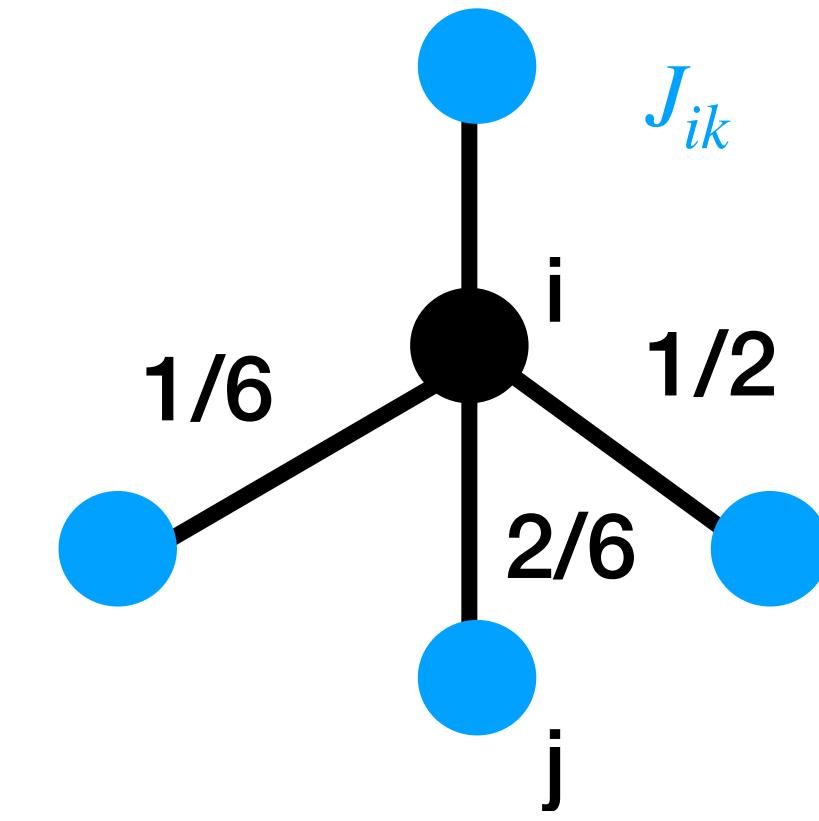
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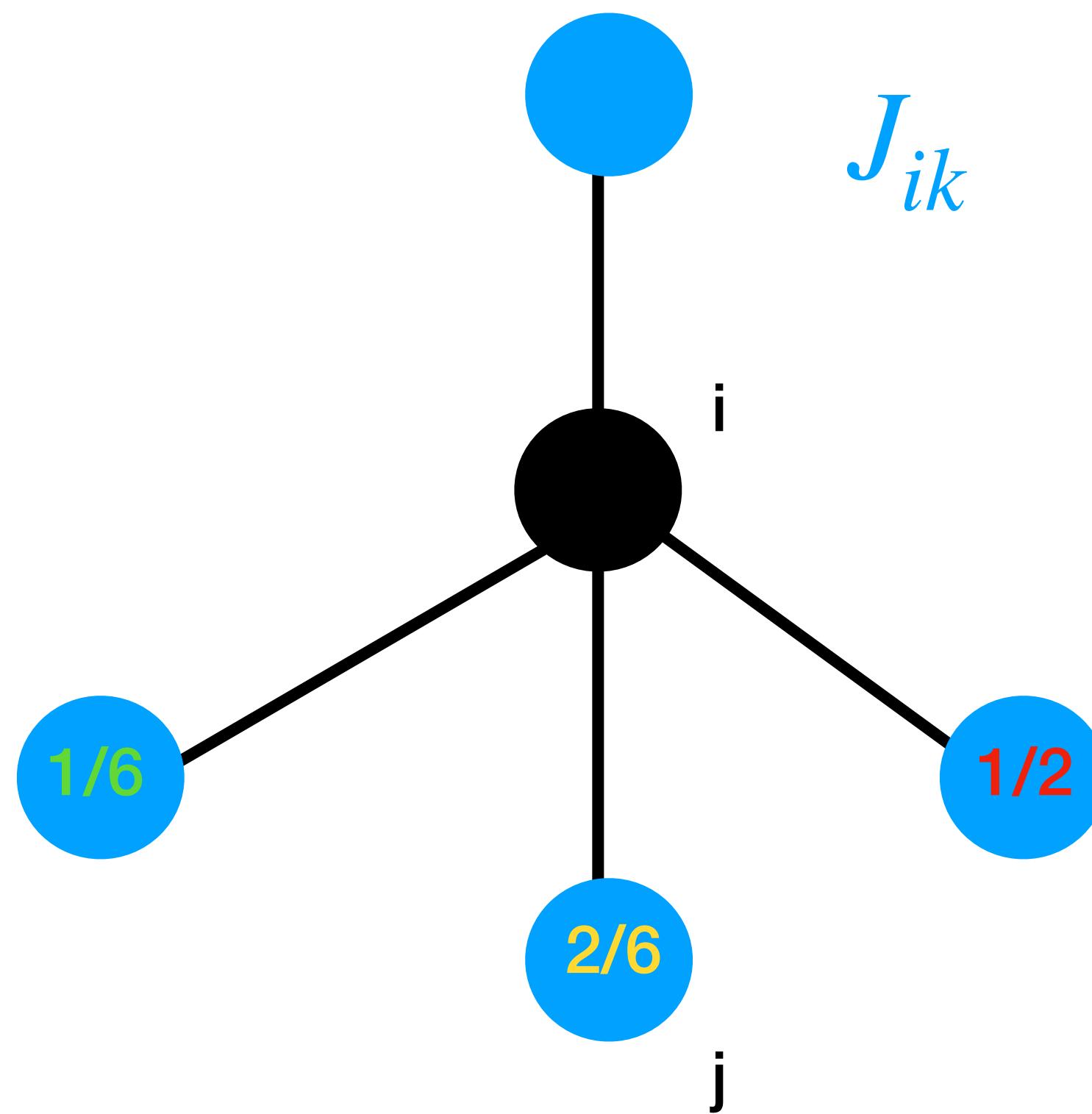
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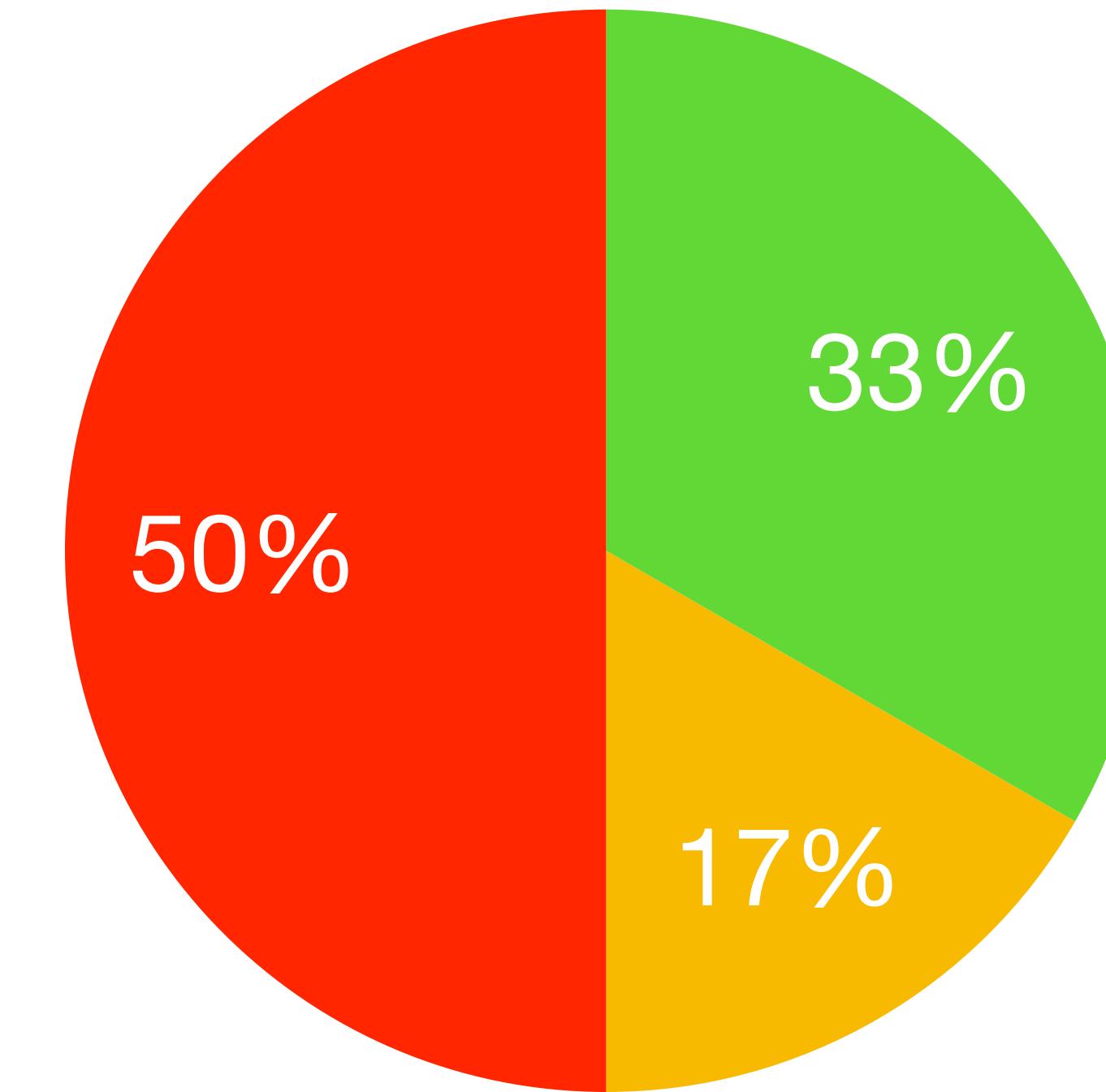


# Ant Colony Optimization (Dorigo, 1992)

## Path selection



Roulette: random number  
in  $[0,1]$



# Ant Colony Optimization (Dorigo, 1992)

## Pheromone distribution

Each ant releases pheromone on its way back to the nest:

$$\Delta\tau_{ij}^k = \frac{Q}{L_k(t)} \quad \forall (i,j) \in T_k(t)$$

Where  $L_k$  is the total length of the path of the  $k$ -th ant.

The total fresh pheromone deposited on the edge  $(i,j)$  becomes

$$\Delta\tau_{ij} = \sum_{k=1}^C \Delta\tau_{ij}^k$$

and the pheromone update rule is

$$\tau_{ij}(t+1) = (1 - \rho) \tau_{ij}(t) + \Delta\tau_{ij}(t)$$

where  $\rho$  is the pheromone evaporation rate.

In the original algorithm, the pheromone is updated post-factum.

# Ant Colony Optimization (Dorigo, 1992)

## Tips

- Standard approach: the number of ants is equal to the number of nodes.  
This basically determines the updating frequency of the pheromone matrix.
- Randomly change the initial point of the search so as to avoid biases.
- Pay attention to the problem definition. The graph structure has a strong impact on the outcome. The problem may not be symmetric, meaning  $\eta_{ij} \neq \eta_{ji}$ .

# Ant Colony Optimization (Dorigo, 1992)

## Pseudocode

$t=0$  #generation counter

$(V, E)$  = problem Graph

$\eta$  = heuristic tensor

$\rho$  = evaporation rate

$v_0$  = generate\_random\_starting\_points( $V$ )

$\tau$  = InitializePheromoneTensor()

While ( $t < G$ ) or not (termination\_criterion):

    Paths=[ ]

    For each  $k \in [0, C]$ :                  *ant in the colony*

        Path= CreatePath( $\tau, \eta, v_0$ )

        Paths.append(Path)

$\tau$  = PheromoneUpdate( $\tau, \eta, \text{Paths}$ )

$v_0$  = generate\_random\_starting\_points( $V$ )

$t=t+1$

# Ant Colony Optimization (Dorigo, 1992)

## Extensions

**Elitist ant system:** some elite ants are used to follow the best route found so far. Push optimal solutions.

**Max-min ant system:** min and max cutoffs to the pheromone update. Expand the search space and keep all parts of the graph visitable. Reinitialize poor trails when the system is near-stagnation.

