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Metaheuristic Optimization
10. Genetic Algorithms

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Outline

website

Section Outline

Introduction

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  9. individuals that reproduce will likely pass on their traits to their offspring
  10. hence, a species will slowly change and adapt to a given environment

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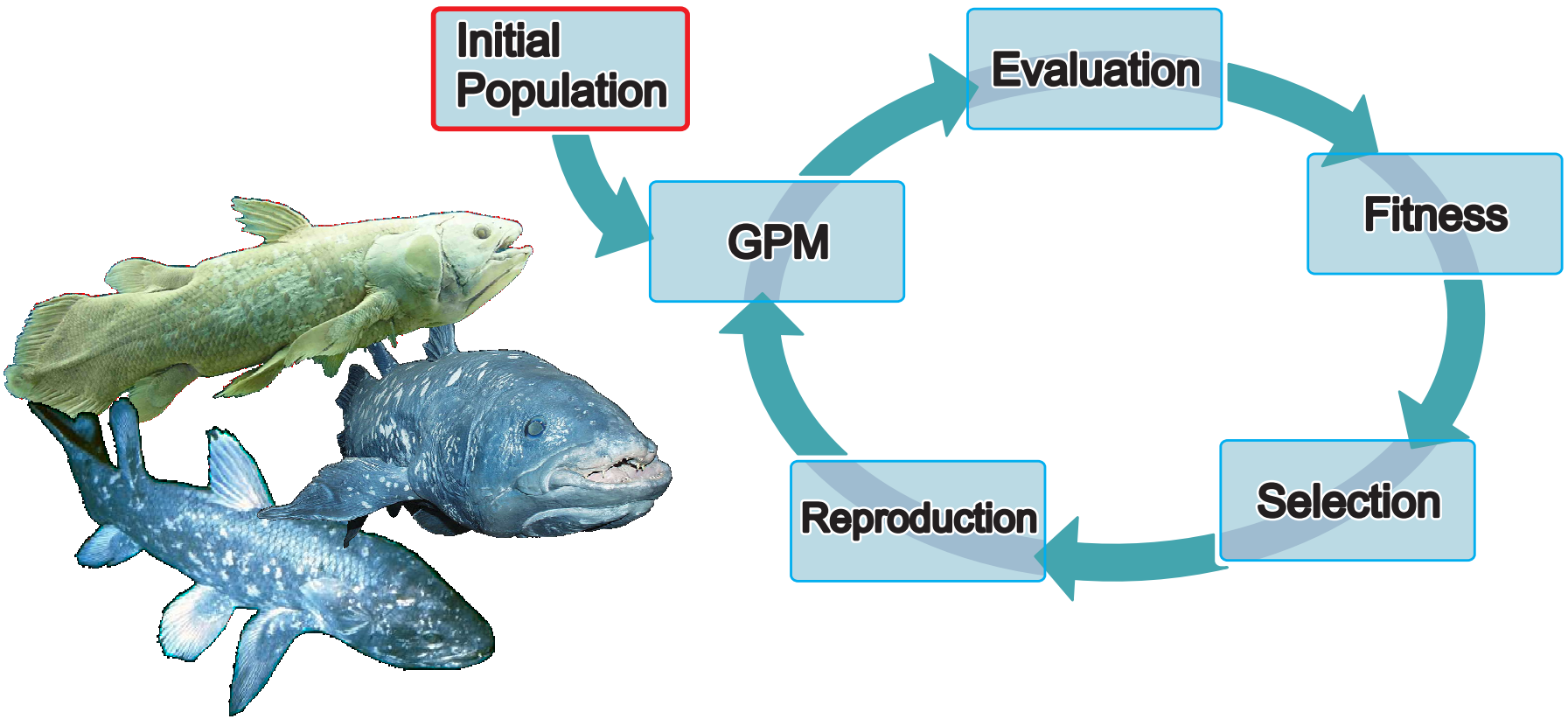
- Individuals which survive become the parents of the next generation

Section Outline

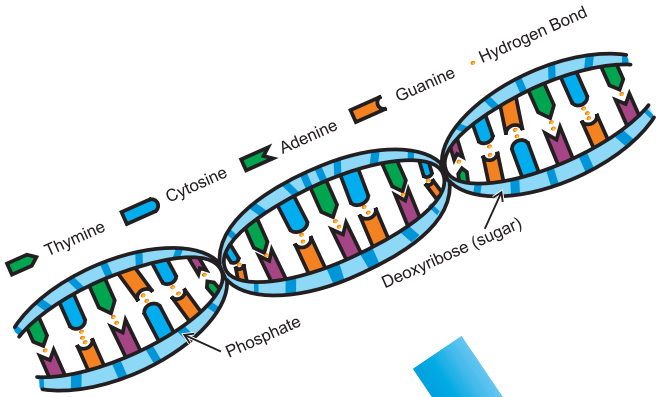
Evolution: First Generation

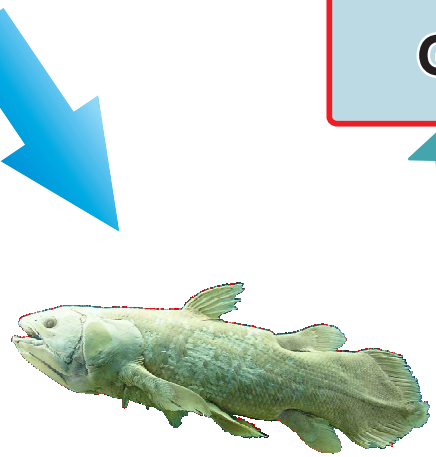
- Start with a random set of individuals (or, their genetic codes)

