UiO : University of Oslo

institutt for informatikk

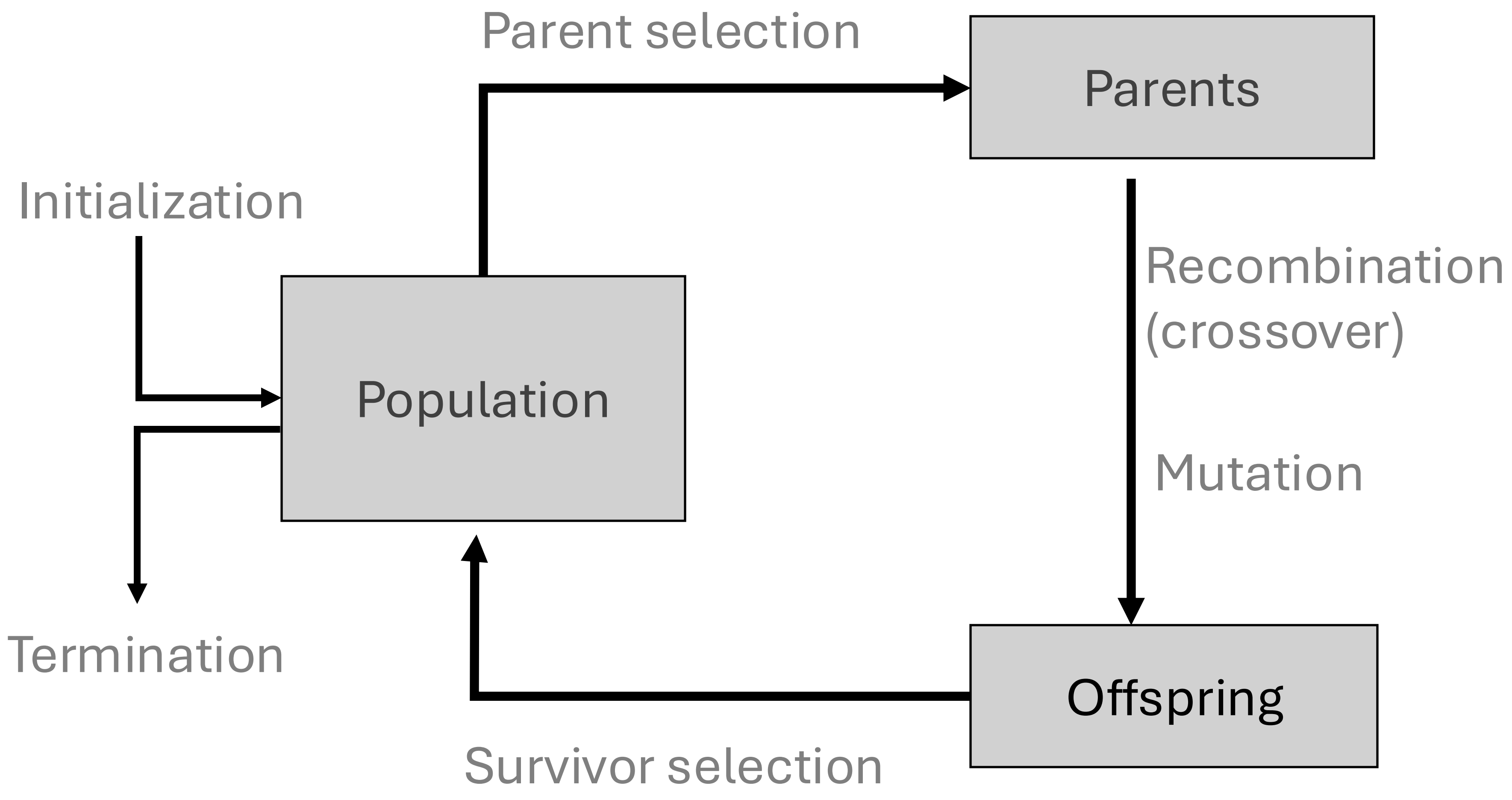
IN3050/IN4050 - Introduction to Artificial Intelligence and Machine Learning