**Rank-based ant system:** solutions are ranked according to their length. Shorter path, higher rank. The amount of pheromone deposited is multiplied by the rank. Ants with low rank leave no pheromones. It increases hierarchy in pheromone release.

...

# Multi-Objective ACO

## What changes?

From heuristic matrix to heuristic tensor: a benefit/cost vector corresponds to each edge

$$\eta_{ij} - > \eta_{ij,m} \quad m = 1, \dots, M \quad \eta_{ij,m} = s_{jk}/c_{ij}$$

Approaches may differ in choosing:

- The number of pheromone matrices
- The number of heuristic matrices
- The aggregation strategy of the above matrices and the hyperparameters associated to it
- The method used to select solutions that update the pheromone information

**we present few examples**

# Multiple Ant Colony System (MACS) (Barán, 2003)

Single pheromone matrix:  $\tau_{ij}$

Pheromone matrix initialized as.  $\tau_0 = \frac{1}{\prod_{i=1}^M \langle f_m \rangle_{\text{initial pop.}}}$

Multiple cost matrices:  $\eta_{ij,m}$   $m = 1, \dots, M$

Each ant uses a different normalized weight for cost aggregation:  $\vec{\lambda}_k = (\lambda_{1,k}, \dots, \lambda_{M,k})$   $k = 1, \dots, C$

The update rule becomes:

$$p_{ij,m}^{(k)}(t) = \frac{\tau_{ij}^\alpha \left( \prod_{m=1}^M \eta_{ij,m}^{\lambda_{m,k}} \right)^\beta}{\sum_{l \in \mathcal{N}_{i,k}} \tau_{il}^\alpha \left( \prod_{m=1}^M \eta_{il,m}^{\lambda_{m,k}} \right)^\beta}$$

$\mathcal{N}_{i,k}$  = neighbors of  $i$  visitable by the  $k$ -th ant

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The pheromone to be distributed at each iteration is given by:

$$\tau'_0 = \frac{1}{\prod_{i=1}^M \langle f_m \rangle_{rank=1}}$$

**If**  $\tau'_0 > \tau_0$  → set  $\tau_0 = \tau'_0$  and re-initialize possible trails using  $\tau_0$

**Else** → perform global updating using

$$\tau_{ij} \leftarrow (1 - \rho) \tau_{ij} + \rho \Delta_k \quad \forall (i, j) \in k \in \text{Paths}_{rank=1} \quad \text{and} \quad \Delta_k = \frac{1}{\prod_{i=1}^M f_m^{(k)}}$$

# Multiple Ant Colony System (MACS) (Barán, 2003)

## Pseudocode

```
t=0 #generation counter  
(V, E ) = problem Graph  
 $\eta, \rho$  = heuristic tensor, evaporation rate  
 $\tau_0 = \text{Estimate}(f_1, \dots, f_M)$  estimate initial pheromone value  
 $\lambda, v_0 = \text{generate_random_starting_point_and_weights(V)}$   
 $\tau = \text{InitializePheromoneMatrix}(\tau_0)$   
NonDominatedPaths=[ ]  
While (t<G) or not (termination_criterion):  
    For each  $k \in [0, C]$ : ant in the colony  
        Path = CreatePath_and( $\tau, \eta, \lambda, v_0$ )  
        If not dominates(NonDominatedPaths, Path):  
            NonDominatedPaths.append(Path)  
            NonDominatedPaths = non_dominated_solutions(NonDominatedPaths)  
 $\tau'_0 = \text{EvaluateNonDominatedPheromone}(\text{NonDominatedPaths})$   
        If  $\tau'_0 > \tau_0$ :  
             $\tau_0 \leftarrow \tau'_0$   
             $\tau = \text{InitializePheromoneMatrix}(\tau_0)$   
        Else:  
             $\tau = \text{PheromoneUpdateOnNonDominatedPaths}(\tau, \eta, \text{Improved_Paths})$   
    t=t+1
```

# Pareto ACO (P-ACO) (*Doerner, 2004*)

Multiple pheromone matrices:  $\tau_{ij,m}$   $m = 1, \dots, M$

Multiple cost matrices:  $\eta_{ij,m}$   $m = 1, \dots, M$

Each ant used a different normalized weight:

$$\vec{\lambda}_k = (\lambda_{1,k} \dots \lambda_{M,k}) \quad k = 1, \dots, C$$

The update rule becomes:

$$p_{ij,m}^{(k)}(t) = \frac{\sum_{m=1}^M \left( \tau_{ij,m}^\alpha \eta_{ij,m}^\beta \lambda_{m,k} \right)}{\sum_{l \in \mathcal{N}_{i,k}} \sum_{m=1}^M \left( \tau_{il,m}^\alpha \eta_{il,m}^\beta \lambda_{m,k} \right)}$$

$\mathcal{N}_{i,k}$  = neighbors of i visitable by the  $k$ -th ant

# Pareto ACO (P-ACO) (*Doerner, 2004*)

The update rule becomes:

$$p_{ij,m}^{(k)}(t) = \frac{\sum_{m=1}^M (\tau_{ij,m}^\alpha \eta_{ij,m}^\beta \lambda_{m,k})}{\sum_{l \in \mathcal{N}_{i,k}} \sum_{m=1}^M (\tau_{il,m}^\alpha \eta_{il,m}^\beta \lambda_{m,k})} \quad \mathcal{N}_{i,k} = \text{neighbors of } i \text{ visitable by the } k\text{-th ant}$$

A local pheromone update ensures diversification

$$\tau_{ij,m} \leftarrow (1 - \rho) \tau_{ij,m} + \rho \tau_0$$

$$(1 - \rho) \tau_{ij,m} + \rho \tau_0 \leq \tau_{ij,m} \implies \tau_{ij,m} \geq \tau_0$$

*Decrease probability if famous and already visited*

A globe pheromone update ensures to highlight rank 1 and 2 solutions

$$\tau_{ij,m} \leftarrow (1 - \rho) \tau_{ij,m} + \rho \Delta \tau_{ij,m}$$

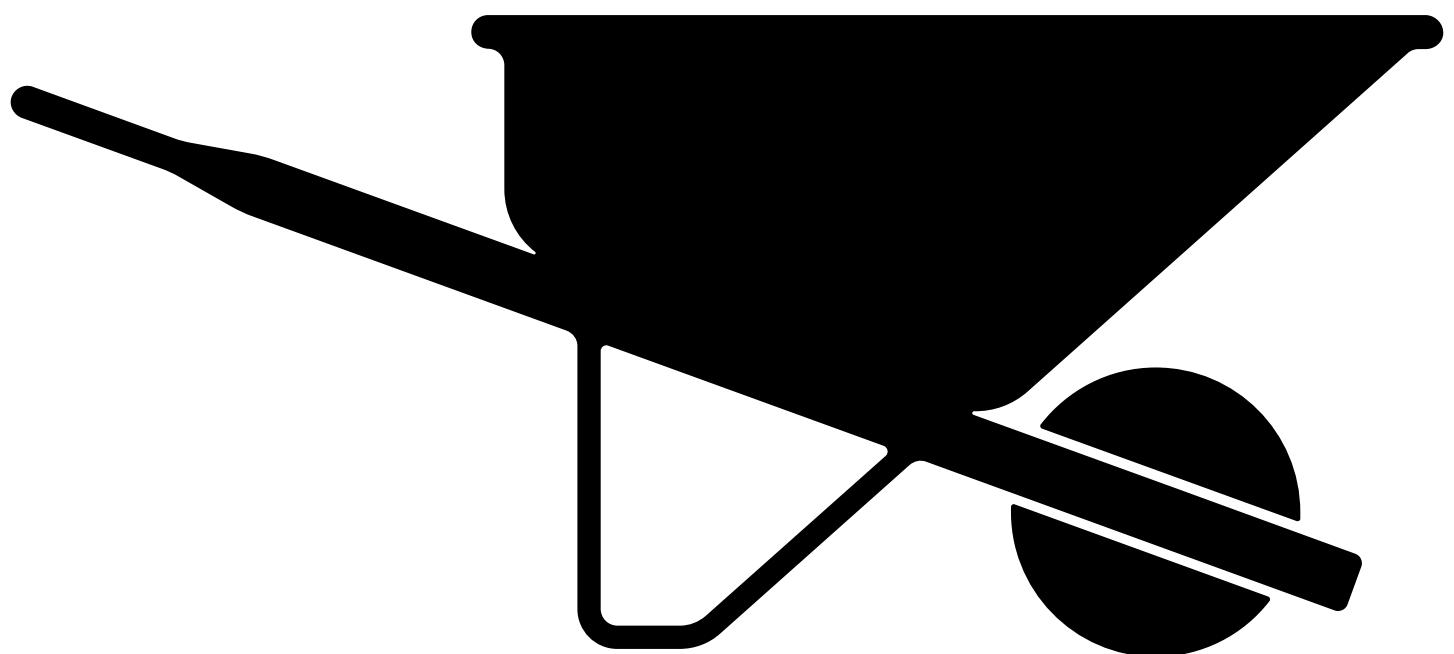
The best empirical value:  $\Delta \tau_{ij,m} = \tau_0$  (rank = 1),  $\frac{\tau_0}{2}$  (rank = 2)

# Pareto ACO (P-ACO) (*Doerner, 2004*)

## Pseudocode

```
t=0 #generation counter  
(V, E ) = problem Graph  
 $\eta$  = heuristic tensor  
 $\rho$  = evaporation rate  
 $\lambda, v_0$  = generate_random_starting_point_and_weights(V)  
 $\tau_0$  = Estimate( $f_1, \dots, f_M$ ) estimate initial pheromone value  
 $\tau$  = InitializePheromoneTensor()  
While (t<G) or not (termination_criterion):  
    Paths=[]  
    For each  $k \in [0,C]$ : ant in the colony  
        Path,  $\tau$  = CreatePath_and_LocalPheromoneUpdate( $\tau, \eta, \lambda, v_0$ )  
        Paths.append(Path)  
    Improved_Paths = Improve_solutions(Paths)  
    Rank1_Paths, Rank2_Paths = SelectBestImprovedSolutions(Improved_Paths)  
     $\tau$  = GlobalPheromoneUpdate( $\tau, \eta, \text{Improved\_Paths}$ )  
 $\lambda, v_0$  = generate_random_starting_point_and_weights(V)  
t=t+1
```