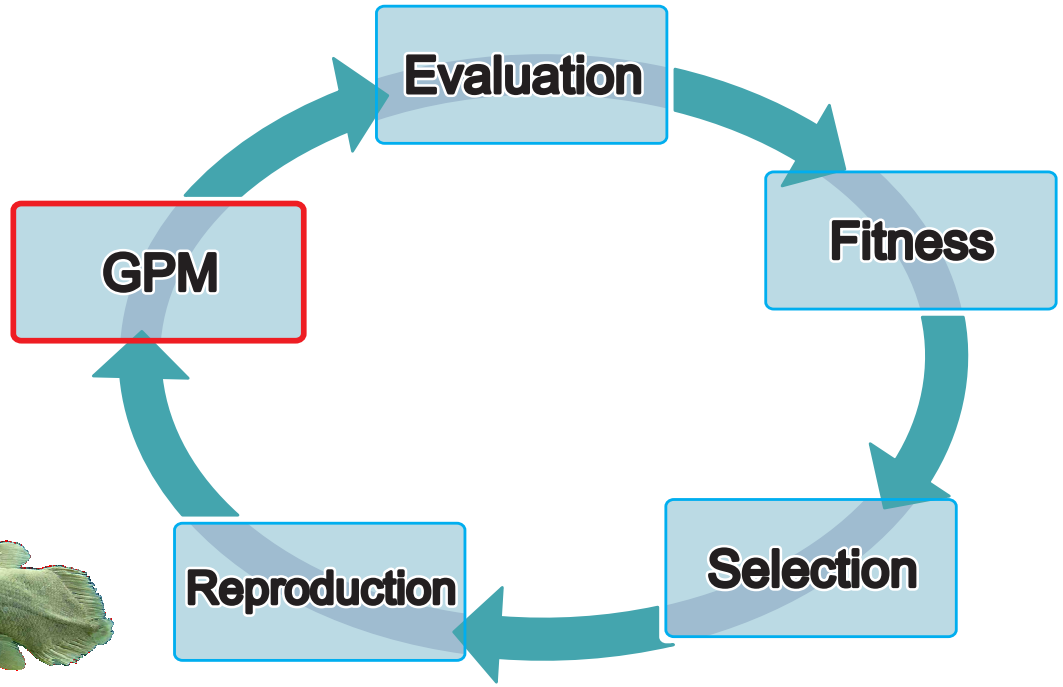


Evolution: Genotype-Phenotype Mapping

- Live begins with the development from genotype to phenotype

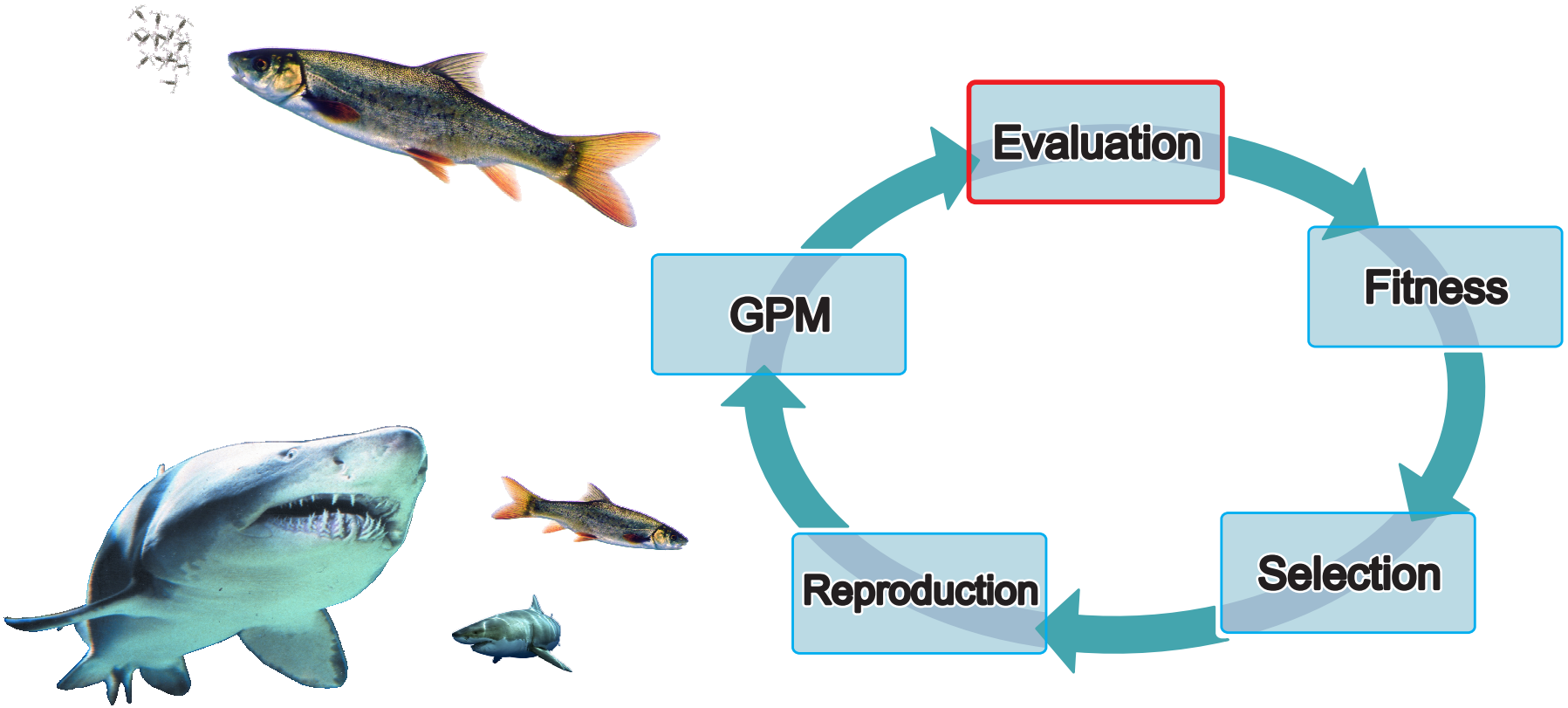






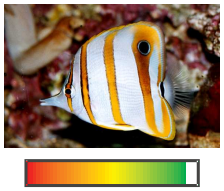
Evolution: Evaluation

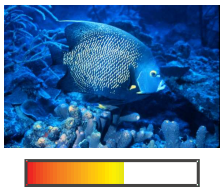
- Test the features of each individual

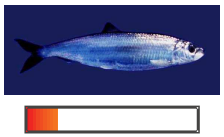


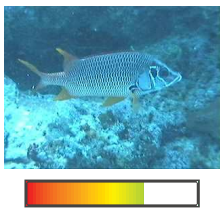
Evolution: Fitness

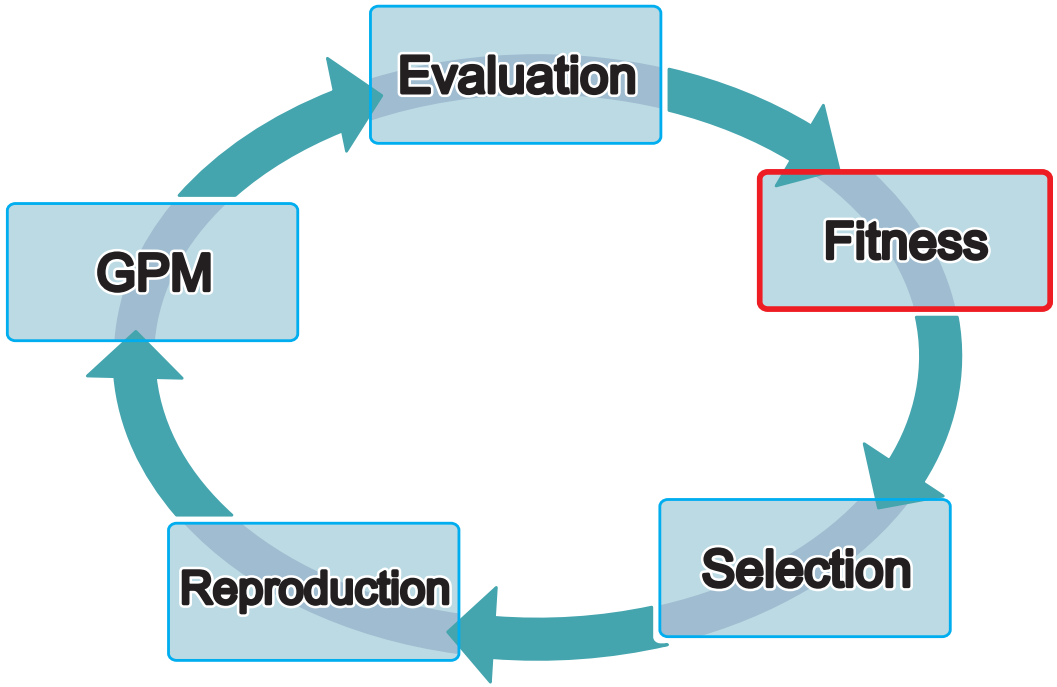
- Fitness is relative, determined/defined as number of offspring





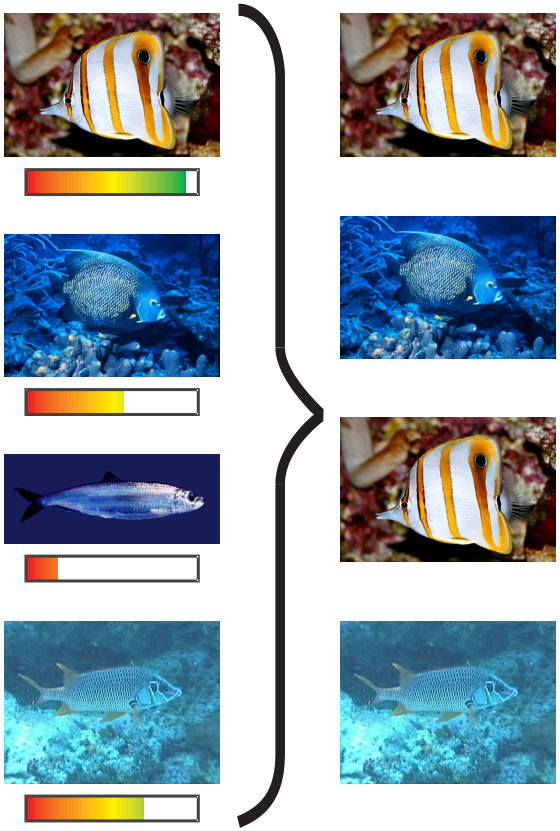


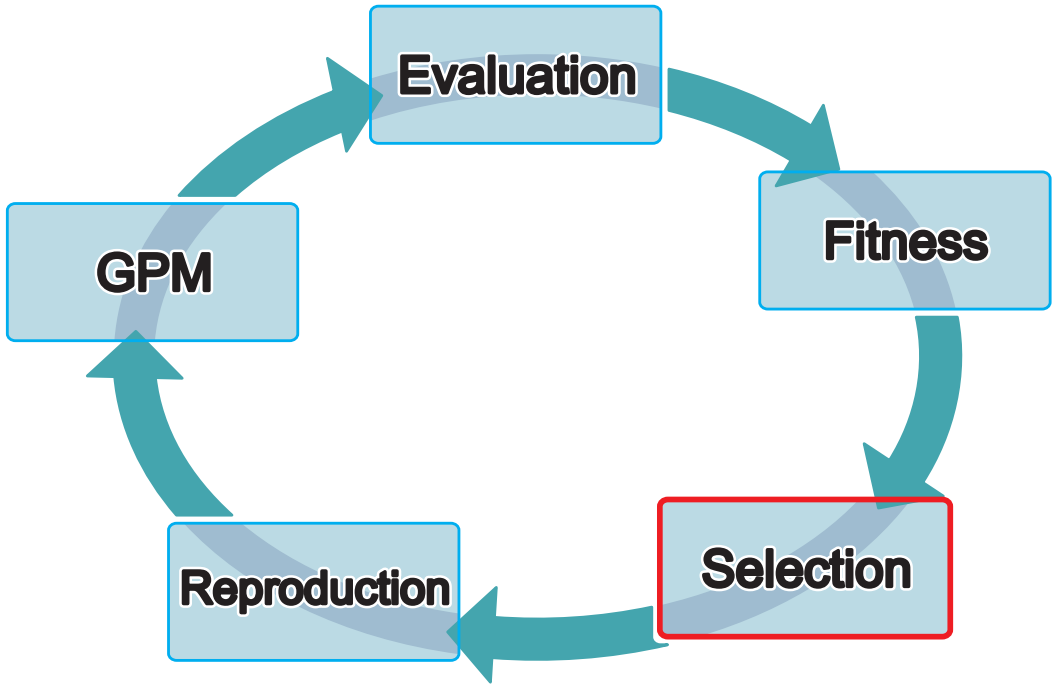




Evolution: Selection

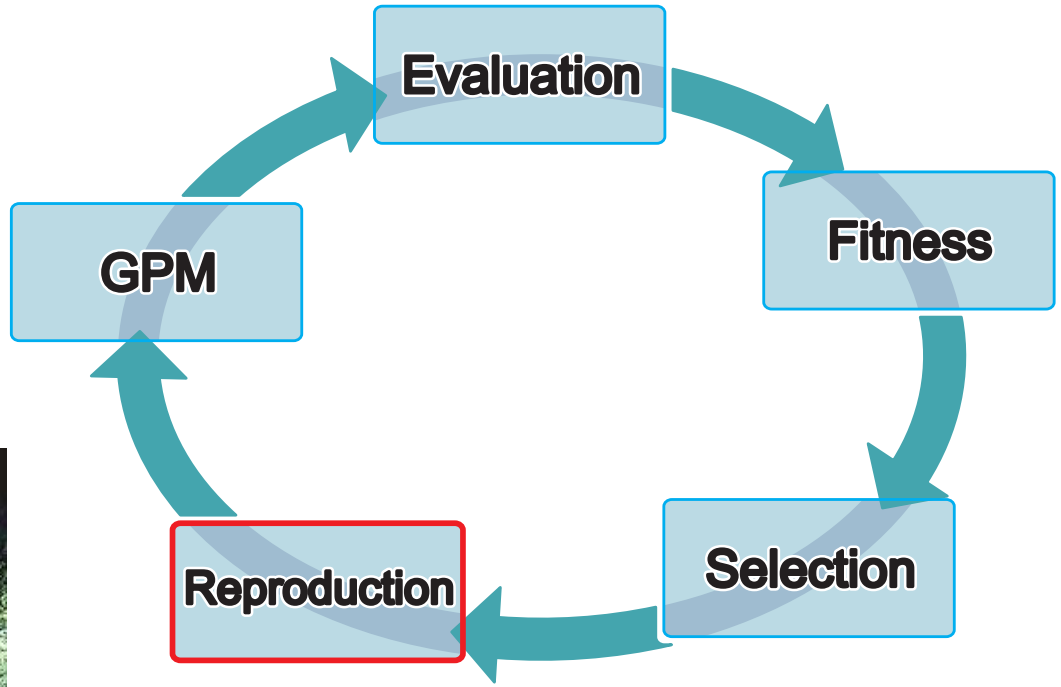
- Fitter individuals usually survive selection, have more offspring





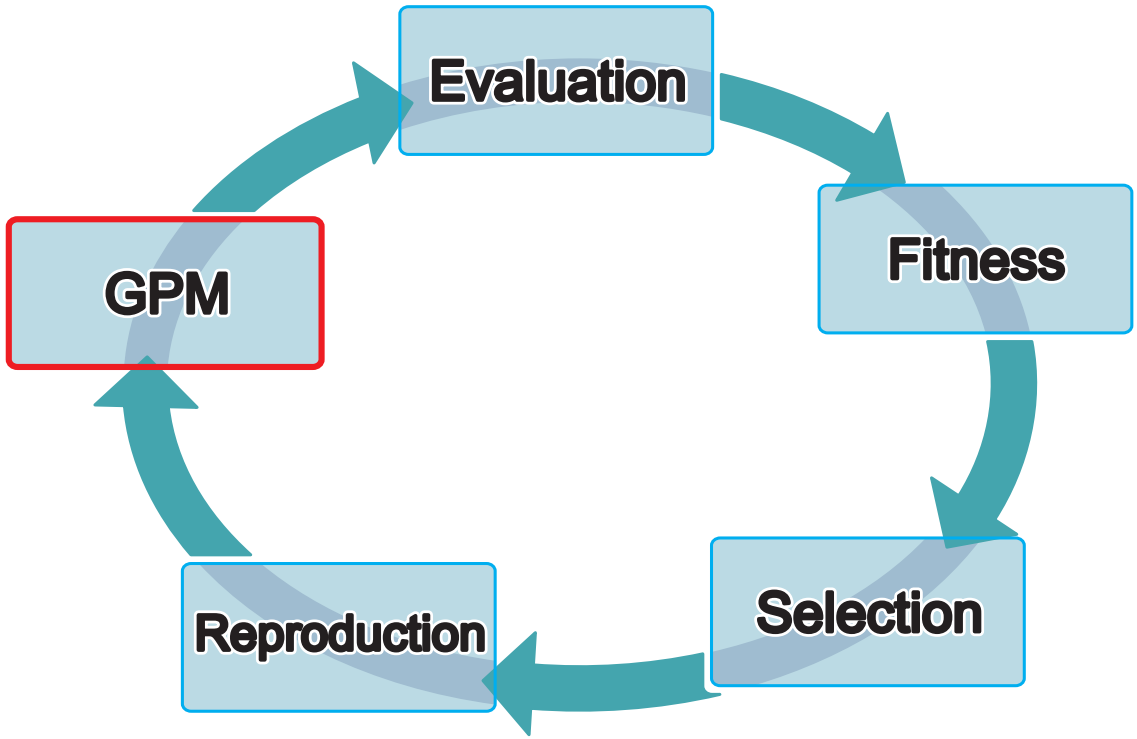
Evolution: Reproduction

- Asexual and sexual reproduction



Evolution: Next Generation

- Cycle starts again with the next "generation"