Lecture 6– Autumn 2024

Evolutionary Algorithms 2 –Population Management and More

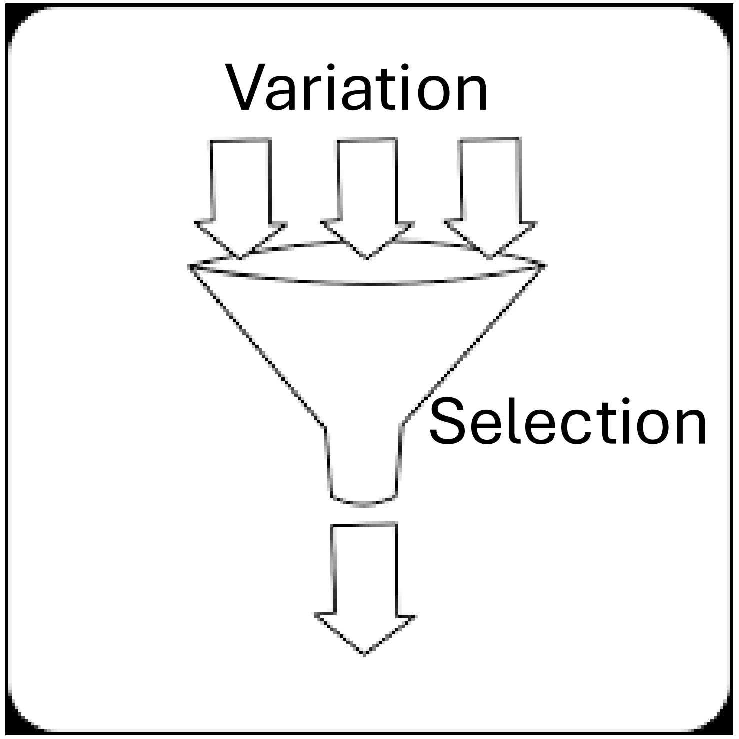
Pooya Zakeri

Repetition: General scheme of EAs

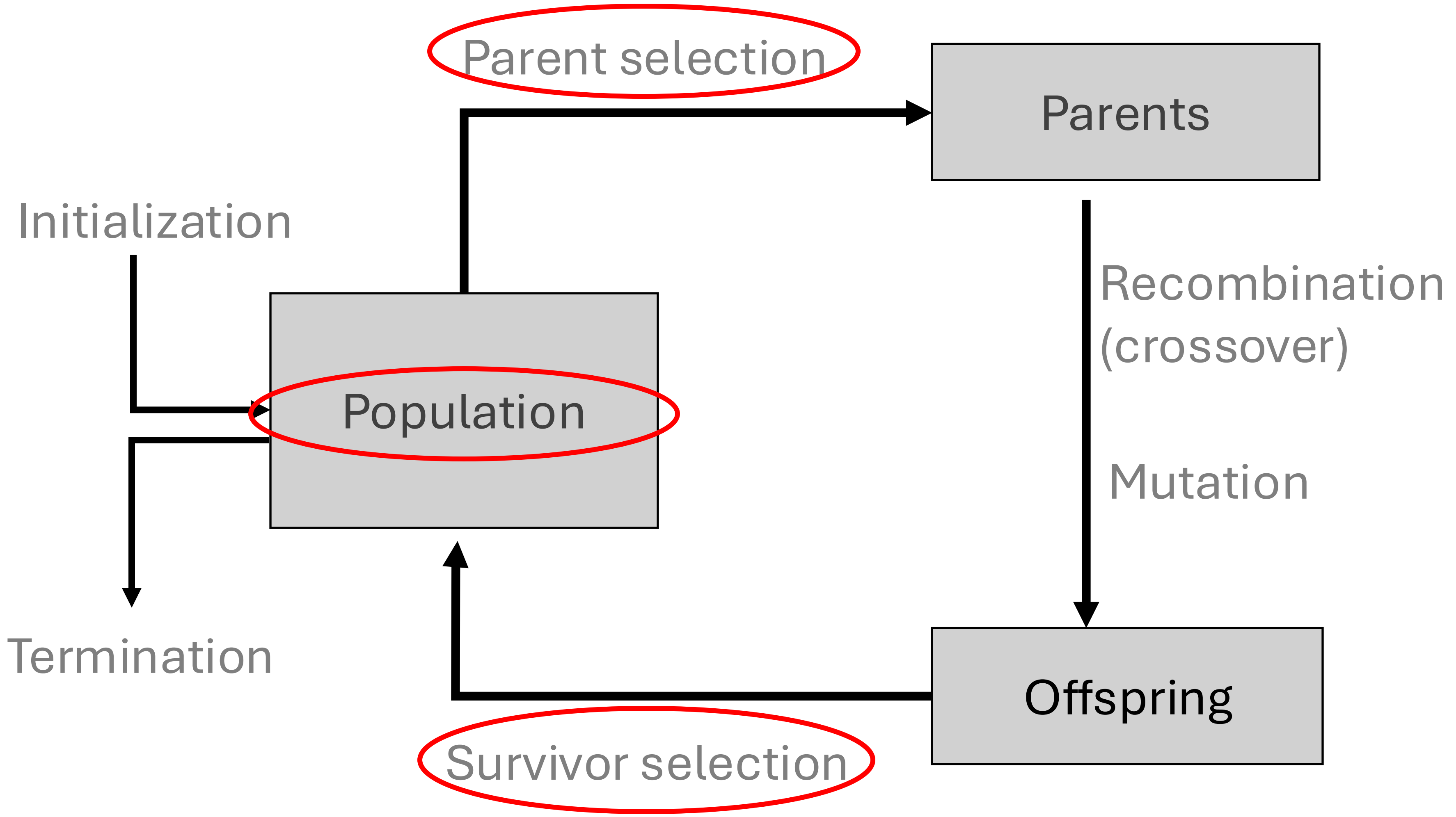


Chapter 5: Fitness, Selection and Population Management

- **Selection** is the second fundamental force for evolutionary systems
- Topics include:
  - Selection operators
  - Preserving diversity



Scheme of an EA: General scheme of EAs



Selection

- Selection can occur in two places:
  - **Parent selection** (selects mating pairs)
  - **Survivor selection** (replaces population)
- Selection works on the population

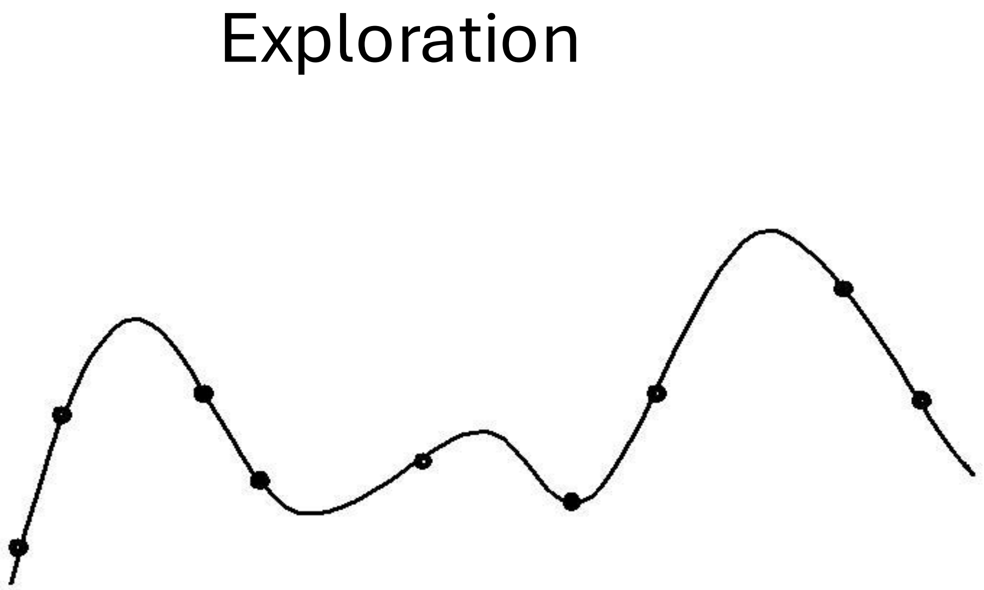
  -> Selection operators are **representation-independent** because they work on the fitness value
- **Selection pressure**: As selection pressure increases, fitter solutions are more likely to survive, or be chosen as parents