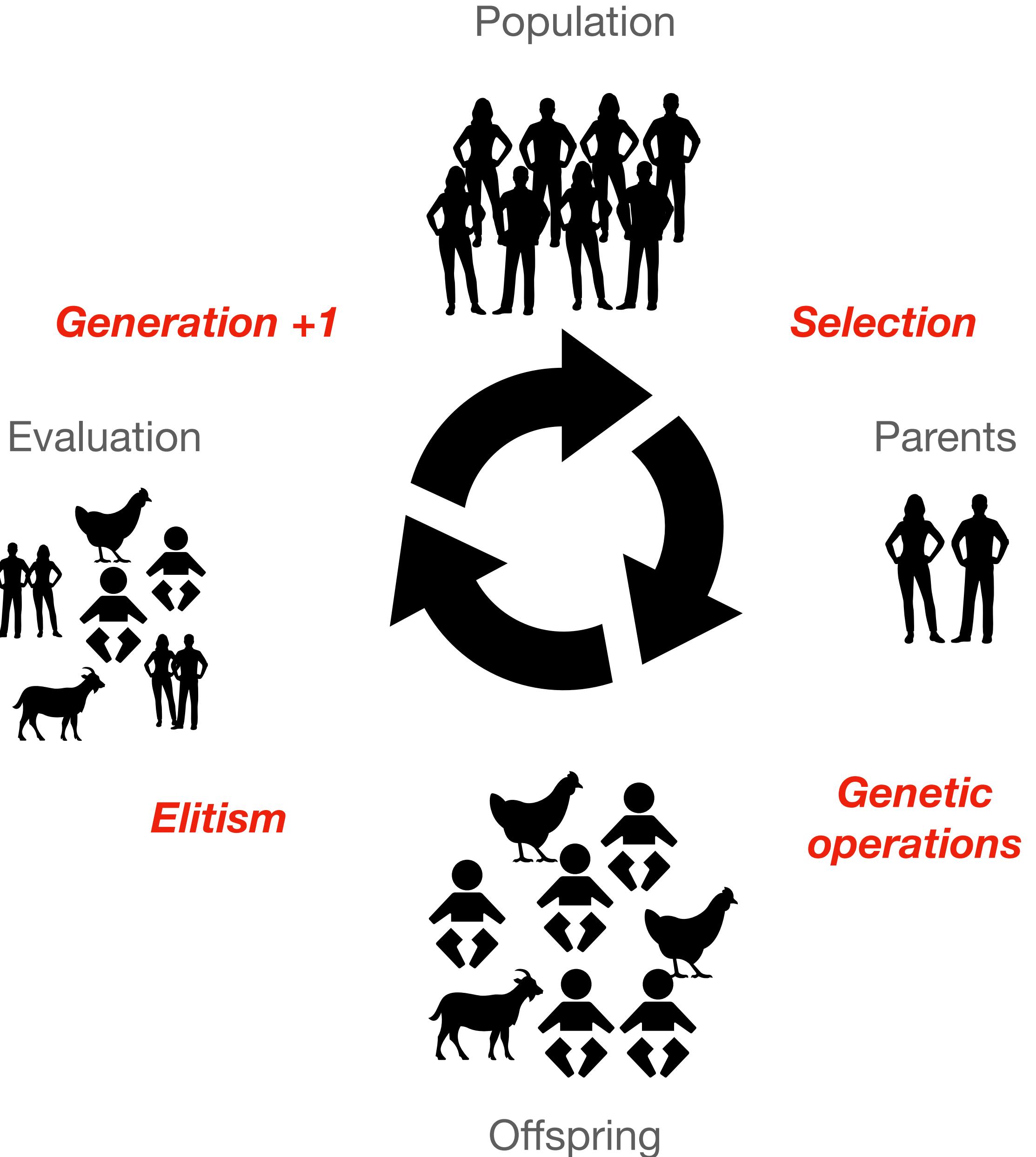
# **Hands on**



# Genetic algorithm

## Nomenclature and outline

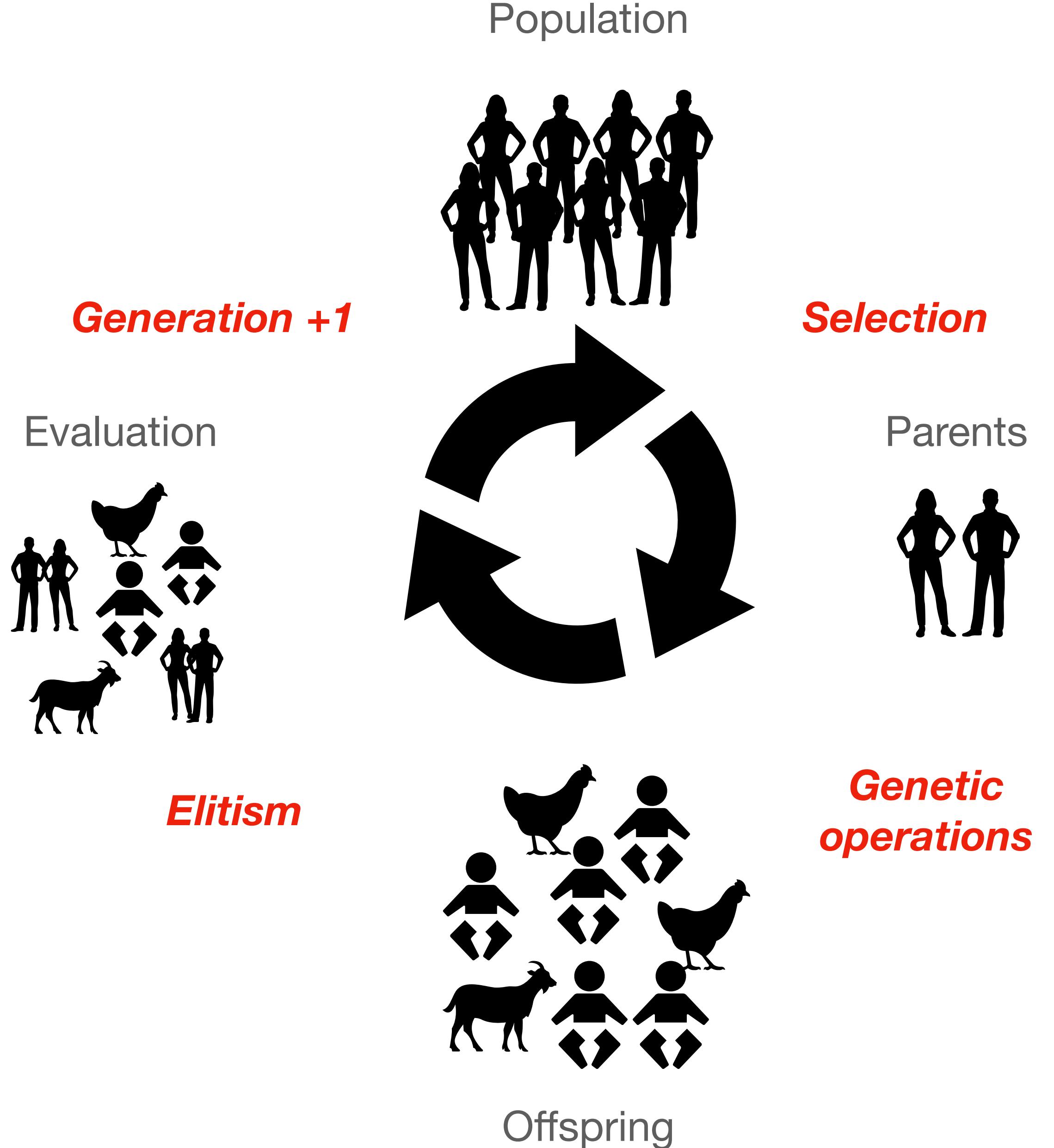
- Individual: feasible solution  $x$
- Population: set of individuals
- Generation: iteration counter
- Genetic operation: operation acting on parents (selected individuals) and outputting children.



# Genetic algorithm

## Nomenclature and outline

- Selection:
  - random
  - random + tournament
- Genetic operations
  - Mutation
  - Crossover
  - Tailored operations
- Elitism/survival
  - define “better” based on objective



# What is tournament selection?

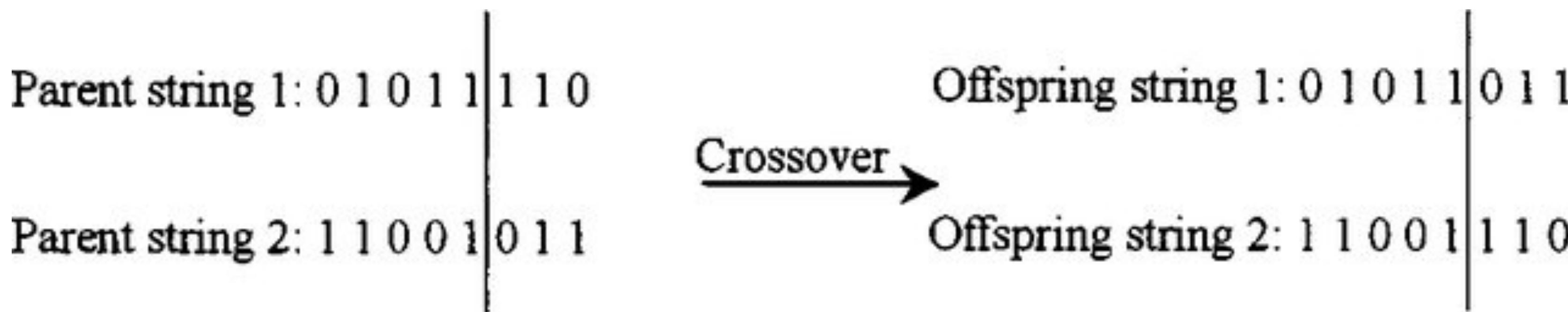
- Define tournament size  $T$
- Select  $T$  individuals from the population at random
- Compare their performance so as to keep only one of them
- The individual (or its variations) are allowed into the next generation



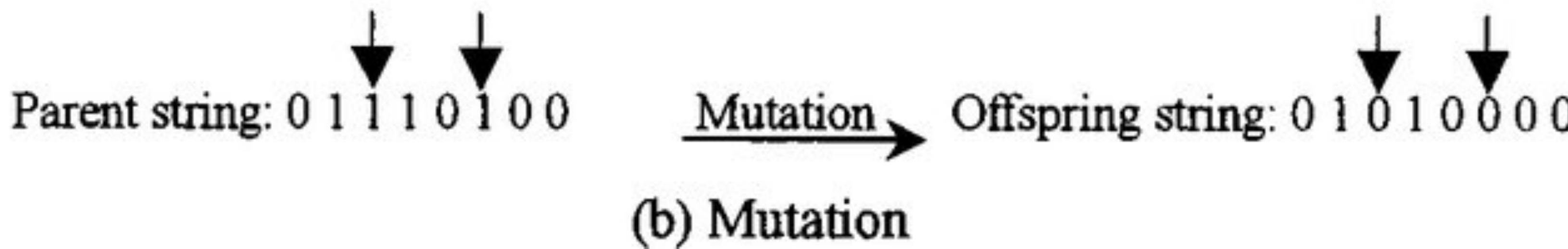
- The higher  $T$  the higher the selection pressure