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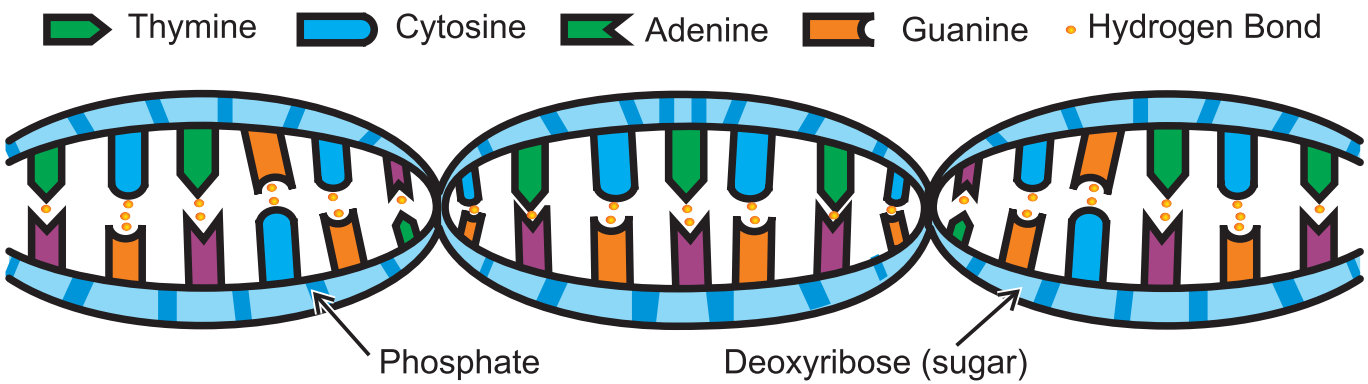
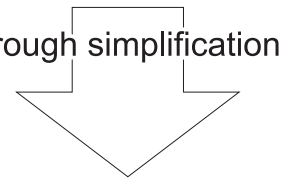
- In the late 1960s/early 1970s, Holland [14–17] formalizes Genetic Algorithms
- De Jong [18] uses them for function optimization

- Idea: Try to emulate the natural process of evolution on a very simple search space $\mathbb{G}$: the bit strings of length n, i.e., $\{\texttt{false}, \texttt{true}\}^n$



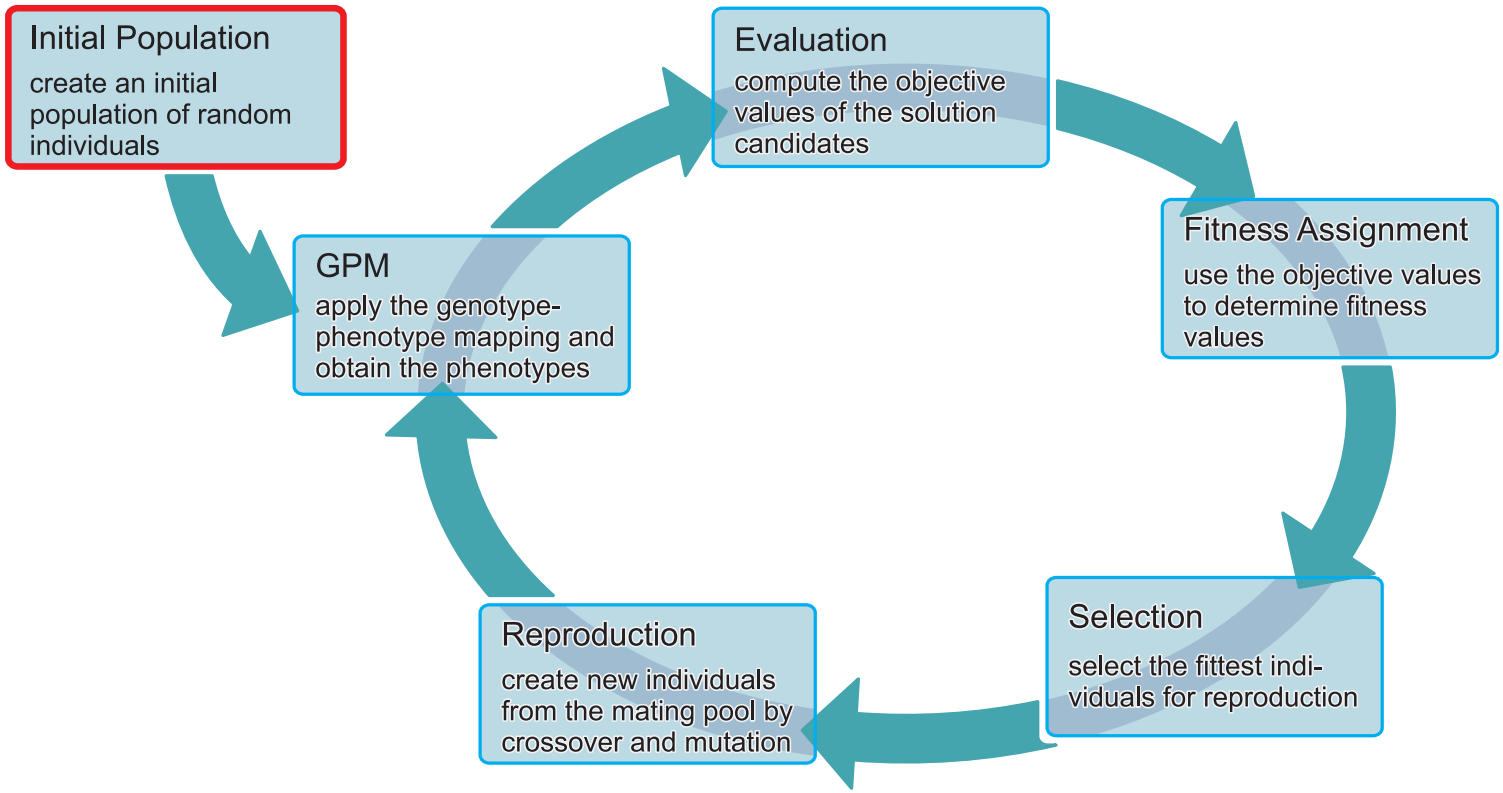


$g \in \mathbb{G}$ | 1 | 0 | 1 | 0 | 0 | 1 | 1 | 0 | 0 | 1 | 1 | 1 | 0 | 1 | 0 | 0 | 0 | 1 |

Search Space $\mathbb{G}$: all bit strings of a given length
Genotypes g: specific bit strings

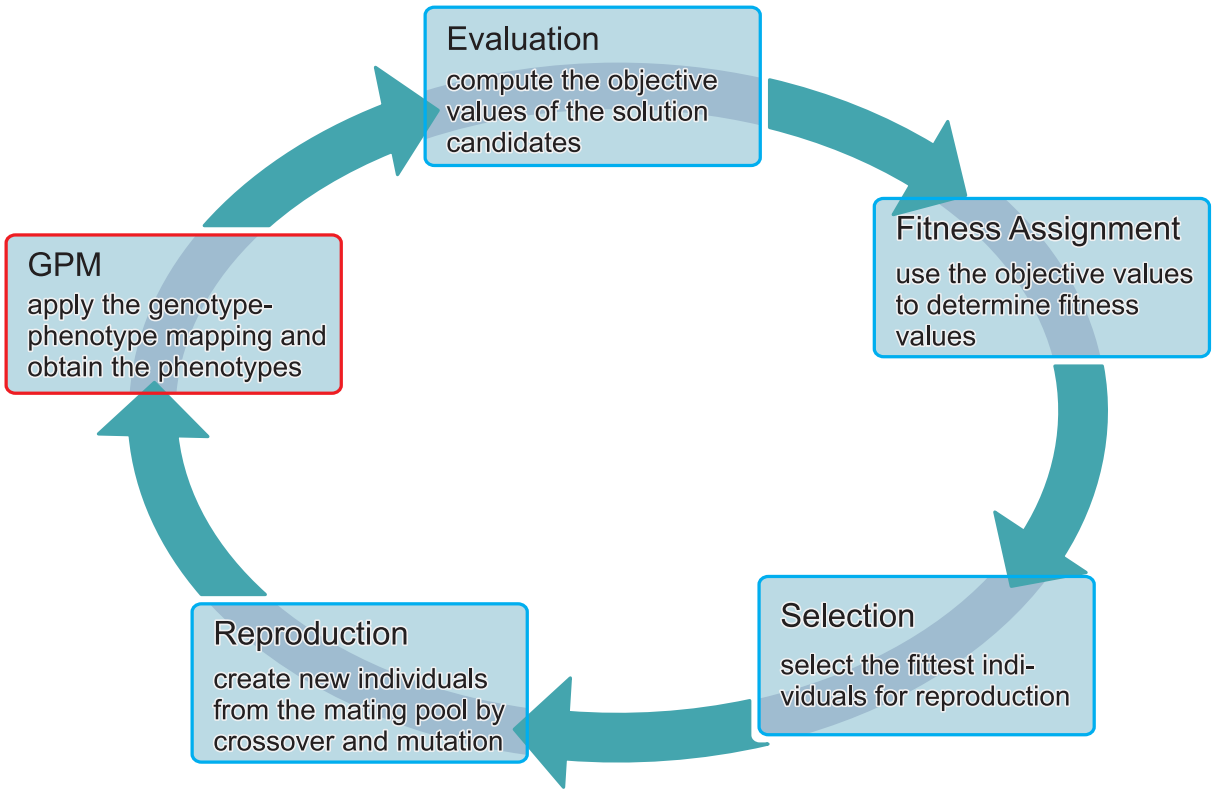
Genetic Algorithms: First Generation

- Each genotype is a bit string of length n
- Nullary search operation to create initial individuals: create a population of random bit strings