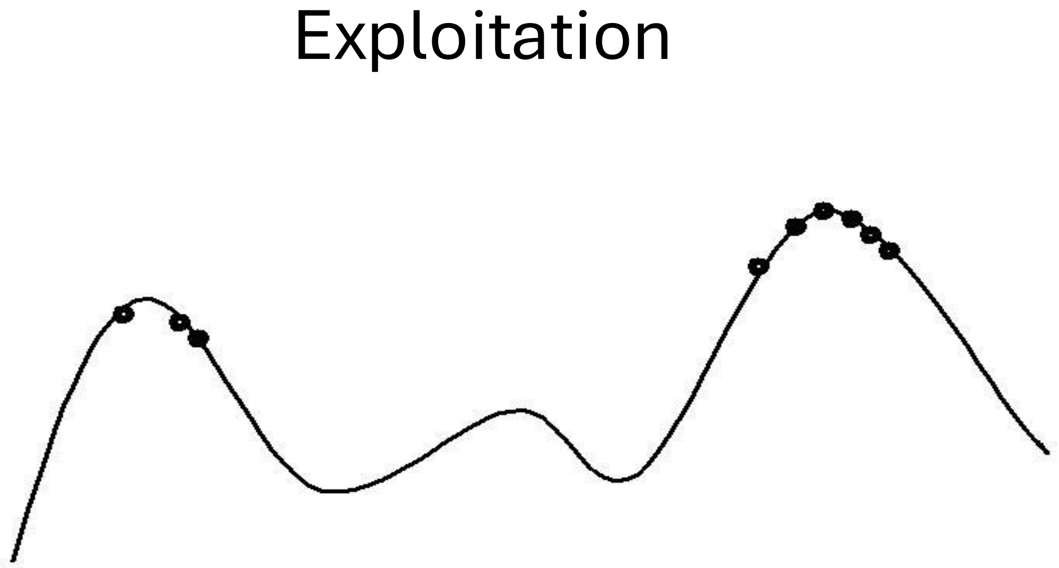
Effect of Selection Pressure

- Low Pressure

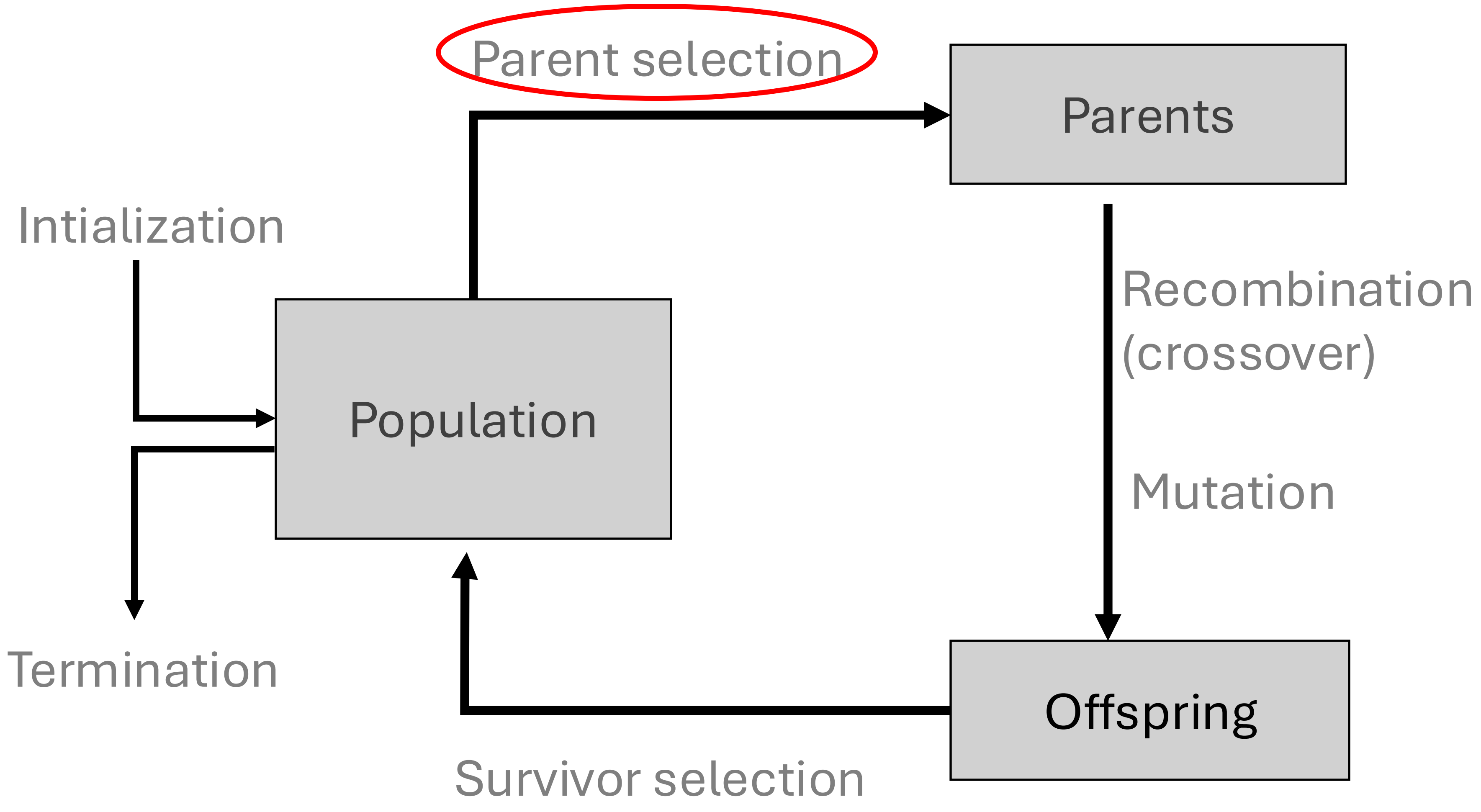
- High Pressure

Why Not Always High Selection Pressure?





Scheme of an EA: General scheme of EAs



Parent Selection: Fitness-Proportionate Selection

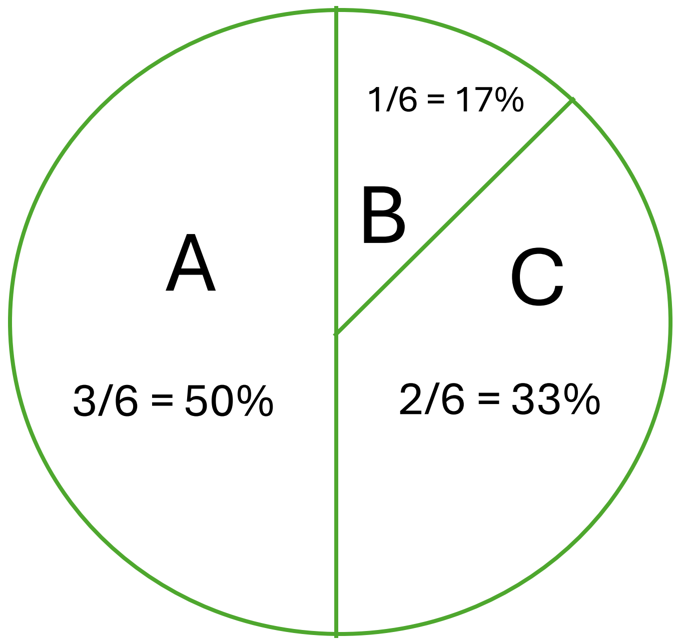
Example: roulette wheel selection

fitness(A) = 3

fitness(B) = 1

fitness(C) = 2

$\longrightarrow$



Parent Selection: Fitness-Proportionate Selection (FPS)

- Probability for individual *i* to be selected for mating in a population size *μ* with FPS is

$$P_{FPS}(i) = f_i \Big/ \sum_{j=1}^{\mu} f_j$$

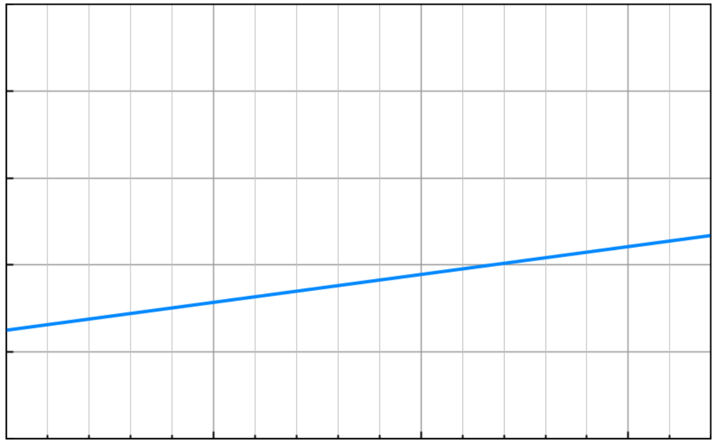
- Problems include
    - One highly fit member can rapidly take over if rest of population is much less fit: **Premature Convergence**
    - At end of runs when finesses are similar, **loss of selection pressure**