# What are genetic operations?

## Classical examples

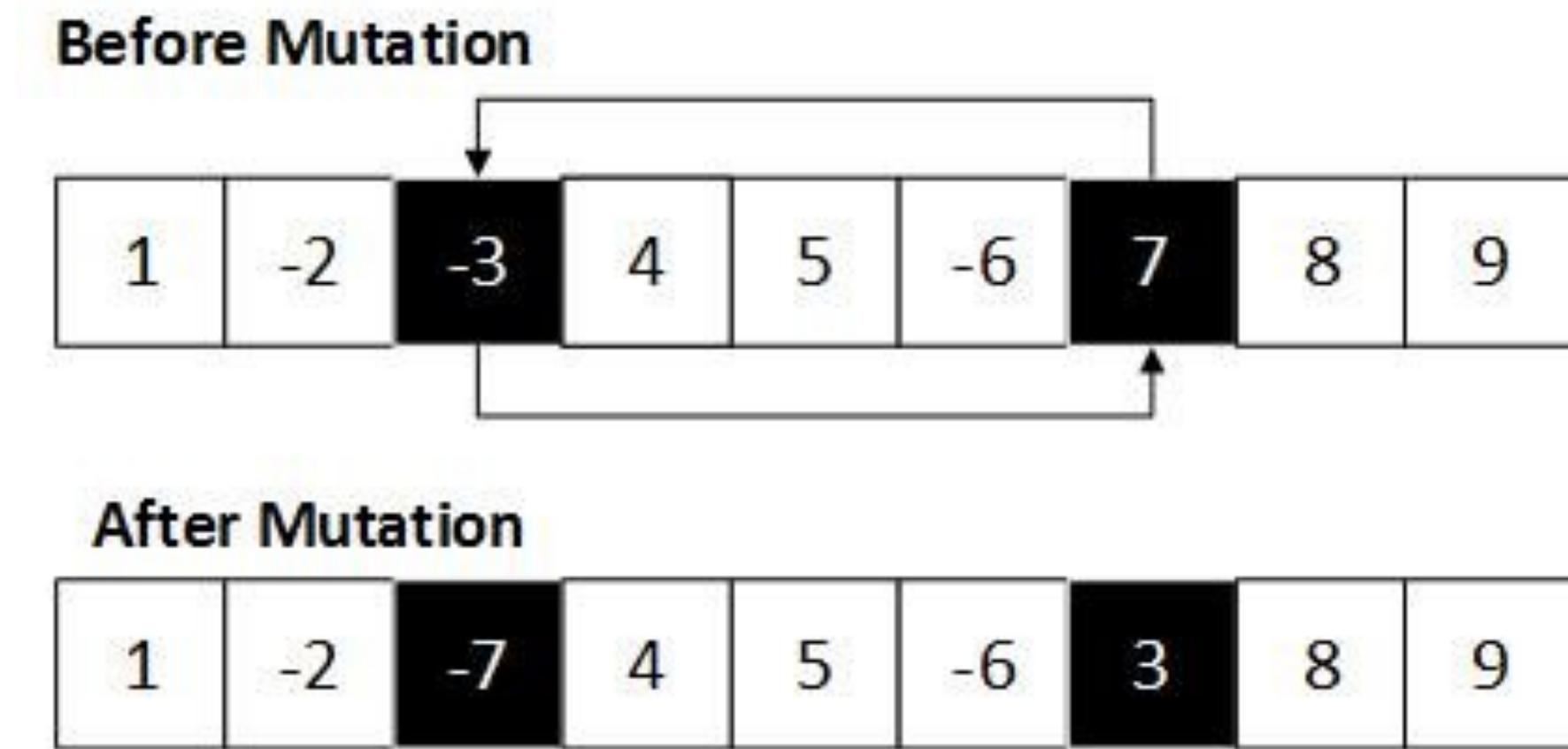
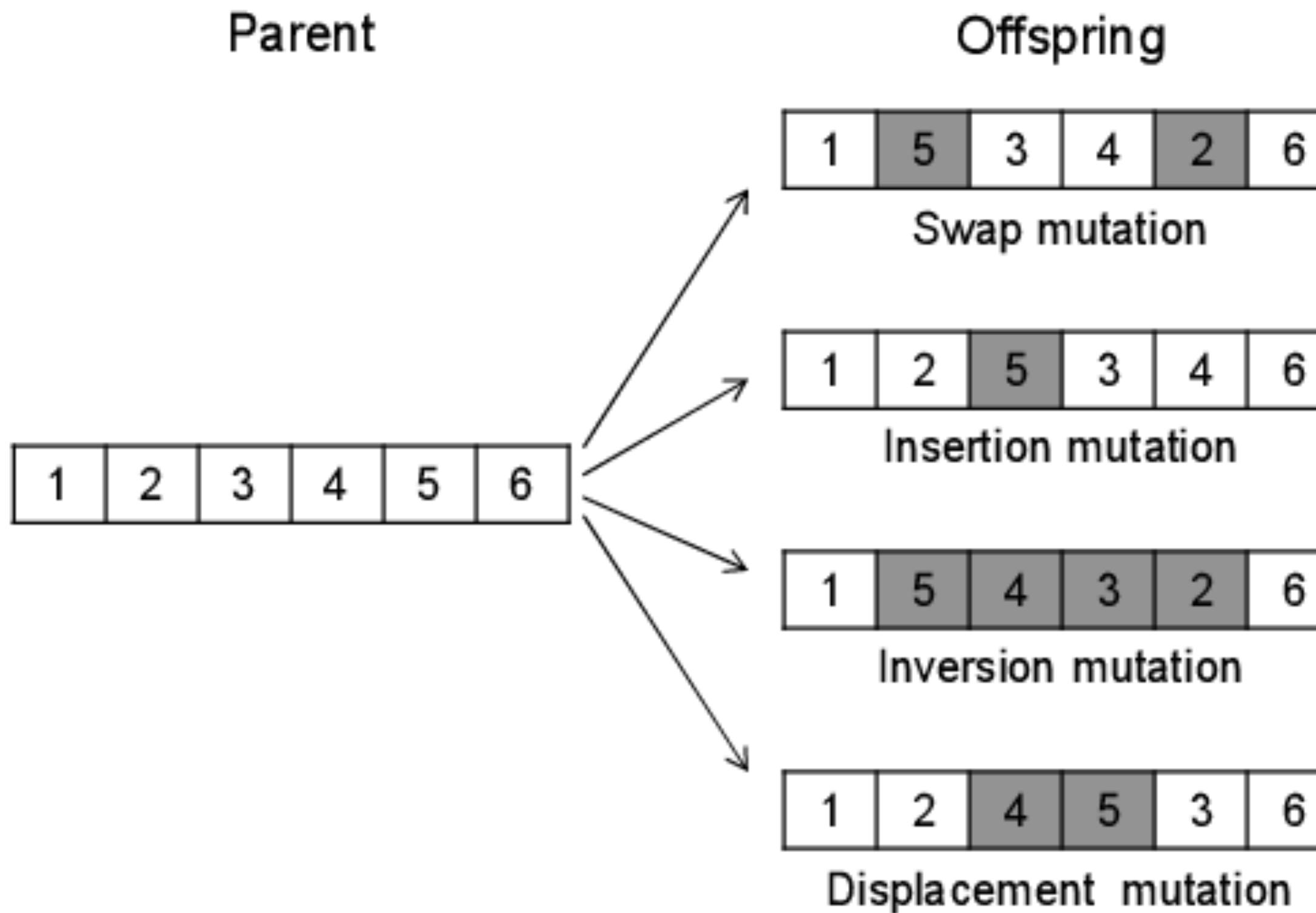


(a) Crossover



(b) Mutation

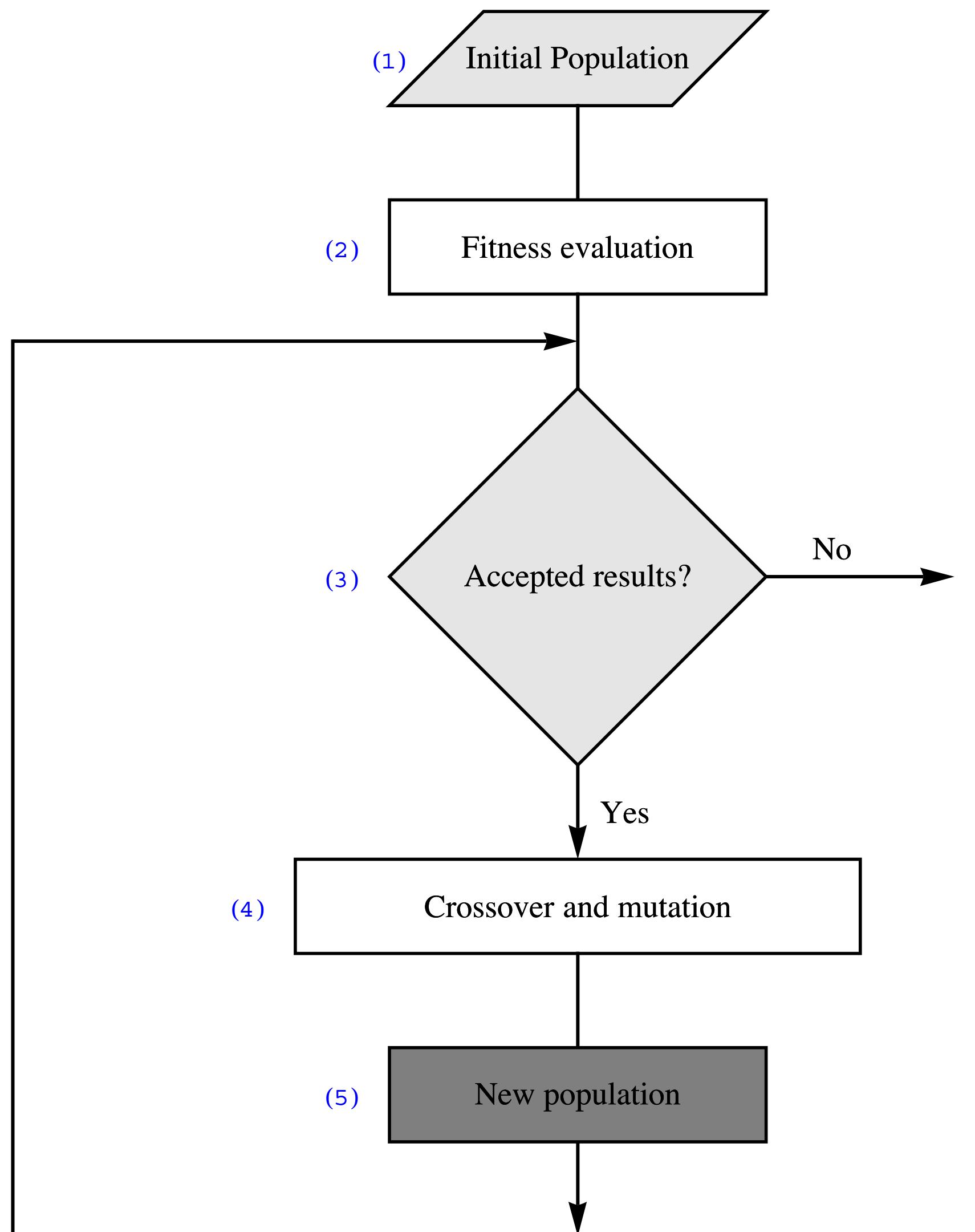
# What are genetic operations?



# Genetic algorithm

## Pseudocode

```
g=0 #generation counter  
P(g) = generate_random_population(N)  
Fitness(g) = evaluate_population_fitness(P(g))  
While (g<G) or not (termination_criterion):  
    g=g+1  
    offspring= []  
    For i=1,...,N:  
        variation = select([mutation,crossover])  
        parents = select_parents(P(g), Fitness(g),variation)  
        child = variation(parents)  
        offspring.append(child)  
    P(g) = [P(g-1) , offspring]  
    Fitness(g) = [Fitness(g-1) , evaluate_population_fitness(offspring)]  
  
    P(g), Fitness(g) = select_best_individuals(P(g), Fitness(g),N)  
    termination_criterium = evaluate_termination_criterium(P(g), Fitness(g))  
  
return P(g), Fitness(g)
```