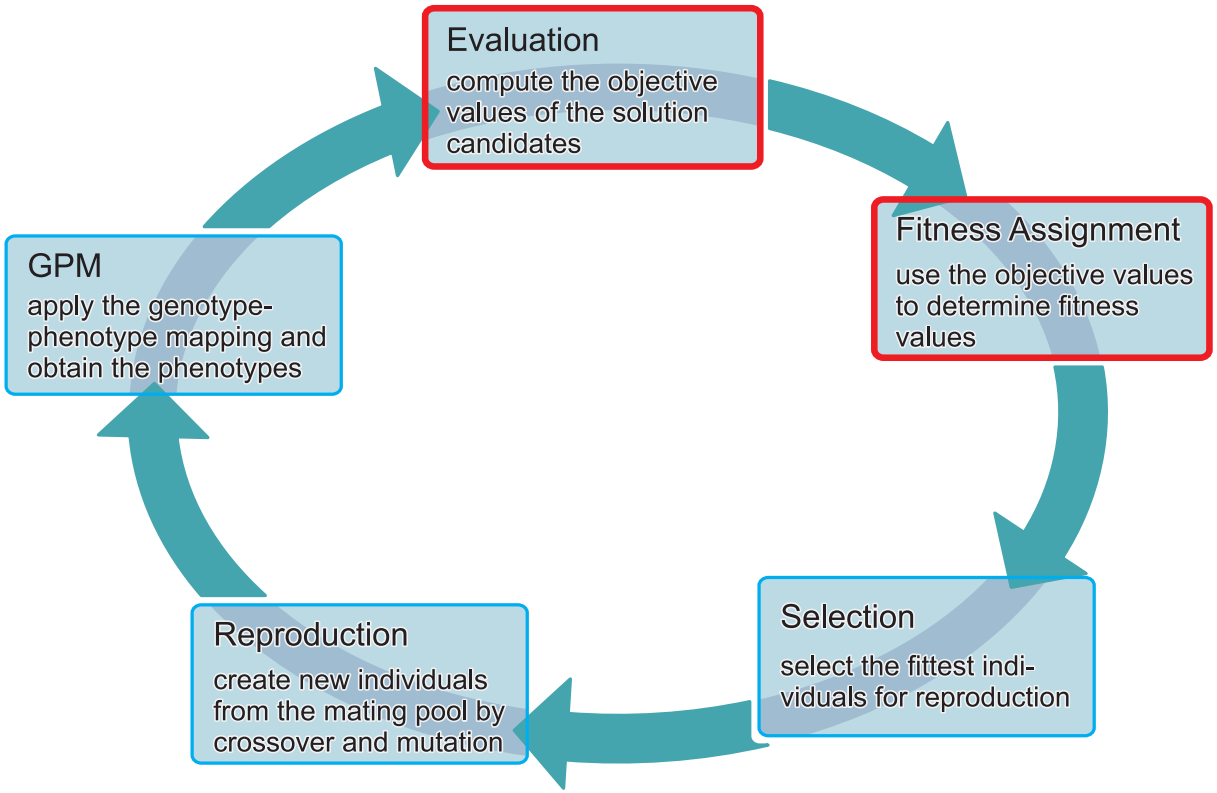
Genetic Algorithms: GPM

- Map the genotypes to phenotypes
- The GPM is usually problem-dependent



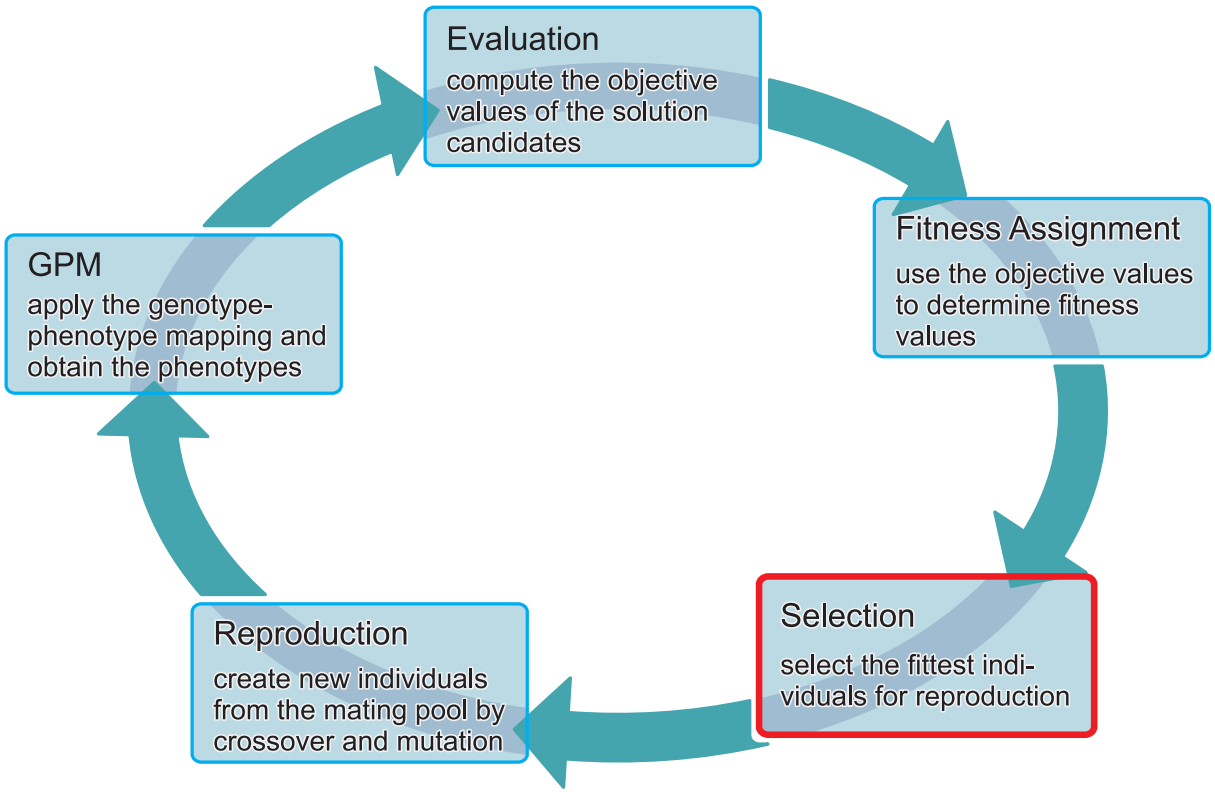
Genetic Algorithms: Evaluation

- Evaluate the objective function(s)
- In the original GA, fitness = objective values. In Multi-Objective Evolutionary Algorithms, this is not the case

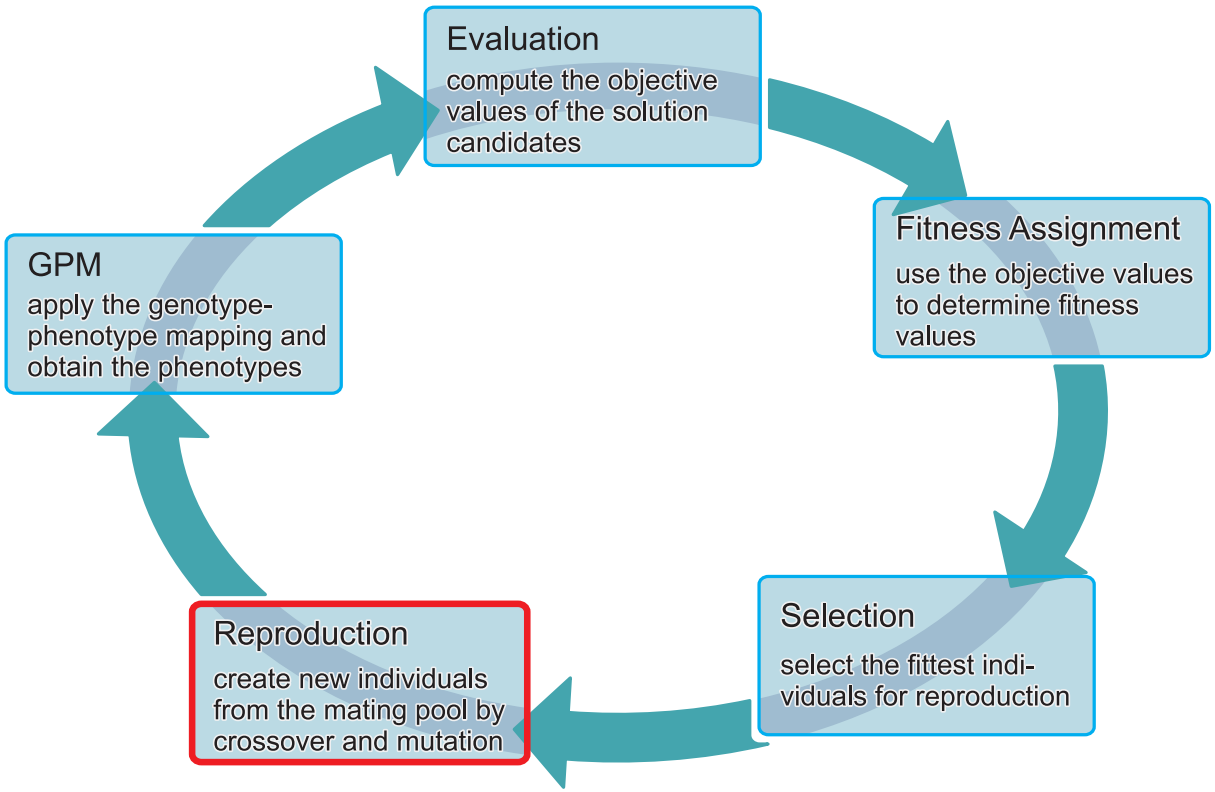


Genetic Algorithms: Selection

- Select the best individuals with highest probability
- Many different selection algorithms exist: Roulette-Wheel Selection, Tournament Selection, etc.

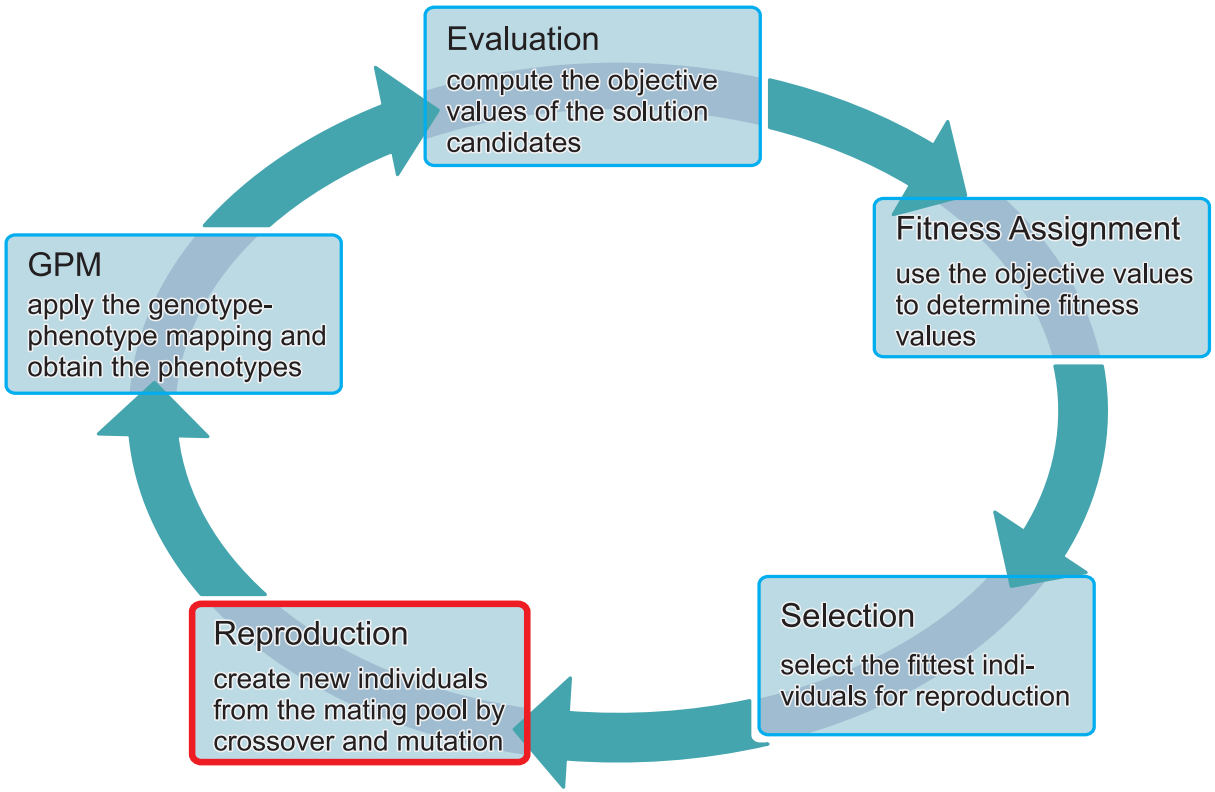


- Recombine genotypes: two genotypes are combined to create a new one (binary search operation); crossover rate cr
- Building Block Hypothesis: Good genes will aggregate [16, 19, 20]