Parent Selection: Rank-based Selection

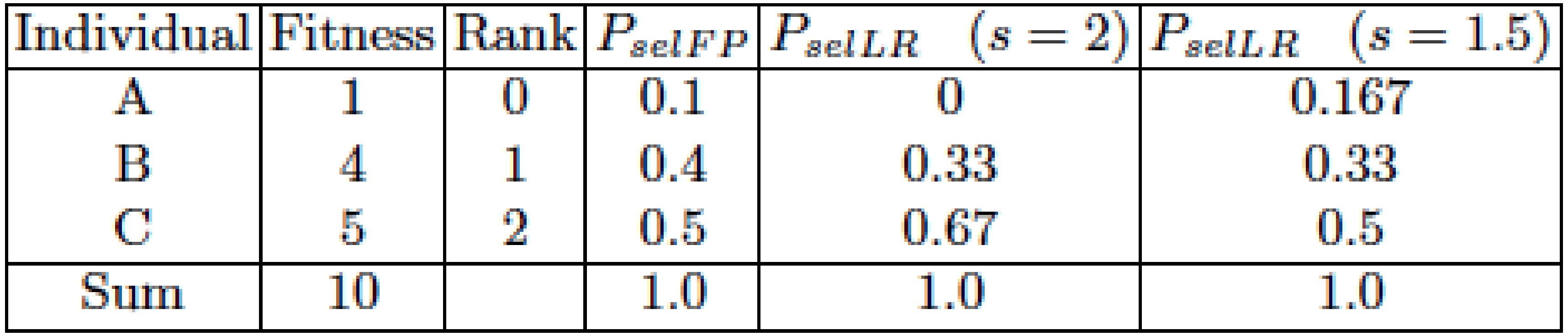
- Attempt to remove problems of FPS by basing selection probabilities on ***relative* rather than *absolute* fitness**
- **Rank population** according to fitness and then base selection probabilities on rank (fittest has rank μ*-1* and worst rank 0)
- This imposes a sorting overhead on the algorithm

Rank-based Selection: Linear Ranking

$$P_{lin-rank}(i) = \frac{(2-s)}{m} + \frac{2i(s-1)}{m(m-1)}$$



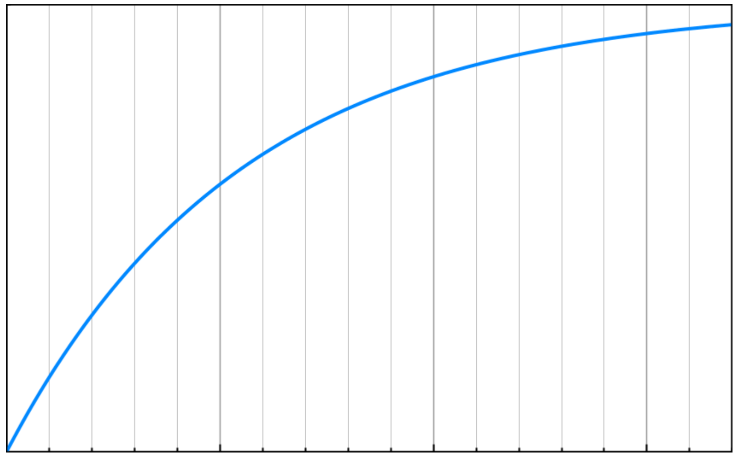
- Parameterized by factor *s*: $1 < s \leq 2$
  - Tunes selection pressure
- Simple 3 - member example



Individual	Fitness	Rank	P_{selFP}	P_{selLR} $(s=2)$	P_{selLR} $(s=1.5)$
A	1	0	0.1	0	0.167
B	4	1	0.4	0.33	0.33
C	5	2	0.5	0.67	0.5
Sum	10		1.0	1.0	1.0

Rank-based selection: Exponential Ranking

$$P_{\exp\text{-}rank}(i) = \frac{1 - e^{-i}}{c}$$



- Linear Ranking is limited in selection pressure
- Exponential Ranking can allocate more than 2 copies to the fittest individual
- Normalize constant factor *c* according to population size

Parent Selection: Tournament Selection (1/3)

- The methods above rely on **global population statistics**
  - This could be a **bottleneck, especially on parallel machines**, very large population
  - Relies on the presence of external fitness functions that might not exist, e.g. evolving game players

Parent Selection: Tournament Selection (2/3)

The idea for a procedure using only local fitness information:

- Pick ***k* members at random,** then select the best of these
- **Repeat to select more** individuals

Parent Selection: Tournament Selection (3/3)

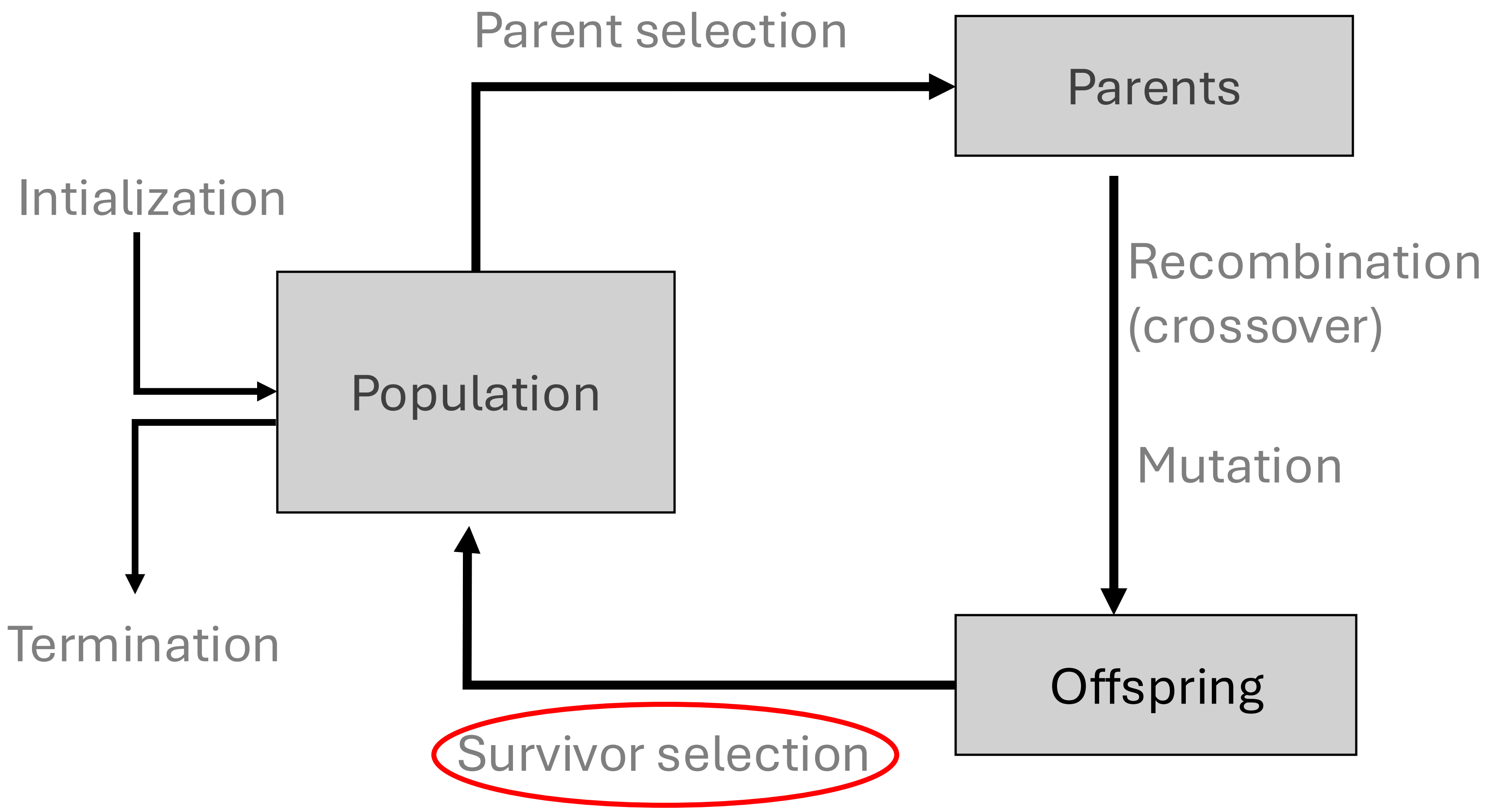
- Probability of selecting *i* will depend on:
  - Rank of *i*
  - Size of sample *k*
    - higher *k* increases selection pressure
  - Whether contestants are picked with replacement
    - Picking without replacement increases selection pressure
  - Whether fittest contestant always wins (deterministic) or this happens with probability *p*