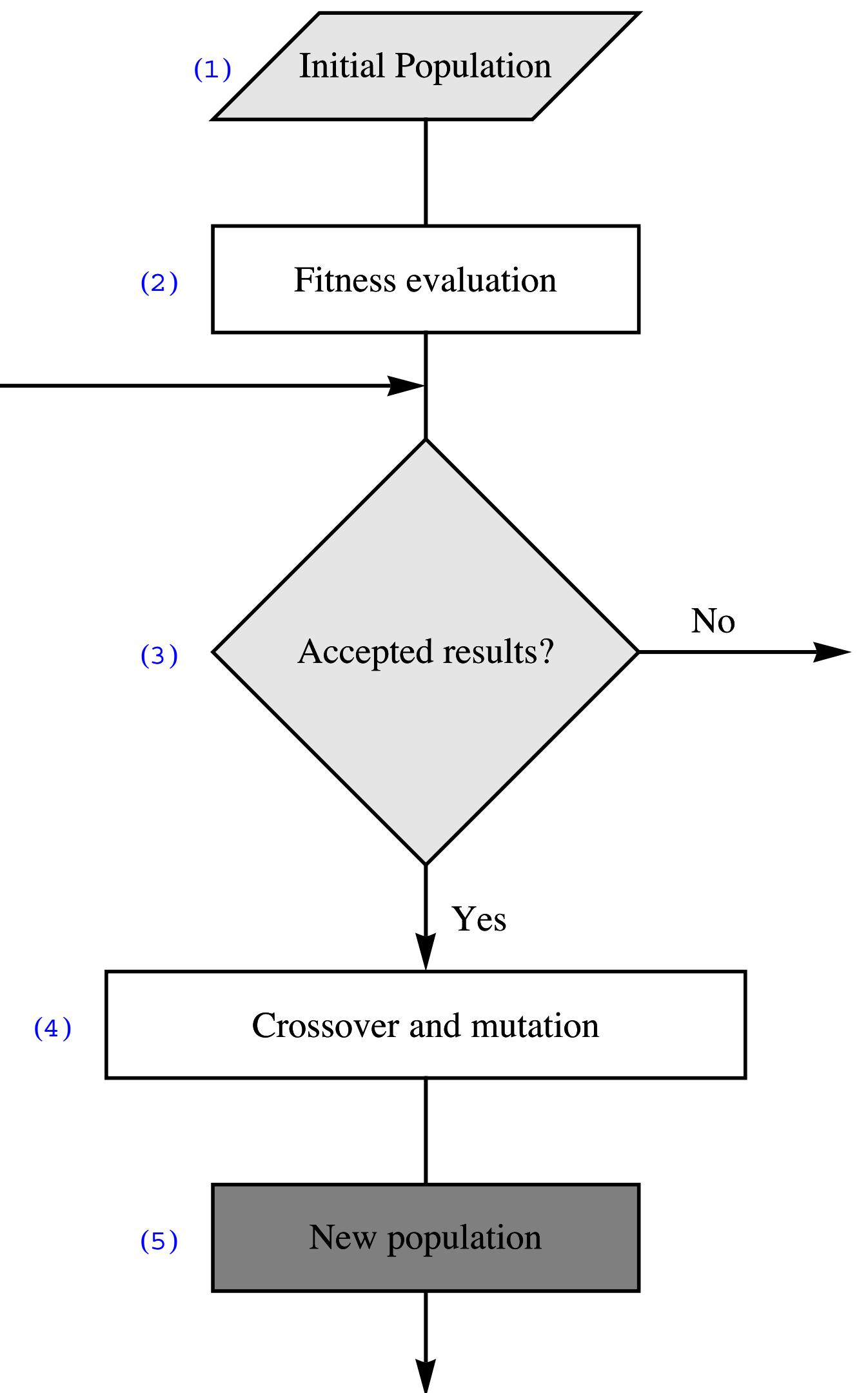


# Genetic algorithm

## Pseudocode

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    offspring= []  
    For i=1,...,N:  
        variation = select([mutation,crossover])  
        parents = select_parents(P(g), Fitness(g),variation)  
        child = variation(parents)  
        offspring.append(child)  
    P(g) = [P(g-1) , offspring]  
    Fitness(g) = [Fitness(g-1) , evaluate_population_fitness(offspring)]  
  
    P(g), Fitness(g) = select_best_individuals(P(g), Fitness(g),N)  
    termination_criterium = evaluate_termination_criterium(P(g), Fitness(g))  
  