Genetic Algorithms: Mutation

- Perform mutation (unary search operation) with probability mr
- Slight perturbations to increase diversity in population



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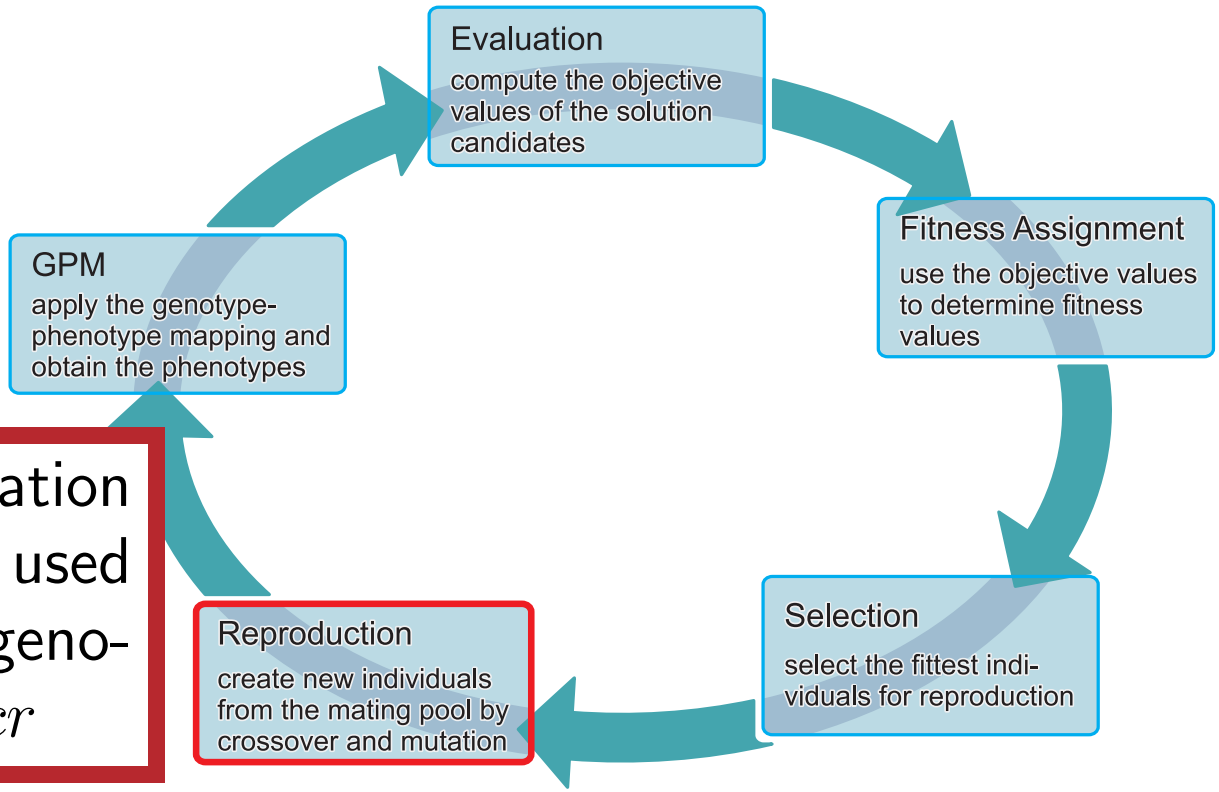
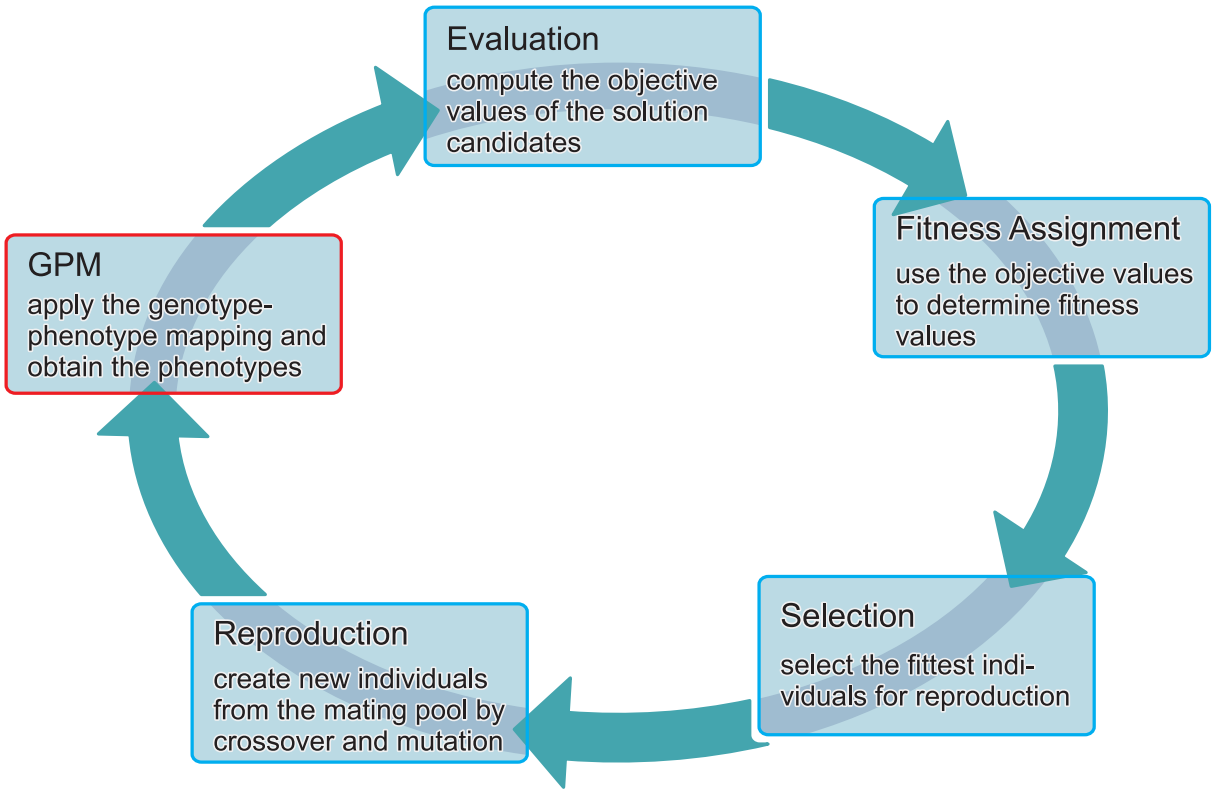


Often either mutation or crossover is used to create a new genotype: $1 = mr + cr$

Genetic Algorithms: New Generation

- Start with new population in next generation.



Genetic Algorithms: Putting it Together

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6. Check the termination criterion (usually done after every objective function evaluation)

Listing: A simple Evolutionary Algorithm

```
public class EA<G, X> extends OptimizationAlgorithm<G, X> {
  public ISelectionAlgorithm selection;
  public int ps;
  public int mps;
  public double cr;
  public IBinarySearchOperation<G> binary;
  public EA() {
    super();
    this.cr = 0.3d;
    this.ps = 128;
    this.mps = 64;
    this.selection = TruncationSelection.INSTANCE;
  }
  public Individual<G, X> solve(final IObjectiveFunction<X> f) {
    Individual<G, X> pbest, pcur;
    Individual<G, X>[] pop, mate;
    int i;

    pbest = new Individual<>();
    pop = new Individual[this.ps];
    mate = new Individual[this.mps];

    for (i = pop.length; (--i) >= 0;) {
      pop[i] = pcur = new Individual<>();
      pcur.g = this.nullary.create(this.random);
    }

    for (;;) {
      for (i = pop.length; (--i) >= 0;) {
        pcur = pop[i];
        pcur.x = this.gpm.gpm(pcur.g);
        pcur.v = f.compute(pcur.x);
        if (pcur.v < pbest.v) {
          pbest.assign(pcur);
        }
        if (this.termination.shouldTerminate()) {
          return pbest;
        }
      }

      this.selection.select(pop, mate, this.random);

      for (i = pop.length; (--i) >= 0;) {
        pop[i] = pcur = new Individual<>();
        if (this.random.nextDouble() < this.cr) {
          pcur.g = this.binary.recombine(mate[i % mate.length].g,
              mate[this.random.nextInt(mate.length)].g, this.random);
        } else {
          pcur.g = this.unary.mutate(mate[i % mate.length].g, this.random);
        }
      }
    }
  }
}
```

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- Two common, basic approaches to choose mps, independent from how selection is done:
  1. $ps > mps$: only a few individuals are selected and these have multiple offspring
  2. $ps = mps$: each selected individual has one offspring, an individual can be selected multiple times

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- In the most simple, single-objective case (only one objective function, i.e., what we did so far):

$$\nu(p) = f(p.x) \quad \forall \text{individuals} \tag{1}$$

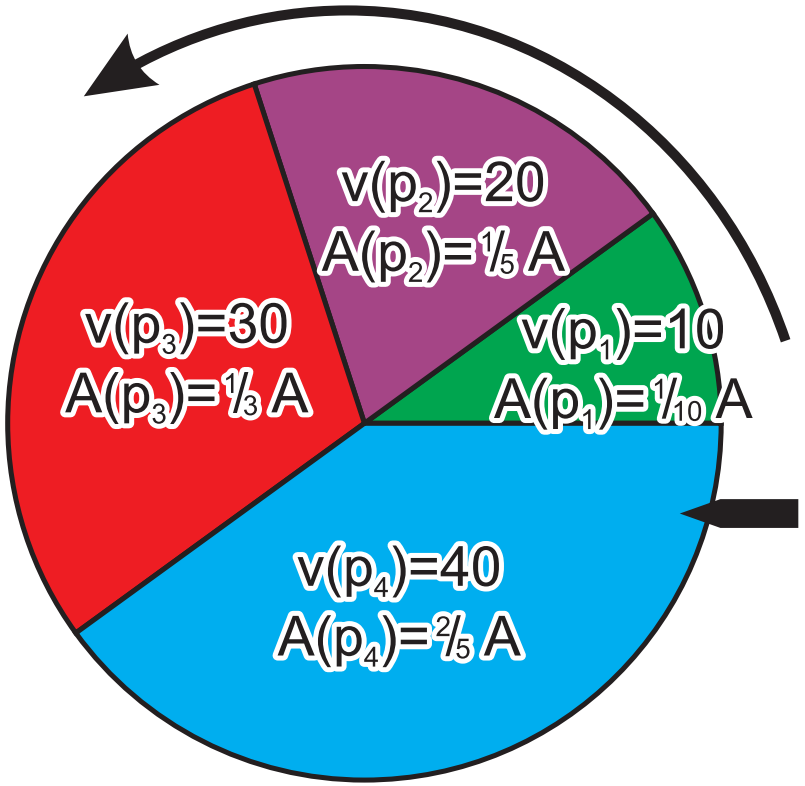
Listing: The Selection Algorithm: Programmer's Perspective

```
package metaheuristicOptimization.algorithms.ea;

import java.util.Random;

import metaheuristicOptimization.Individual;

/** the interface for selection algorithms */
public interface ISelectionAlgorithm {
  /**
   * Fill the mating pool with selected individuals from the population
   *
   * @param pop
   *          the population of the current individuals
   * @param mate
   *          the mating pool to be filled with individuals
   * @param r
   *          the random number generator
   */
  public abstract void select(final Individual<?, ?>[] pop, final
      Individual<?, ?>[] mate,
      final Random r);
}
```