Parent Selection: Uniform

$$P_{uniform}(i) = \frac{1}{m}$$

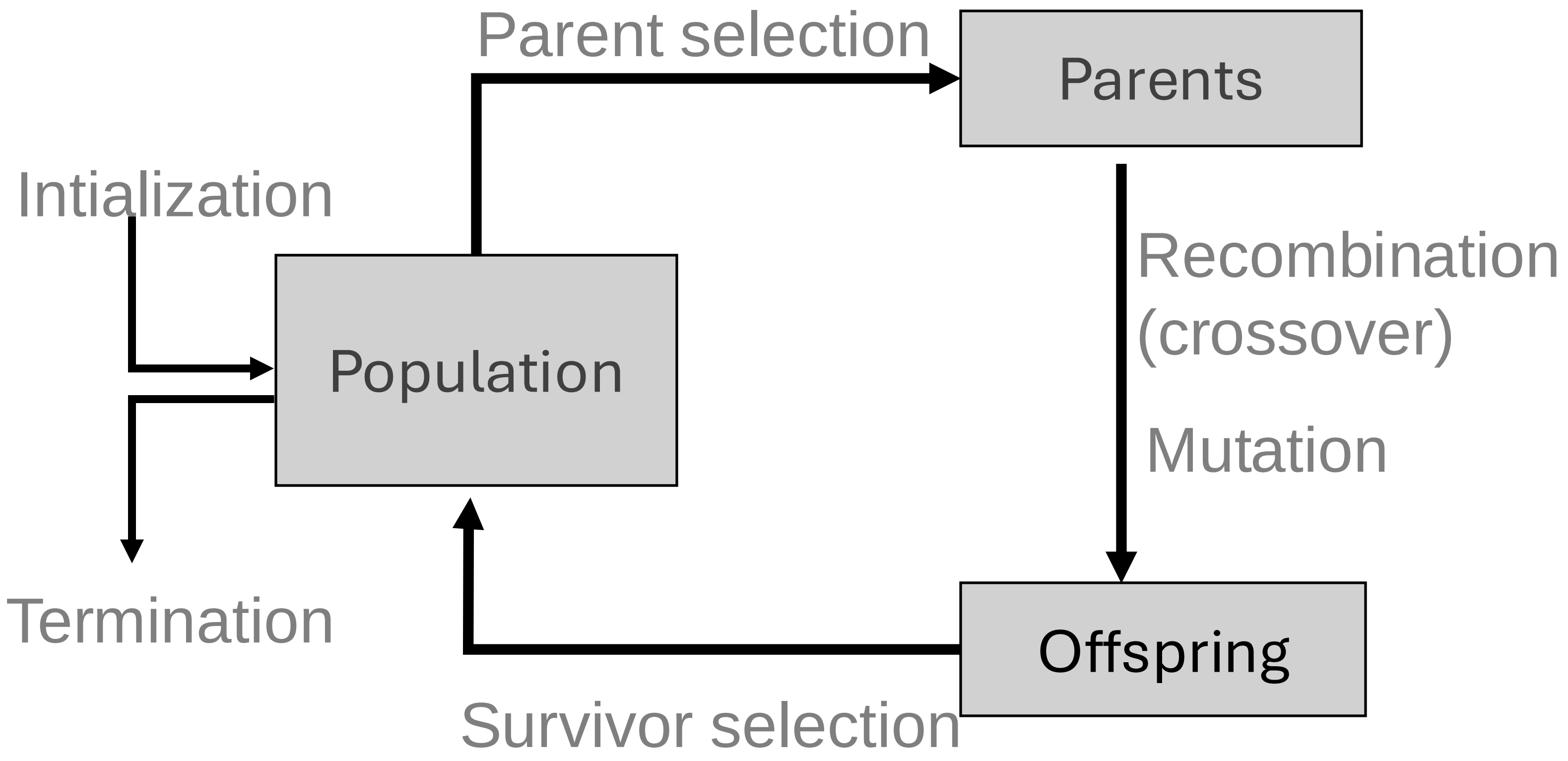
- Parents are selected by uniform random distribution whenever an operator needs one/some
- Uniform parent selection is unbiased - every individual has the **same probability** to be selected

Scheme of an EA:
General scheme of EAs



Survivor Selection (Replacement)

- From a set of μ old solutions and λ offspring: Select a set of μ individuals **forming the next generation**

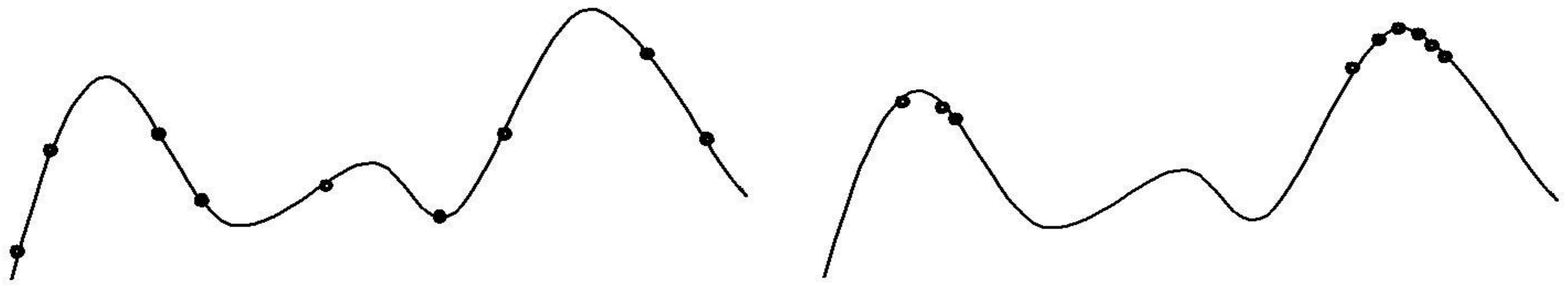


Fitness-based replacement – examples

- Elitism
  - Always **keep** at least one copy of **the N fittest solution(s)** so far
  - Widely used in most EA-variants
- **(μ,λ)-selection** (best candidates can be lost)
  - based on the set of **children only** ($\lambda > \mu$)
  - choose the **best** μ offspring for next generation
- **(μ+λ)-selection** (elitist strategy)
  - based on the set of **parents and children**
  - choose the **best** μ individuals for next generation
- (μ,λ)-selection may loose the best solution, but is better at leaving local optima

Multimodality

- Often might want to identify several possible peaks
- Different peaks may be different good ways to solve the problem.
- We therefore need methods to **preserve diversity** (instead of converging to one peak)



Approaches for Preserving Diversity: Introduction

- Explicit vs implicit
- **Implicit** approaches:
    - Impose an equivalent of **geographical separation**
    - Impose an equivalent of **speciation**
- **Explicit** approaches
    - Make **similar individuals compete** for resources (**fitness**)
    - Make **similar individuals compete** with each other for **survival**