return P(g), Fitness(g)
```

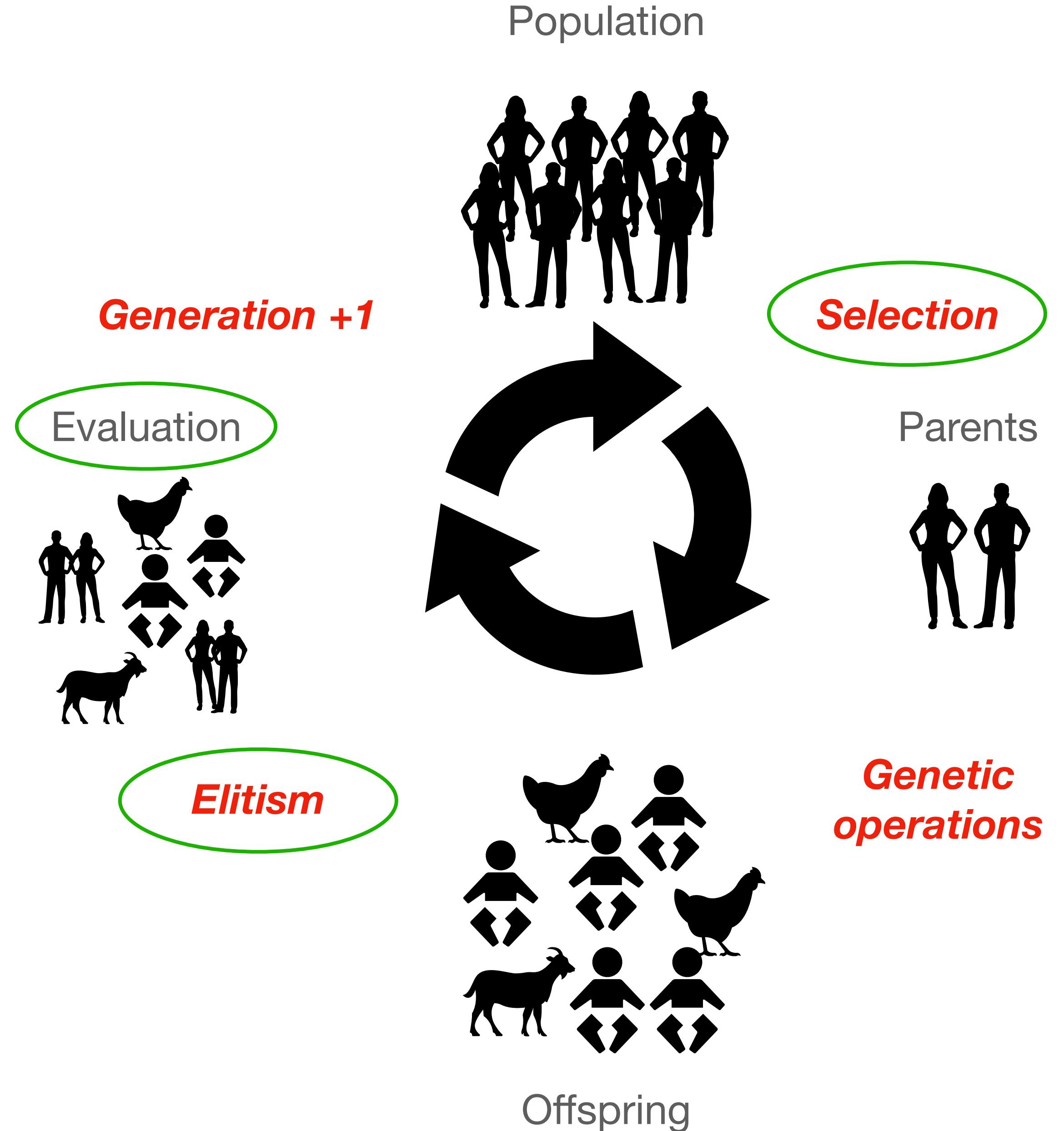
**There exist variants contemplating that only a fraction of selected individuals are subject to genetic mutations!**



# MO Genetic algorithm

## Where does MO appear?

- Evaluation:
  - multiple objectives/constraints
- Selection:
  - tournament selection rules
- Elitism/Survival
  - rank
  - rank + density
  - rank + niching

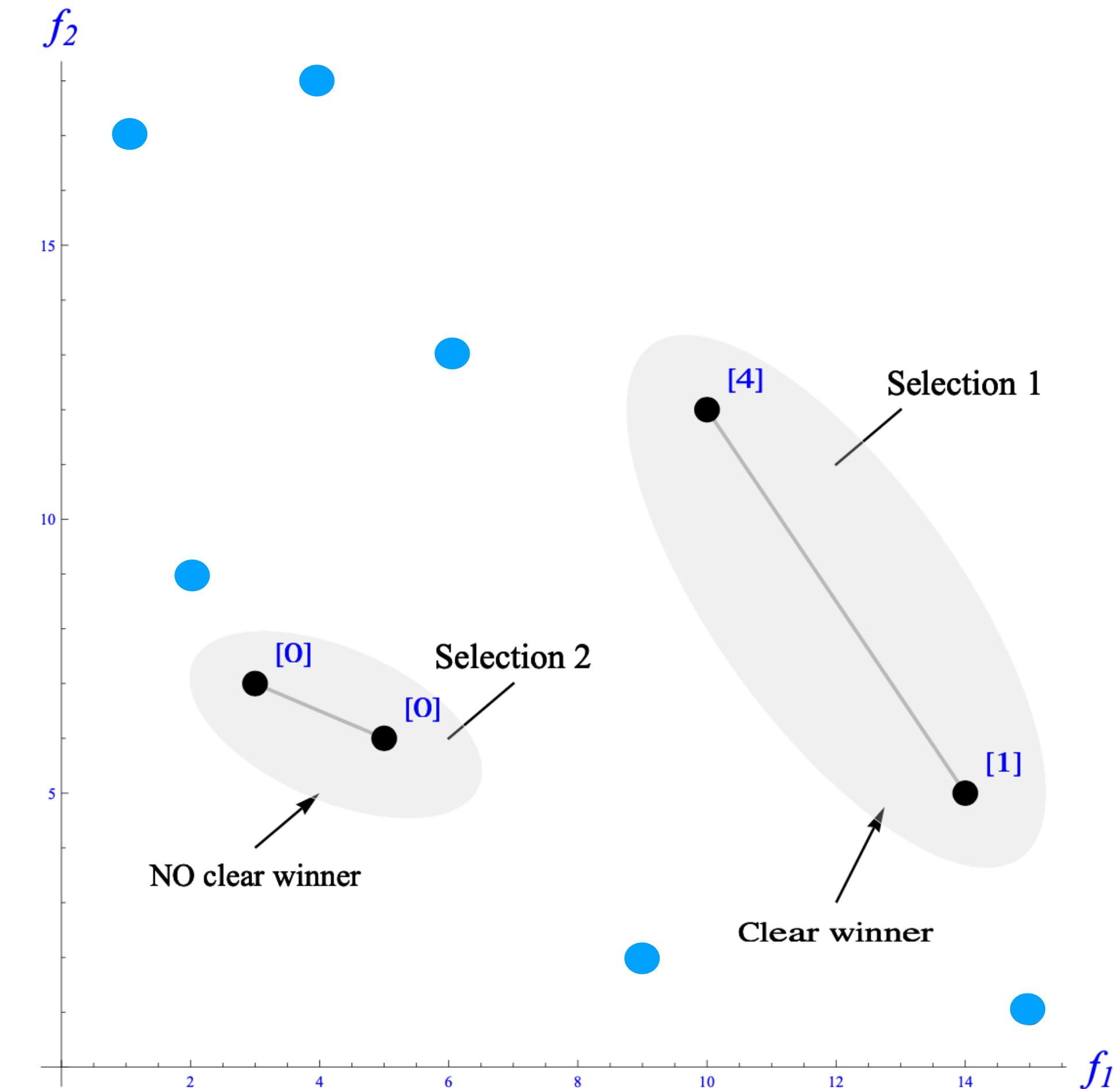


# Niched Pareto Genetic Algorithm (*Horn et al. 1994*)

Selection for parenting uses rank and niche count

- Select at random  $T$  (2) individuals
- Select at random a comparison set (control over selection pressure)
- Primary criterion: compare ranks (Fonseca/Fleming)
- Secondary criterion: compare counts within a niche radius

The main aim is to preserve diversity and prevent early convergence

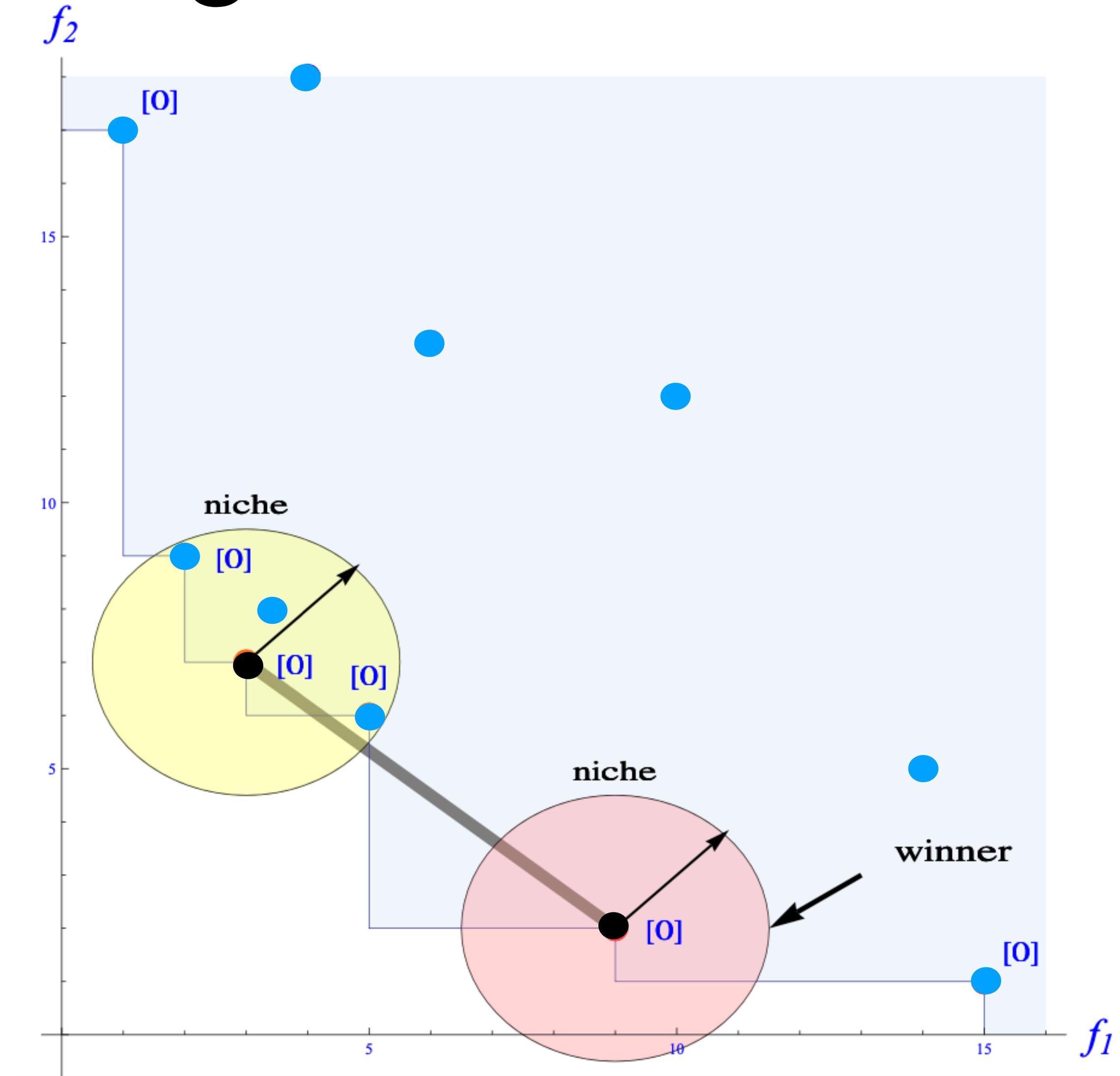


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# NPGA (*Horn et al. 1994*)

Niche counts and fitness rescaling are computed starting from a sharing function

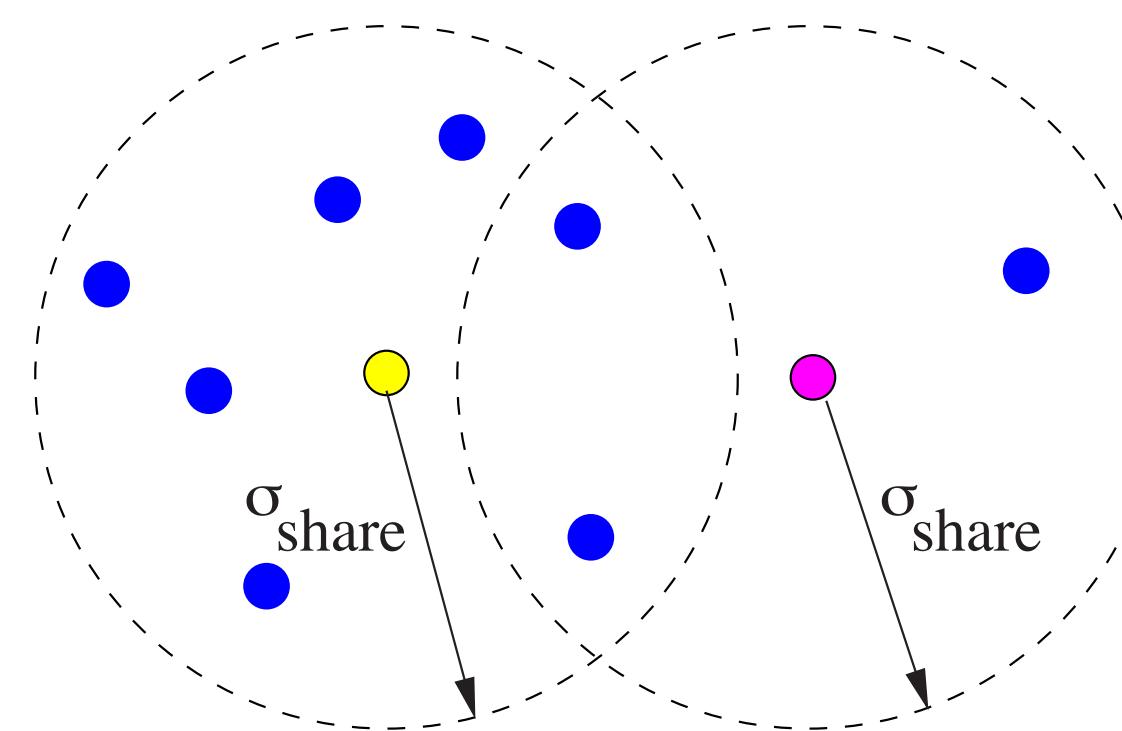
Niche counting becomes

$$m_i = \sum_{j=1}^N sh(d_{ij})$$

$$sh(d_{ij}) = 1 - \left( \frac{d_{ij}}{\sigma_{share}} \right)^\alpha \quad \text{if } d_{ij} < \sigma_{share}$$

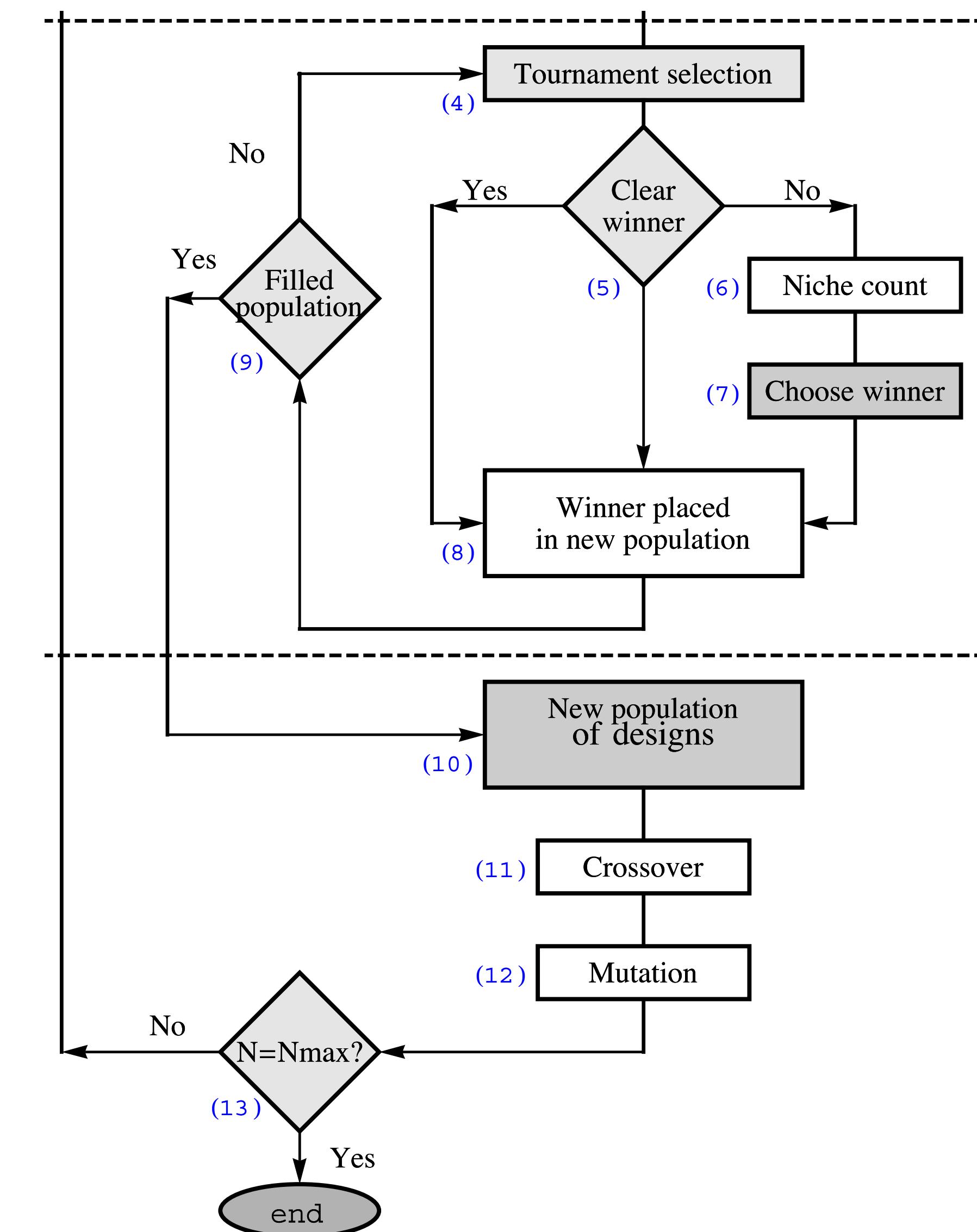
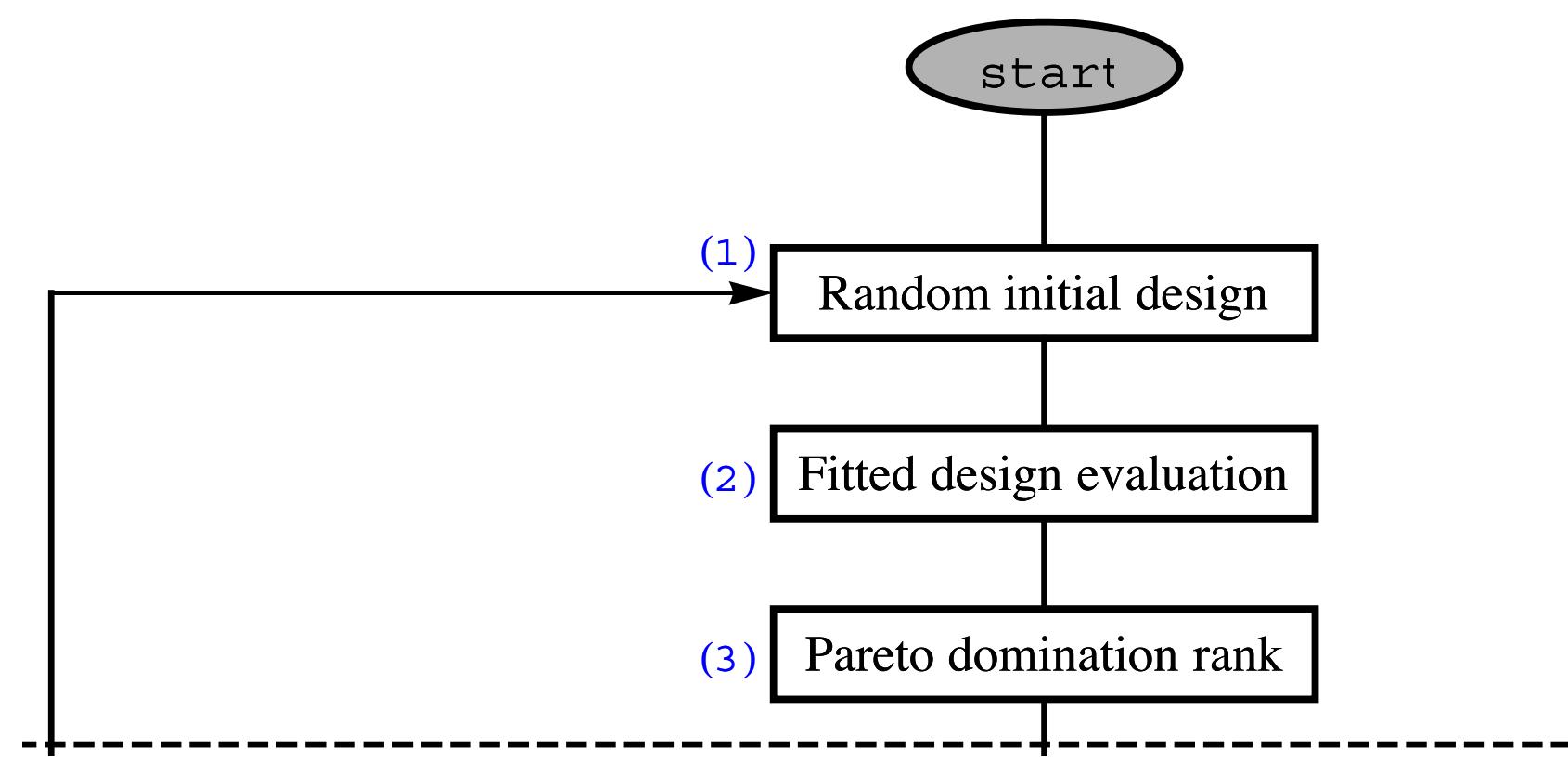
Fitness rescaling

$$f'_i = \frac{f_i}{m_i}$$



“The goal of fitness sharing is to distribute the population over a number of different peaks in the search space, with each peak receiving a fraction of the population proportional to the height of that peak”

# NPGA (Horn et al. 1994)

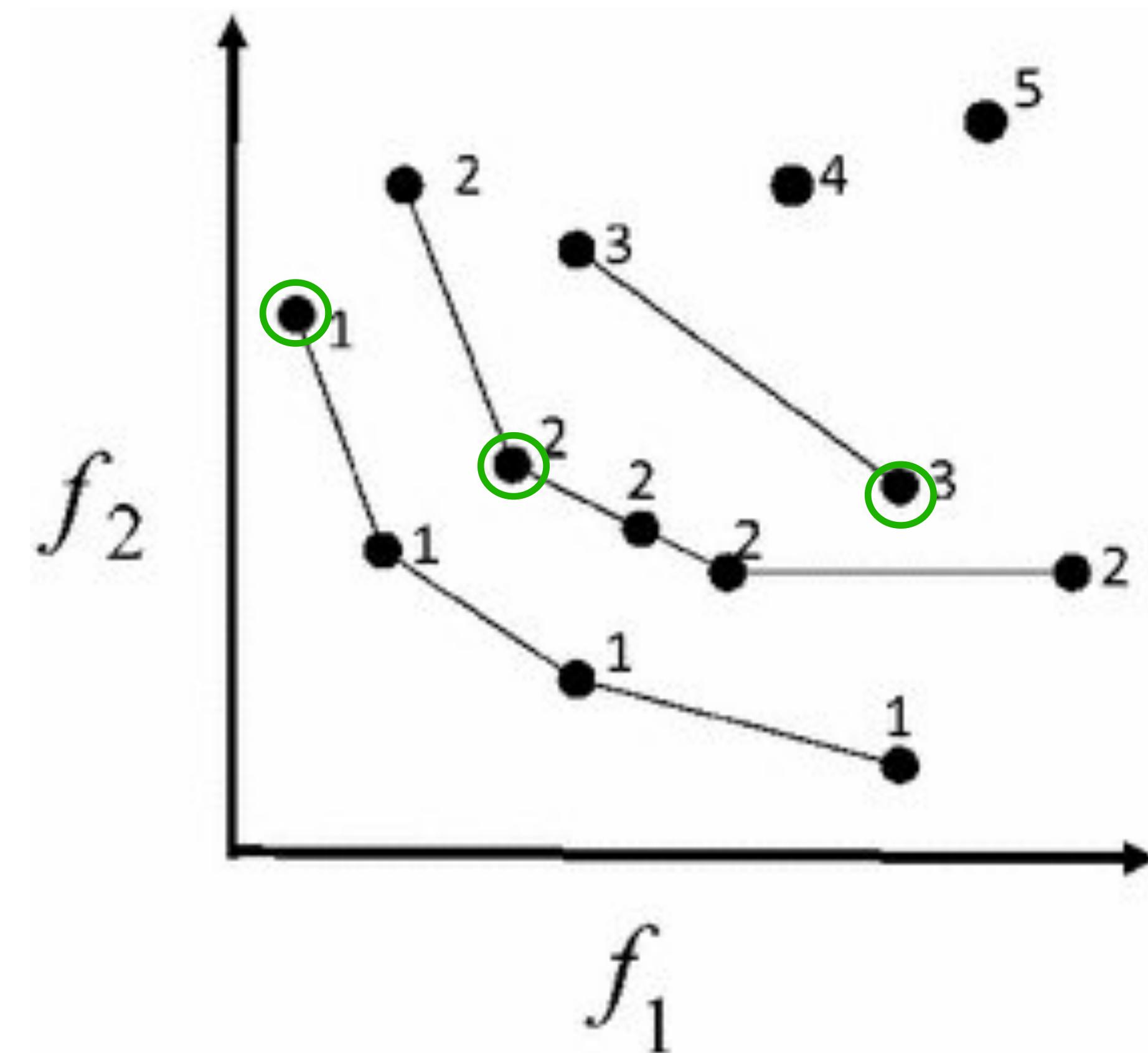


# Non-dominated Sorting GA II (*Deb et al. 2002*)

Selection for parenting uses rank and crowding distance.