Traditional: Roulette-Wheel Selection

- Traditional method: *Roulette-Wheel Selection* – Number of offspring is proportional to fitness (fitness is maximized!) [16, 18, 21–25]

$$P(\text{select}(p)) = \frac{f(p.x)}{\sum_{\forall p' \in \text{pop}} f(p'.x)} \quad (2)$$



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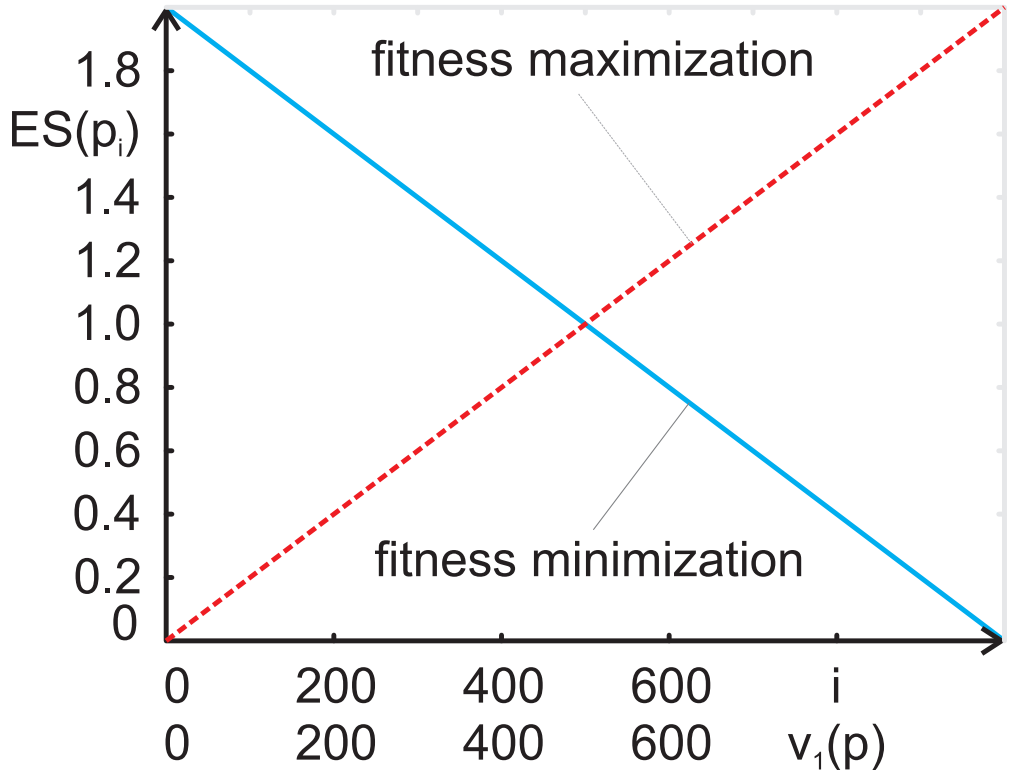

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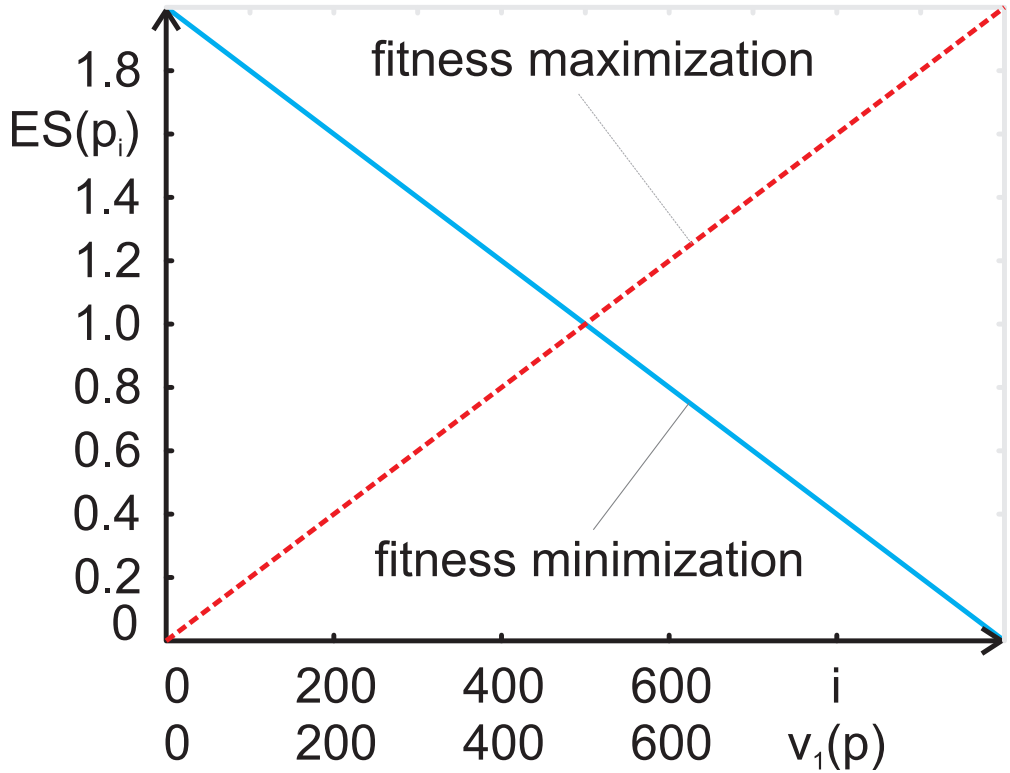

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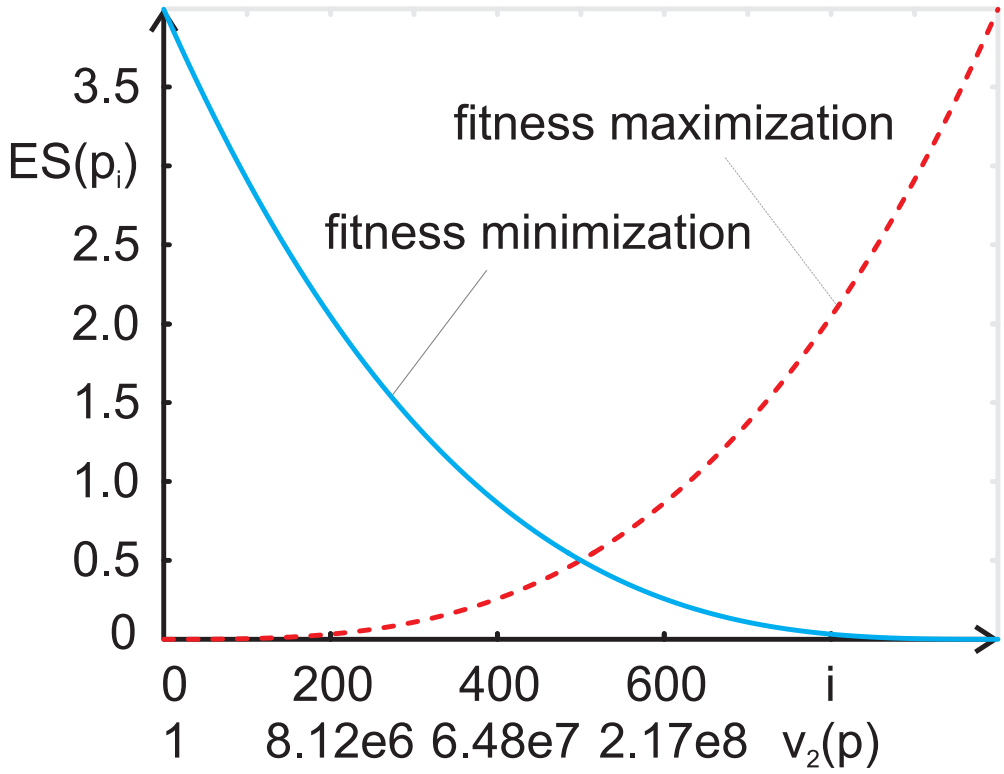

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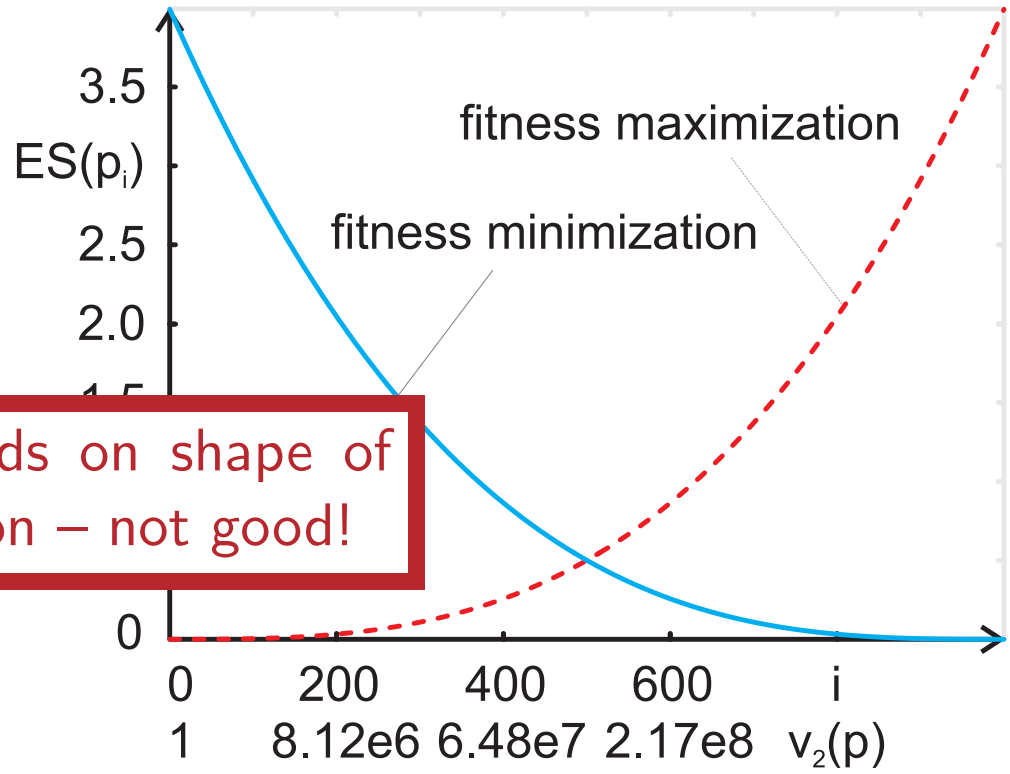