Explicit Approaches for Preserving Diversity: Fitness Sharing (1/2)

- Restricts the number of individuals within a given niche by "sharing" their fitness
- Need to set the size of the niche σ_{share} in either genotype or phenotype space
- run EA as normal but after each generation set

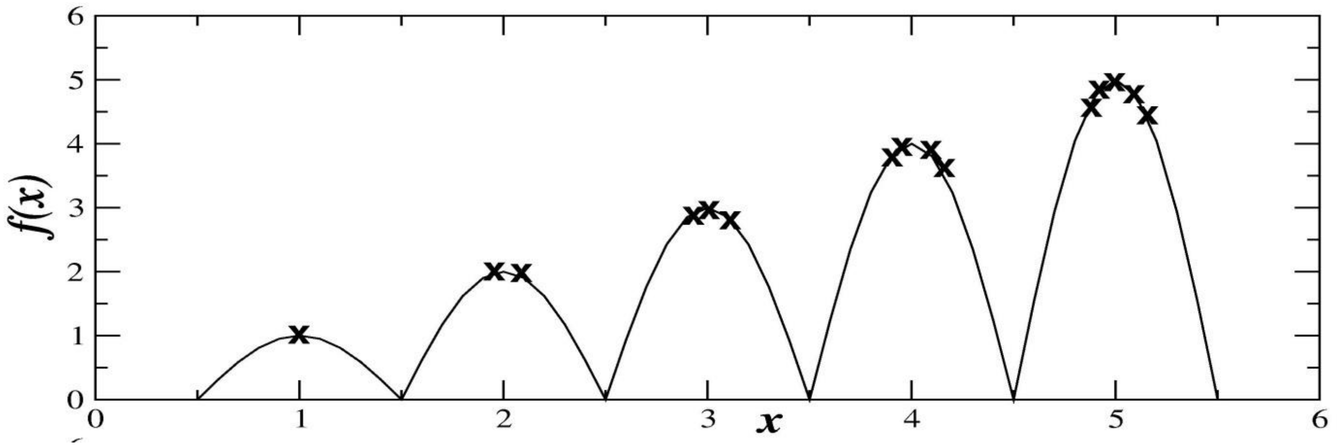
$$f'(i) = \frac{f(i)}{\sum_{j=1}^{\mu} sh(d(i,j))}$$

$$sh(d) = \begin{cases} 1 - d/\sigma & d \le \sigma \\ 0 & otherwise \end{cases}$$

Explicit Approaches for Preserving Diversity: Fitness Sharing (2/2)

$$f'(i) = \frac{f(i)}{\sum_{j=1}^{\mu} sh(d(i,j))}$$

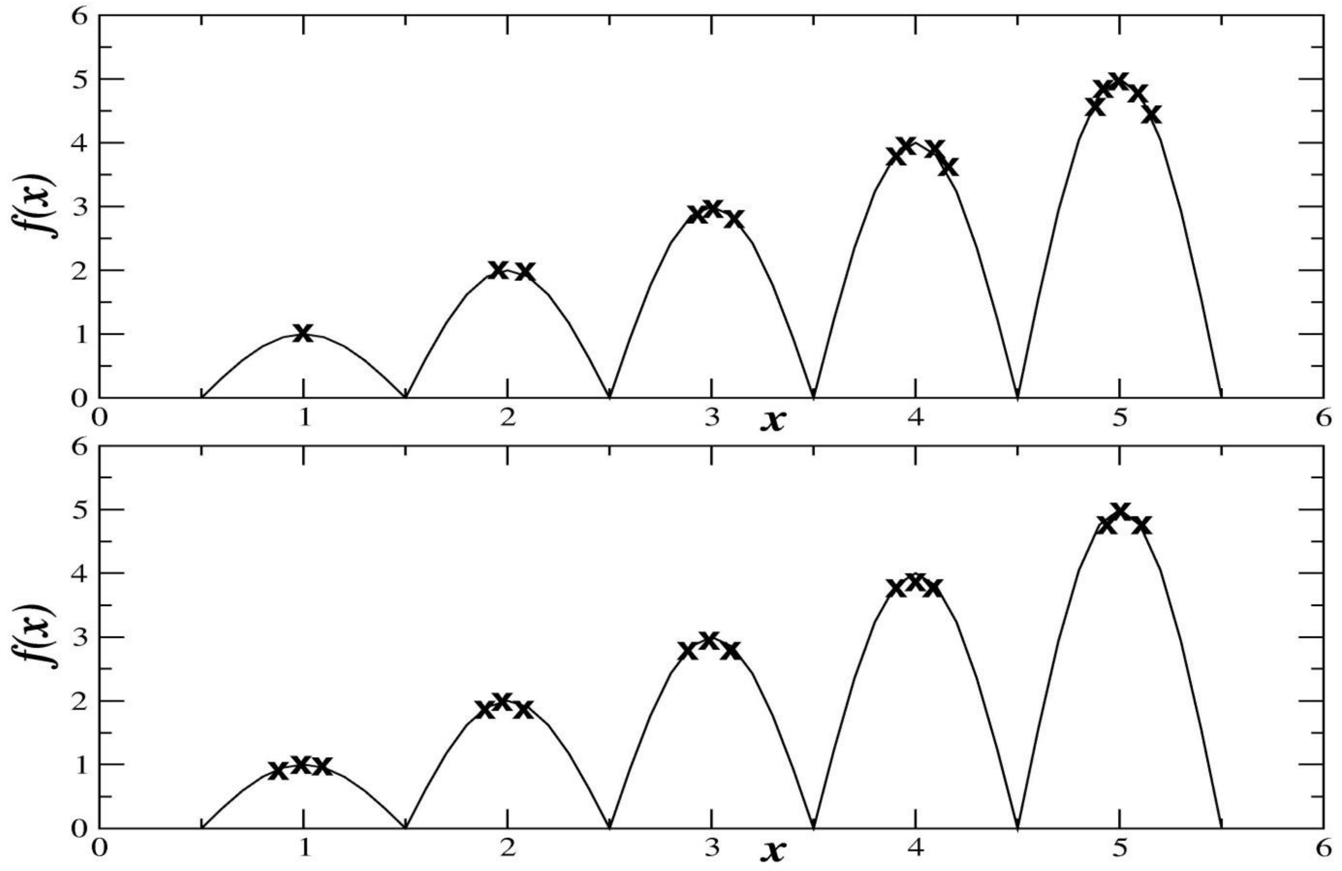
$$sh(d) = \begin{cases} 1 - d/\sigma & d \le \sigma \\ 0 & otherwise \end{cases}$$



Explicit Approaches for Preserving Diversity: Crowding

- Idea: New individuals replace *similar* individuals
- Randomly shuffle and pair parents, produce 2 offspring
- Each offspring competes with their **nearest** parent for survival (using a distance measure)
- Result: Even distribution among niches.