Select at random T individuals (control over selection pressure)

- Primary criterion: compare ranks (Goldberg)



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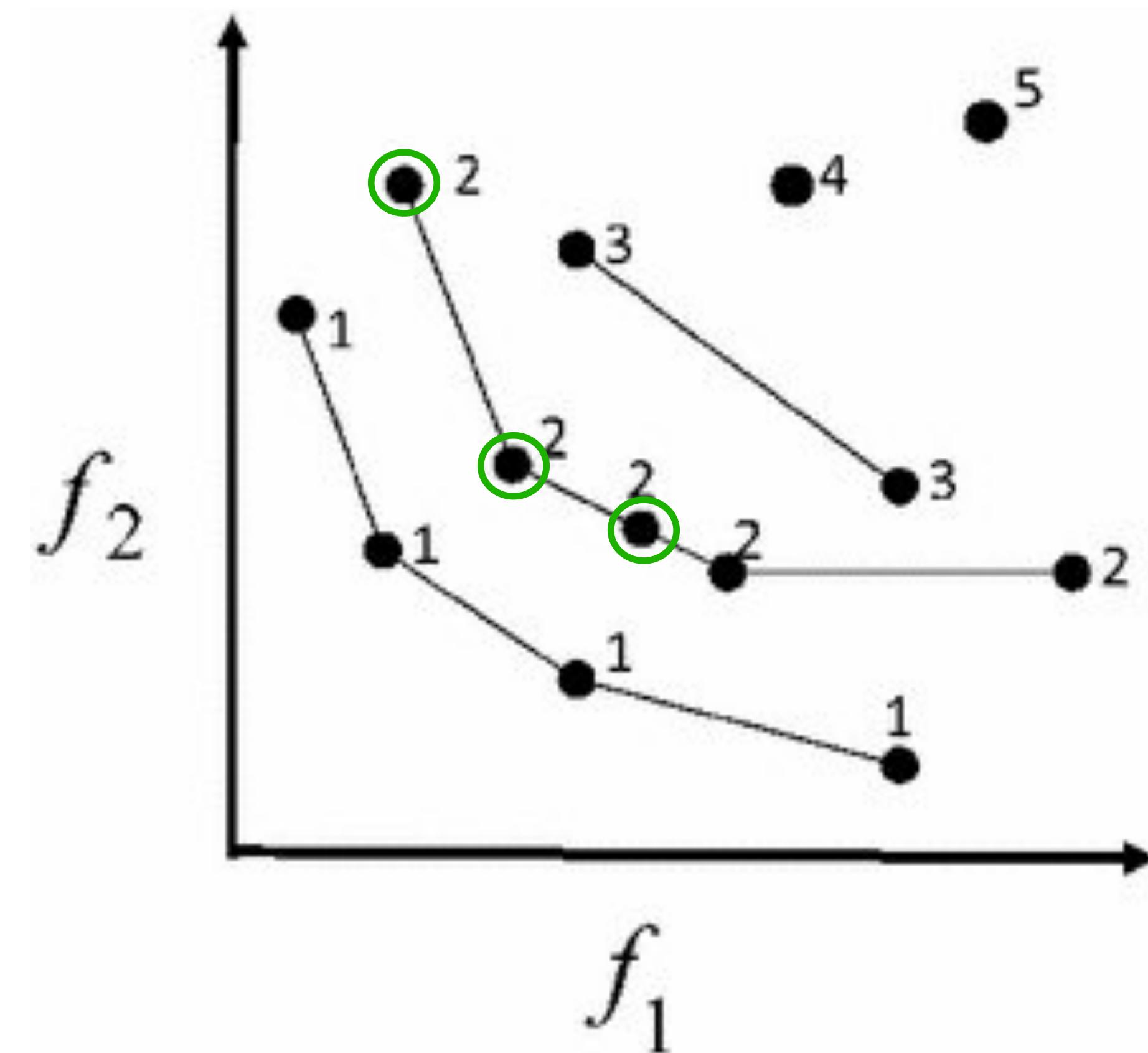
```
fast-non-dominated-sort( $P$ )
for each  $p \in P$ 
     $S_p = \emptyset$            <- individuals dominated by  $p$ 
     $n_p = 0$               <- number of individuals dominating  $p$ 
    for each  $q \in P$ 
        if  $(p \prec q)$  then
             $S_p = S_p \cup \{q\}$ 
        else if  $(q \prec p)$  then
             $n_p = n_p + 1$ 
        if  $n_p = 0$  then
             $p_{\text{rank}} = 1$ 
             $\mathcal{F}_1 = \mathcal{F}_1 \cup \{p\}$ 
     $i = 1$                   Initialize the front counter
    while  $\mathcal{F}_i \neq \emptyset$ 
         $Q = \emptyset$           Used to store the members of the next front
        for each  $p \in \mathcal{F}_i$    <- for each element belonging to the current Pareto front
            for each  $q \in S_p$    <- for each element dominated by  $p$ 
                 $n_q = n_q - 1$     <- decrease its domination number
                if  $n_q = 0$  then
                     $q_{\text{rank}} = i + 1$ 
                     $Q = Q \cup \{q\}$ 
         $i = i + 1$ 
         $\mathcal{F}_i = Q$ 
```

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Selection for parenting uses rank and crowding distance.

Select at random T individuals (control over selection pressure)

- Primary criterion: compare ranks (Goldberg)



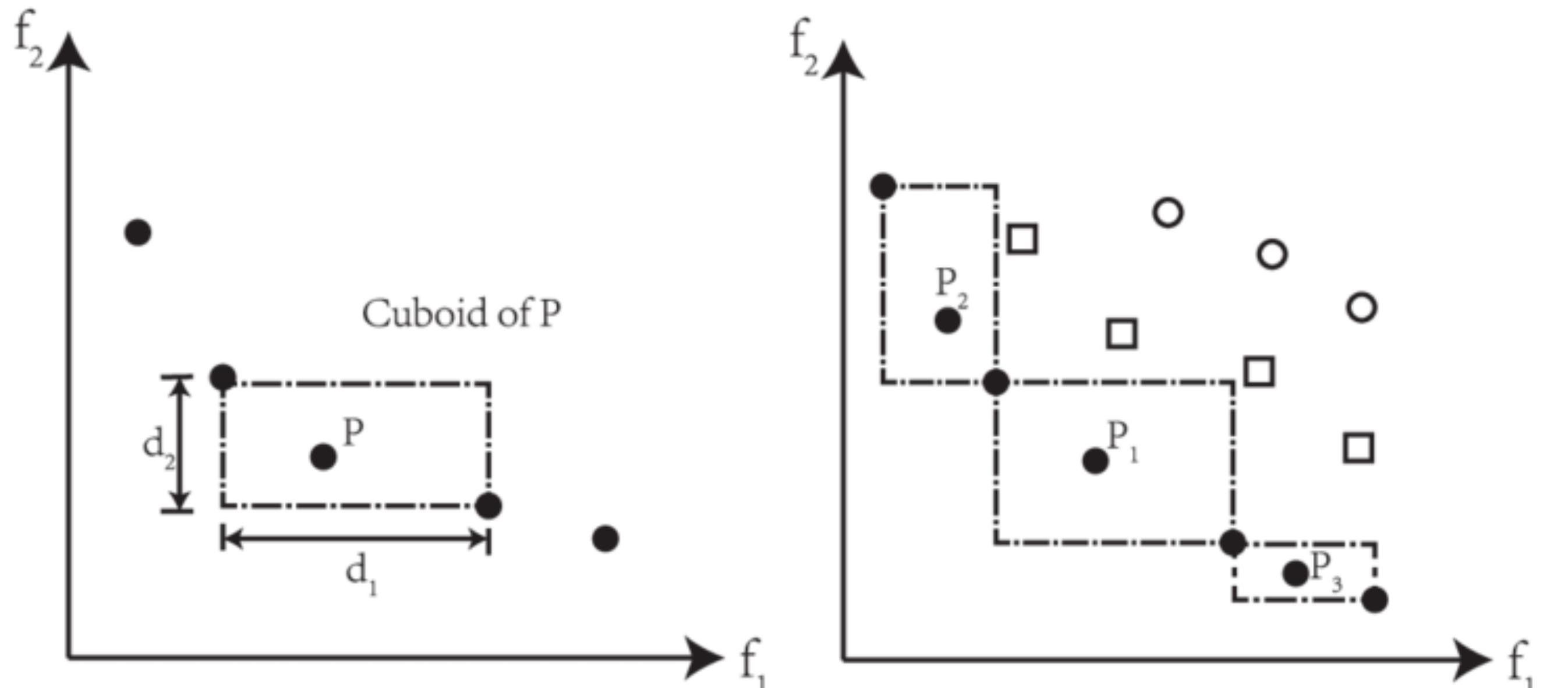
# Non-dominated Sorting GA II (Deb et al. 2002)

Selection for parenting uses rank and crowding distance.

Select at random T individuals (control over selection pressure)

- Primary criterion: compare ranks (Goldberg)
- Secondary criterion: compare crowding distance