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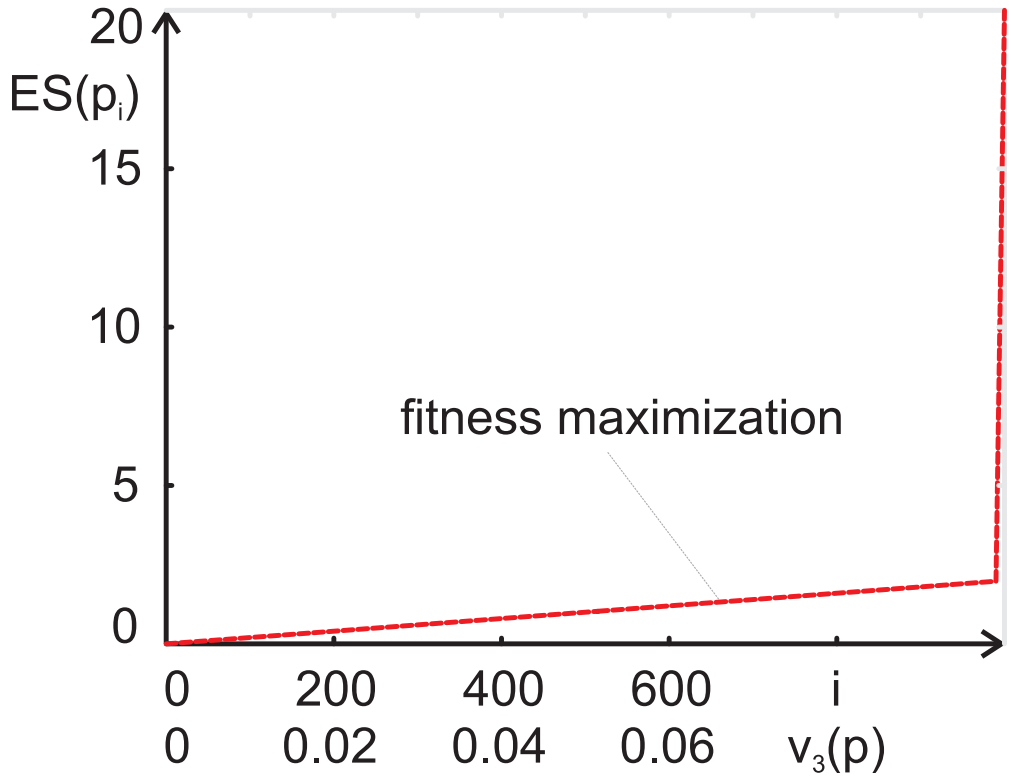

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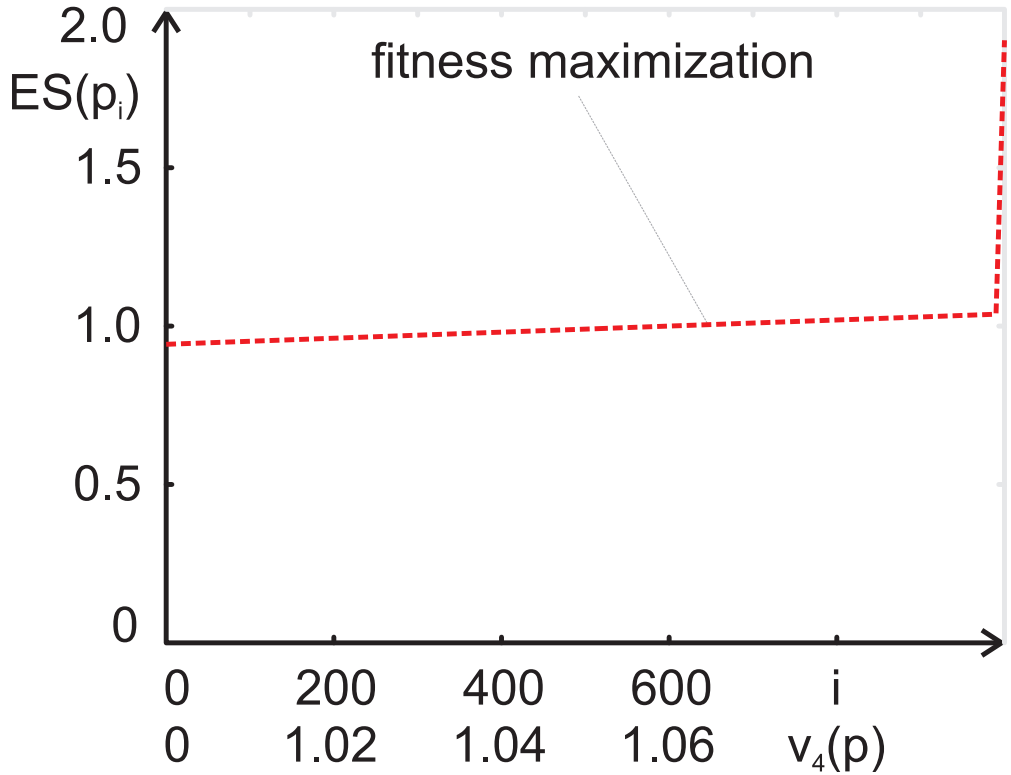

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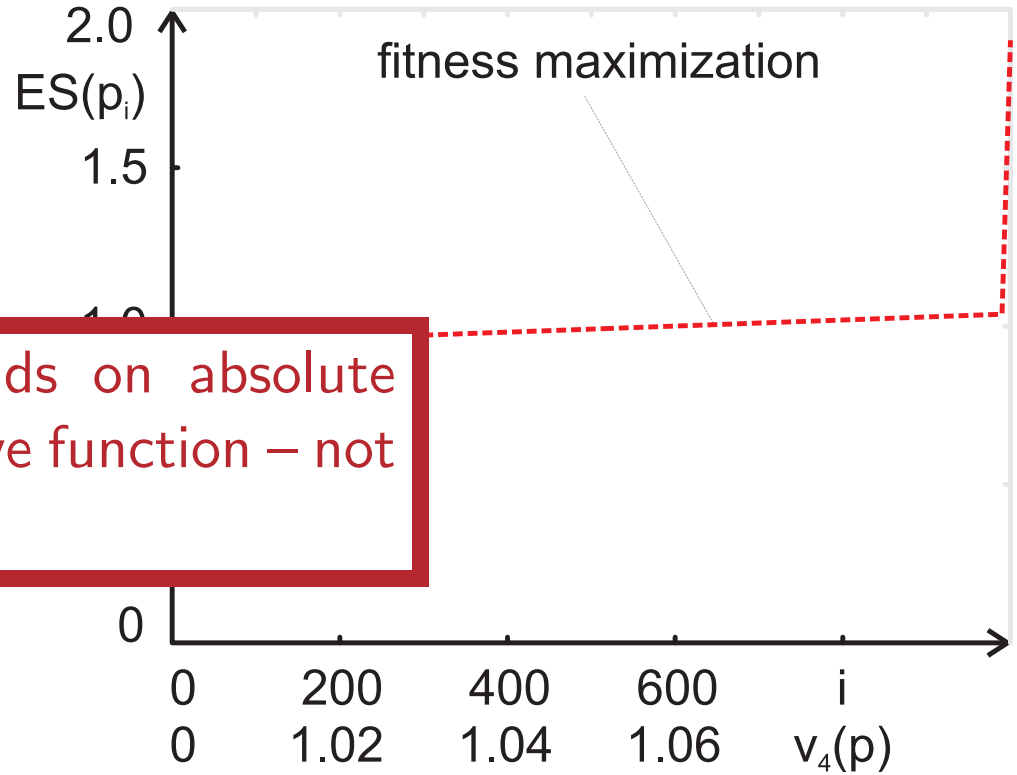

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- An optimization algorithm should work good regardless whether we add an offset to an objective function or use the squared functions...
- ...but Roulette-Wheel Selection gives different results in these cases!
- Avoid to use this directly
- Good only if fitness "*fits*" to this method, as e.g., in Pareto ranking [19, 26, 27]

matePool $\longleftarrow$ rouletteWheelSelection(pop)mps

Input: pop: the list of individuals to select from
Input: [implicit] ps: the population size
Input: mps: the number of individuals to be placed into the mating pool matePool
Output: matePool: the mating pool

begin
- $A \longleftarrow$ create empty list
- $max \longleftarrow -\infty$
- `// Initialize fitness array and find extreme fitnesses`
- **for** $i \longleftarrow 0$ **up to** $ps - 1$ **do**
  - $a \longleftarrow \text{pop}[i].y$
  - $A[i] \longleftarrow a$
  - **if** $a > max$ **then** $max \longleftarrow a$
- $sum \longleftarrow 0$
- **for** $i \longleftarrow 0$ **up to** $ps - 1$ **do**
  - $sum \longleftarrow sum + (max - A[i])$
  - $A[i] \longleftarrow sum$
- **for** $i \longleftarrow 0$ **up to** $mps - 1$ **do**
  - $a \longleftarrow$ {randomly from $[0, sum]$}
  - append $\text{pop}[\max\{i : A[i] \leq a\}]$ to matePool
- **return** $matePool$

Listing: The Roulette-Wheel Selection Algorithm

```
public class RouletteWheelSelection implements ISelectionAlgorithm {
  public void select(final Individual<?, ?>[] pop, final Individual<?, ?>[] mate, final Random r) {
    double[] t;
    double max, last;
    int i, j;

    t = this.temp;
    if ((t == null) || (t.length < pop.length)) {
      this.temp = t = new double[pop.length];
    }

    max = Double.NEGATIVE_INFINITY;
    for (Individual<?, ?> indi : pop) {
      max = Math.max(indi.v, max);
    }

    max = Math.nextUp(max);
    last = 0d;
    for (i = 0; i < t.length; i++) {
      last += (max - pop[i].v);
      t[i] = last;
    }
    t[t.length - 1] = Double.POSITIVE_INFINITY;

    for (i = 0; i < mate.length; i++) {
      j = Arrays.binarySearch(t, last * r.nextDouble());
      if (j < 0) {
        j = ((-j) - 1);
      }
      mate[i] = pop[j];
    }
  }
}
```

Tournament Selection

- *Tournament Selection*: k individuals compete to produce 1 offspring, the best wins!