Explicit Approaches for Preserving Diversity: Crowding vs Fitness sharing



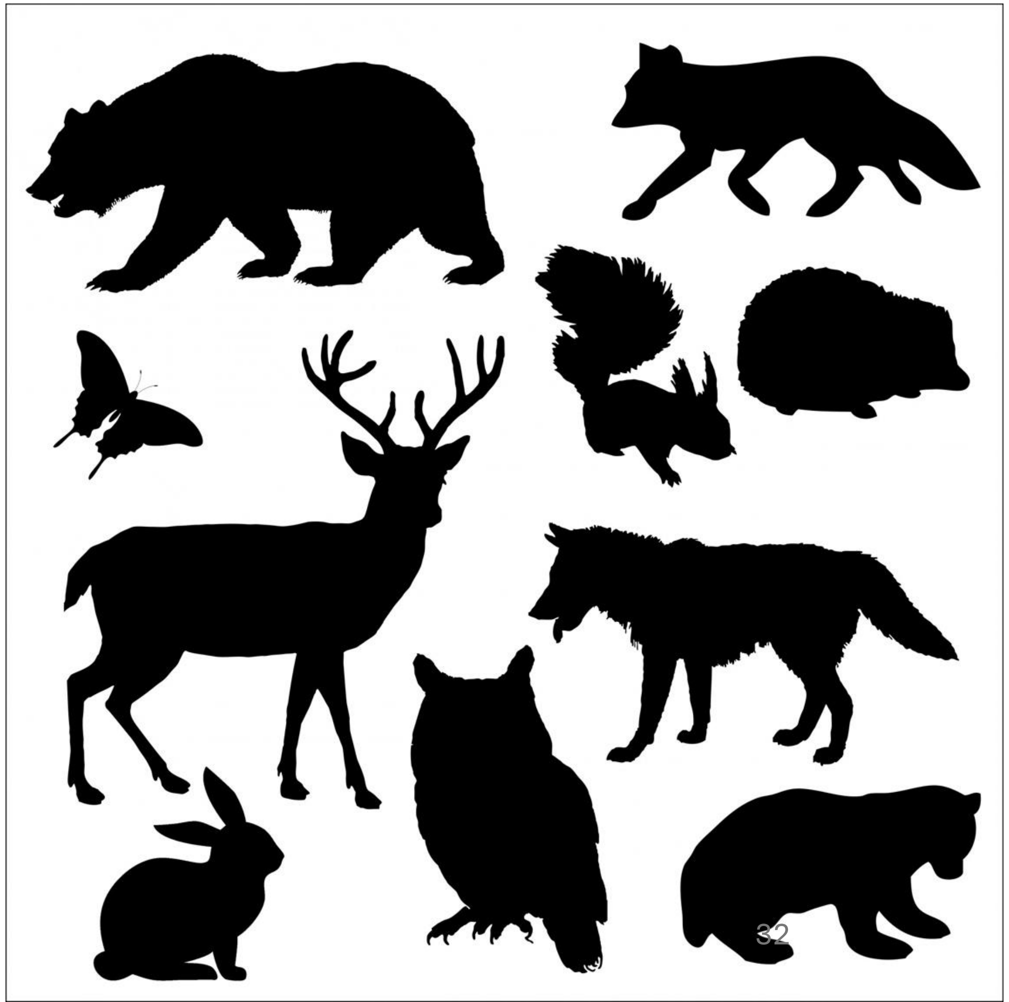
Fitness Sharing

Crowding

Observe the number of individuals per niche

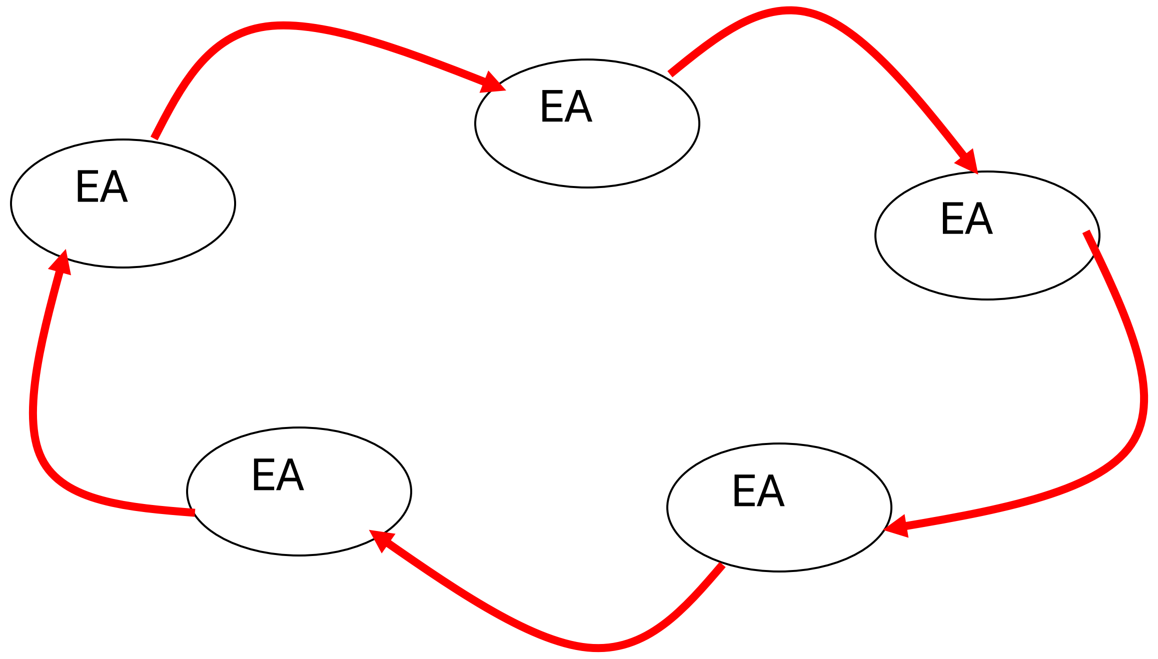
Implicit Approaches for Preserving Diversity: Automatic Speciation

- Either only mate with genotypically / phenotypically similar members or
- Add species-tags to the genotype
  - initially randomly set
  - when selecting a partner for recombination, only pick members with a good match



Implicit Approaches for Preserving Diversity: Geographical Separation

- “Island” Model Parallel EA
- Periodic migration of individual solutions between populations



Implicit Approaches for Preserving Diversity: "Island" Model Parallel EAs

- Run multiple populations in parallel
- After a (usually fixed) number of generations (an ***Epoch***), exchange individuals with neighbours
- Repeat until ending criteria met
- Partially inspired by parallel/clustered systems

Genetic Algorithms for Hyperparameter Optimization

- GAs are commonly used in various ML methods to **tune hyperparameters**
- Hyperparameters govern the model's performance.
- Manual tuning can be inefficient and time-consuming.
  - Such as *grid search* or *random search*
- GAs provide an effective way to automate this process by searching for optimal hyperparameter combinations—e.g.,applying **Differential Evolution**
- Popular ML methods and techniques where GAs are employed for hyperparameter optimization:
  - Neural Networks/Deep Learning, Support Vector Machines (SVM), 3. Decision Trees / Random Forest, Kernel Ridge Regression, k- Nearest Neighbors (k-NN), Clustering Algorithms (e.g., K-Means, DBSCAN)

Why GAs for Hyperparameter Tuning?

- **Exploration and Exploitation Balance**: GAs maintain a good balance between exploring new solutions and exploiting known good solutions, avoiding the risk of getting stuck in local optima.
- **Flexibility**: GAs can handle various types of hyperparameters, including discrete, continuous, and categorical variables.
- **Global Search**: Compared to grid search or random search, GAs offer a more global exploration of the hyperparameter space, making them suitable for complex or non-convex optimization problems.
- **Parallelizable**: GAs are inherently parallelizable, meaning they can be easily distributed across multiple processors, speeding up the optimization process.
- **Efficient**: They reduce the computational expense of grid or random search.