The main aim is to preserve diversity and prevent early convergence



The crowding distance is defined as the sum of the edge length of the cuboid.

crowding-distance-assignment( $\mathcal{I}$ )

$$l = |\mathcal{I}|$$

for each  $i$ , set  $\mathcal{I}[i]_{\text{distance}} = 0$

for each objective  $m$

$$\mathcal{I} = \text{sort}(\mathcal{I}, m)$$

$$\mathcal{I}[1]_{\text{distance}} = \mathcal{I}[l]_{\text{distance}} = \infty$$

for  $i = 2$  to  $(l - 1)$

$$\mathcal{I}[i]_{\text{distance}} = \mathcal{I}[i]_{\text{distance}} + (\mathcal{I}[i + 1].m - \mathcal{I}[i - 1].m)/(f_m^{\max} - f_m^{\min})$$

number of solutions in  $\mathcal{I}$   
initialize distance

sort using each objective value  
so that boundary points are always selected  
for all other points

# NSGA-II (*Deb et al. 2002*)

t=0 #generation counter

P(t) = generate\_random\_population(N)

Fitness(t) = evaluate\_population\_fitness(P(t))

Ranks = ComputeRanks(P(t), Fitness(t))

CrowdingDist = ComputeCrowdingDist(P(t) , Fitness(t) ,Ranks)

While (t<G) or not (termination\_criterion):

    Q(t) =[]

    For i=1,...,N:

        variation = select([mutation,crossover])

        parents = select\_parents(variation, P(g), Ranks , CrowdingDist,T)

        child = variation(parents)

        Q(t).append(child)

    P(t+1) = [P(t) , Q(t)]

    Fitness(t+1) = [Fitness(t) , evaluate\_population\_fitness(Q(t))]

    Ranks = ComputeRanks(P(t+1), Fitness(t+1))

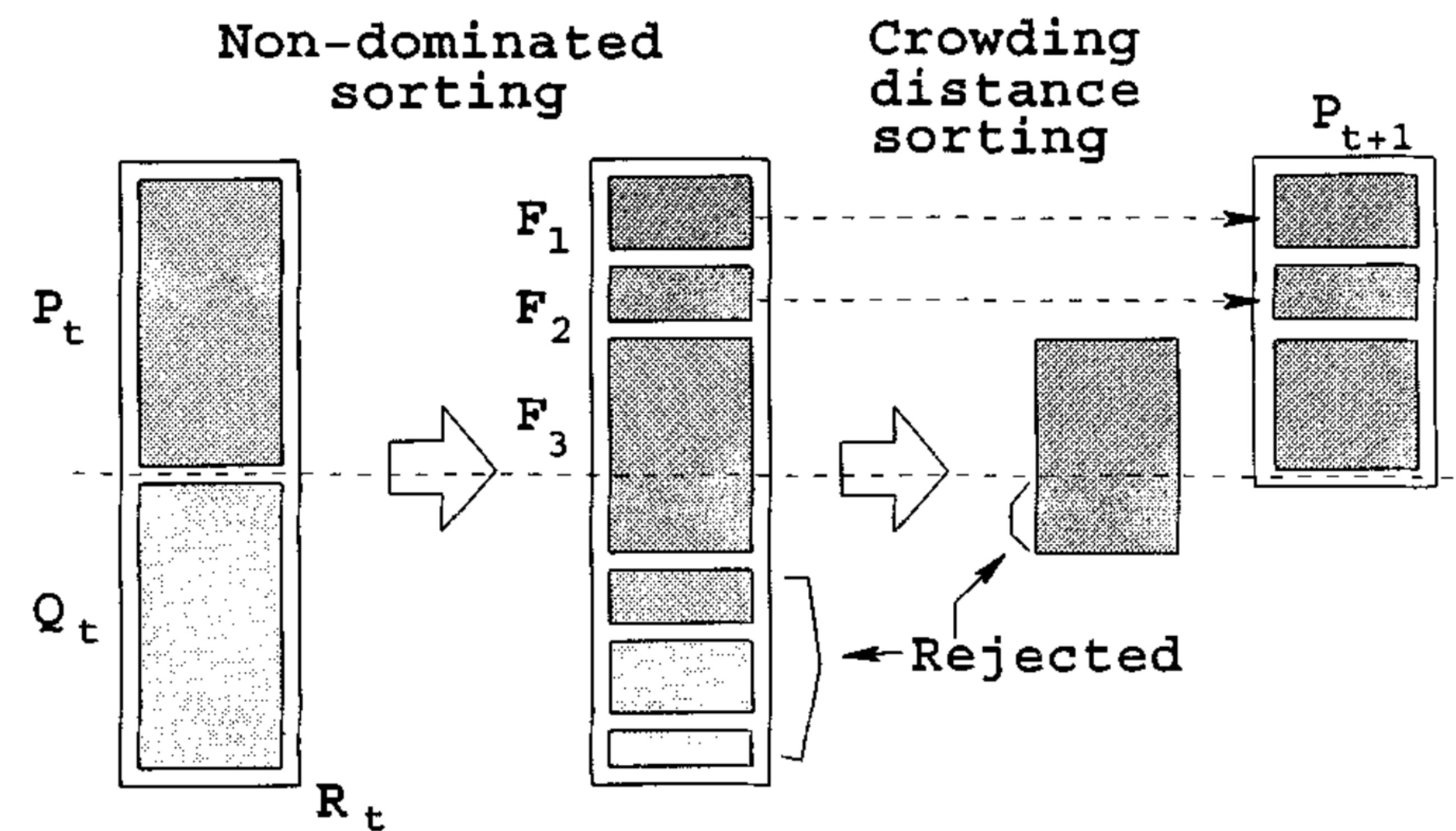
    CrowdingDist = ComputeCrowdingDist(P(t+1) , Fitness(t+1) ,Ranks)

    P(t+1), Fitness(t+1), Ranks, CrowdingDist = SelectElite( P(t+1), Fitness(t+1), Ranks, CrowdingDist)

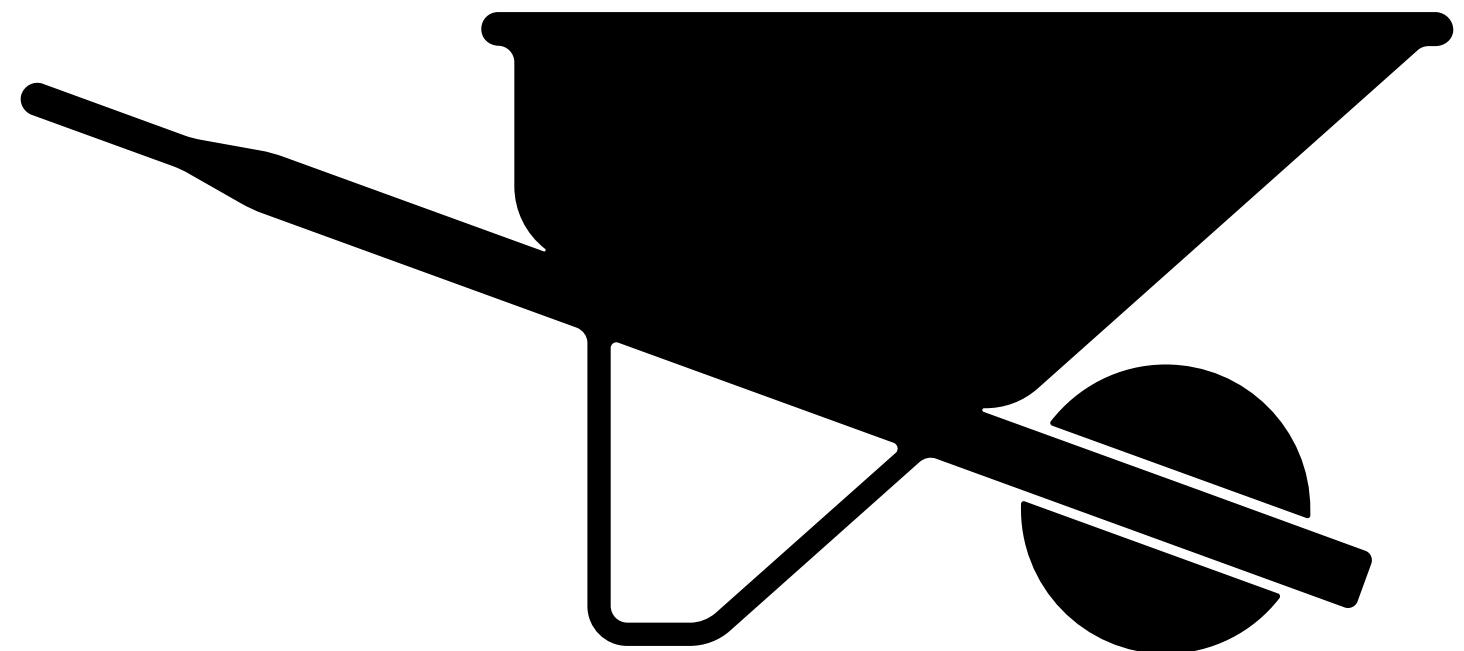
    t=t+1

# NSGA-II (*Deb et al. 2002*)

## Pseudocode



# Hands on



**Using the pymoo library**  
<https://pymoo.org/interface/display.html>