Overview of Differential Evolution Algorithm for Hyperparameter Tuning (1/2)

- **Differential Evolution** is a type of genetic algorithm that uses a population of solutions (vectors) to evolve the best parameters and iteratively optimizes a function by evolving a population of candidate solutions.
- Each vector contains **parameters** that represent the hyperparameters of the model.

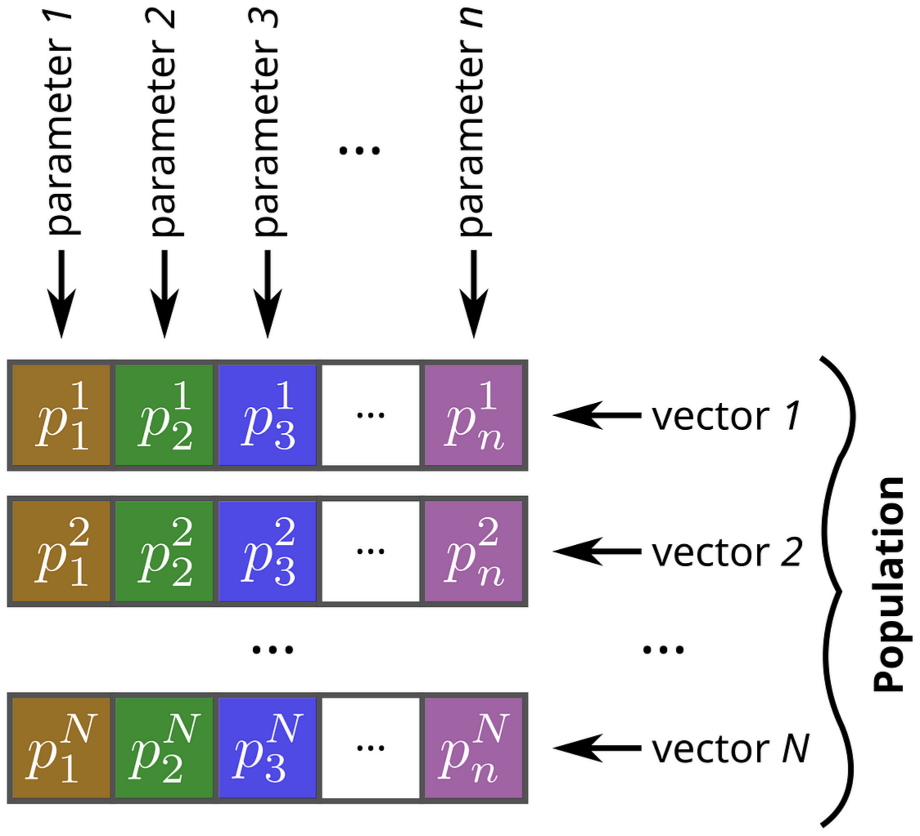

parameter 1
parameter 2
parameter 3
...
parameter n
p_1^1 p_2^1 p_3^1 ... p_n^1
p_1^2 p_2^2 p_3^2 ... p_n^2
p_1^N p_2^N p_3^N ... p_n^N
vector 1
vector 2
vector N
Population

Image source

Overview of Differential Evolution Algorithm for Hyperparameter Tuning (2/2)

- **Initialization**: Create an initial population of vectors with random parameter values within predefined boundaries. The size of the population is NP (number of vectors).
- **Evaluation**: Evaluate the fitness of each vector in the population by calculating its function value. (e.g., mean squared errors on a validation set)
- For each vector in the population, Iterate until convergence is achieved (**repeat**)
  1. **Mutation**: Build a new vector by mutating the parameters of existing vectors.
     - The **best1bin strategy** is commonly used:
       - The mutant parameter is a variation of the best vector plus a mutation rate (F) times the difference between two other random vectors.

$$p_i^{mut} = p_i^{best} + F \cdot (p_i^{r_1} - p_i^{r_2})$$

  2. **Recombination**: Combine parameters from the current vector and mutant vector to create a trial vector.
     - For each parameter, a random uniform number R is generated.
     - If R < recombination rate, the mutant parameter is selected; otherwise, the current parameter is retained.
  3. **Replacement**:
     - Evaluate the fitness of the trial vector.
     - If the trial vector has a better fitness than the current vector, it replaces the current vector in the population.

Further Reading

Using Gas for Weight Optimization in NN (1/3)

- Neural networks are traditionally trained using **gradient descent**, which adjusts weights based on error.
- Genetic algorithms can be used to **encode neural network weights** as a set of strings.
- **Fitness Function**: Measures performance using **sum-of-squares error**, similar to how gradient descent minimizes error.
- **Drawbacks**:
  - Local information at each node is discarded and reduced to a single fitness value.
  - GA-based optimization ignores **gradient information**, losing a valuable source of guidance.
  - Results can be good, but this approach loses some valuable information compared to gradient descent.

Evolving Neural Network Topology with GAs (2/3)

- **Topology Optimization**: GAs are more effectively applied to evolve the structure or topology of the neural network, such as:
    - Adding or deleting neurons.
    - Adding or deleting weight connections.
- **Mutation Operators**:
    - **Delete a neuron**: Simplifies the network.
    - **Delete a weight connection**: Reduces complexity.
    - **Add a neuron**: Increases complexity.
    - **Add a connection**: Enhances inter-neuron communication.
- Deletion operations bias the learning toward **simpler networks**. GAs provide an automated way to explore different network architectures instead of manually trying different structures.

Neuroevolution (3/3)

- ***Neuroevolution*** merges genetic algorithms with neural networks.
- Iterative process of improving neural networks through generations.
- NEAT (Neuroevolution of Augmented Topologies) is a specific algorithm that evolves both the architecture and weights of neural networks.
  - It starts with simple networks and gradually increases complexity, allowing the emergence of efficient architectures.
  - Particularly useful for tasks requiring complex decision-making and adaptation.

Further Reading

Limitations of Evolutionary Algorithms (1/2)

- **Slow Convergence/Computational Cost** :

  GAs can be **slow**, especially after reaching a local maximum. It may take a long time to escape and find a better solution.

- **Fitness Landscape**

  Without knowing the **fitness landscape**, it’s difficult to gauge how well the GA is performing.

- **Difficult to Analyze**

  The behavior of GAs is hard to analyze and predict. we cannot guarantee that the algorithm will converge at all

  - It’s hard to prove that the GA will converge to the optimal solution.

- **Black Box Approach**

  GAs are often treated as a black box, which makes it difficult to improve or interpret the results.

Limitations of Evolutionary Algorithms (1/2)

- **Difficulties in Parameter Tuning**
  - EAs have several hyperparameters (e.g., *population size*, *mutation rate*, *crossover rate*) that significantly impact their performance.
  - Incorrect hyperparameter choices can lead to poor convergence, premature convergence, or excessively slow search.
- **Brittle Representation**
  - Finding a suitable representation for complex problems can be challenging and can make or break the performance of the EA.
- **Fitness Function Design**
  - Designing a good fitness function is often non-trivial and problem-specific, making EAs difficult to apply in certain cases.
- **Not Applicable everywhere?**
  - Particularly when the **fitness landscape** is not continuous

Concluding Insights: Evolutionary Algorithms

- How unrealistic are Evolutionary Algorithms as representations of biological evolution?

- Are computer scientists truly inspired by evolutionary theory?