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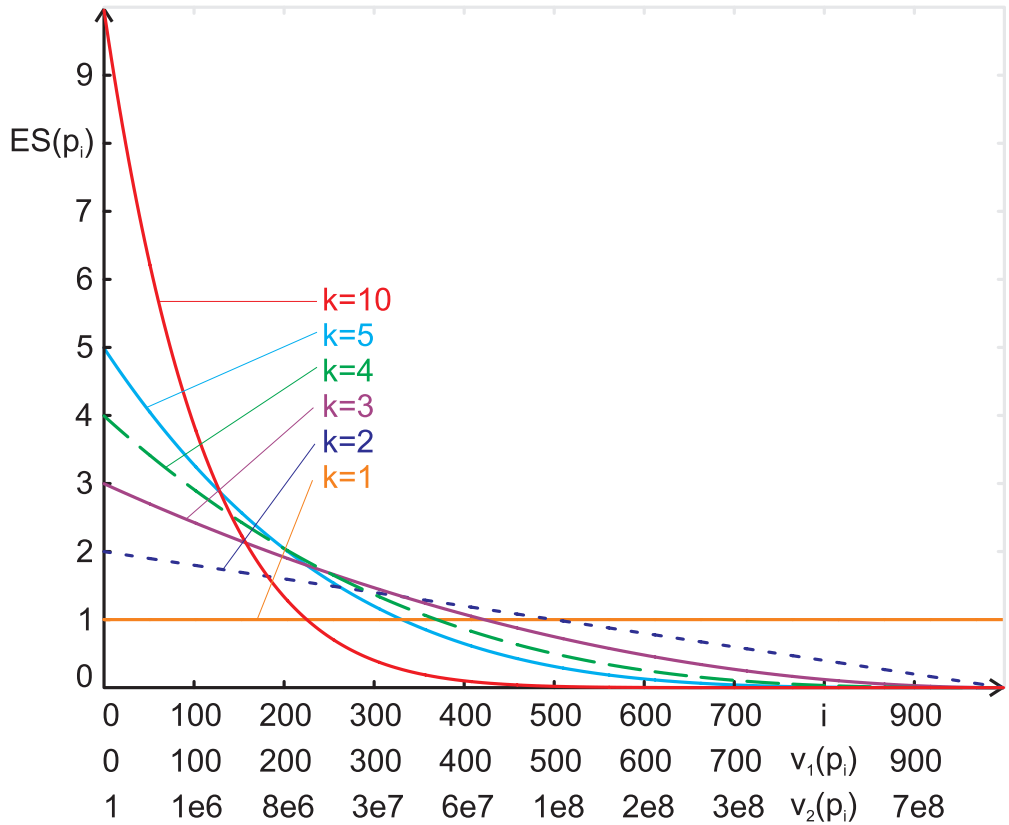

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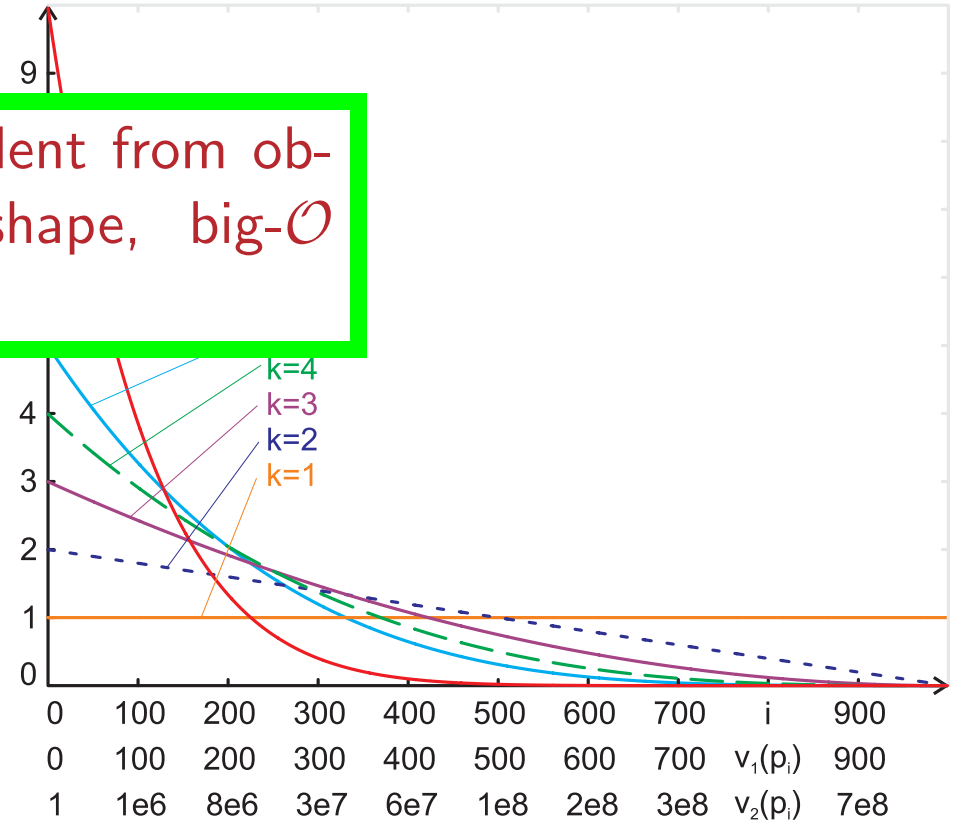
Selection independent from objective function shape, big-$\mathcal{O}$ class, or offset



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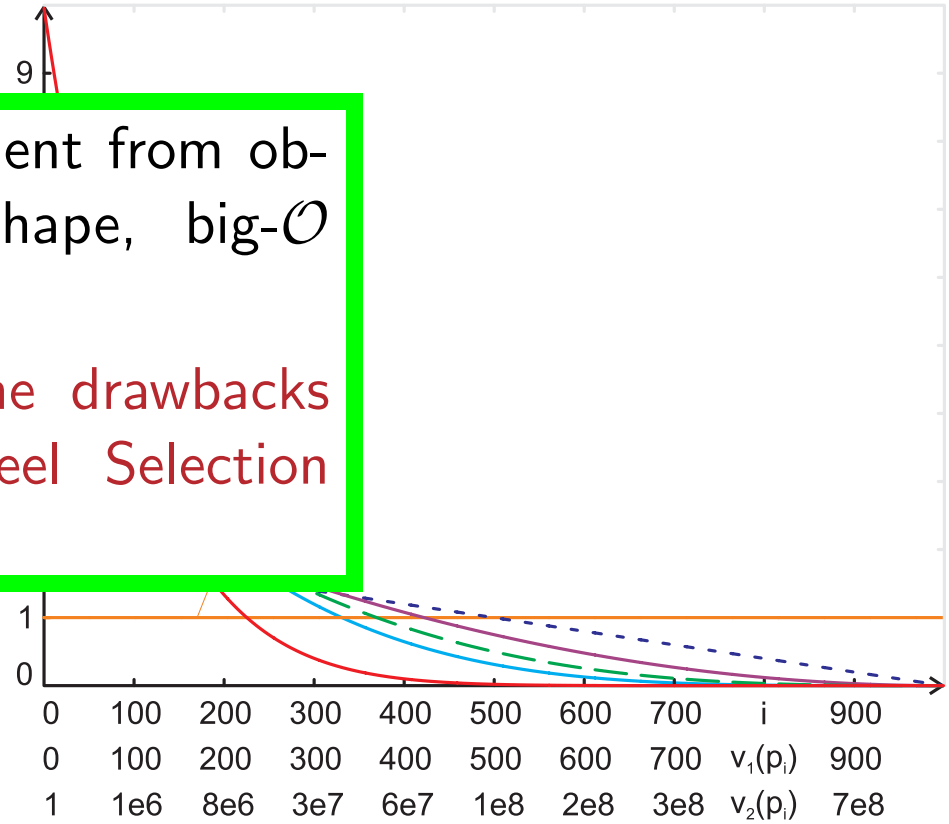

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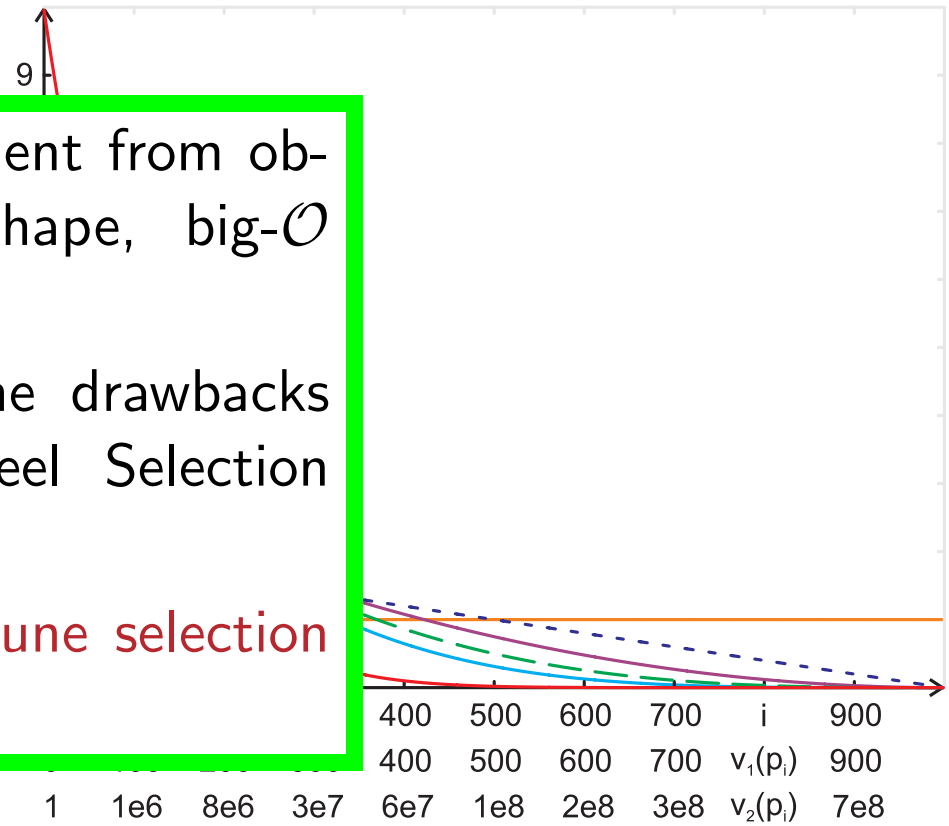
Plus we can fine-tune selection pressure via k



matePool ⟵ tournamentSelection(k, pop, mps)

Input: pop: the list of individuals to select from
Input: [implicit] ps: the population size
Input: mps: the number of individuals to be placed into the mating pool matePool
Input: [implicit] k: the tournament size
Output: matePool: the winners of the tournaments which now form the mating pool

begin
- matePool ⟵ create empty list
- **for** $i \longleftarrow 1$ **up to** mps **do**
  - $a \longleftarrow$ {randomly from $0..sum-1$}
  - **for** $j \longleftarrow 1$ **up to** $k-1$ **do**
    - $b \longleftarrow$ {randomly from $0..sum-1$}
    - **if** $pop[b].y < pop[a].y$ **then** $a \longleftarrow b$
  - append pop[a] to matePool
- **return** *matePool*

Listing: The Tournament Selection Algorithm

```
public class TournamentSelection implements ISelectionAlgorithm {
  public void select(final Individual<?, ?>[] pop, final Individual<?, ?>[]
      mate, final Random r) {
    int i, j;
    Individual<?, ?> x, y;

    for (i = 0; i < mate.length; i++) {
      x = pop[r.nextInt(pop.length)];
      for (j = 1; j < this.k; j++) {
        y = pop[r.nextInt(pop.length)];
        if (y.v < x.v) {
          x = y;
        }
      }
      mate[i] = x;
    }
  }
}
```

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- Also used in Evolution Strategies [35–41] (see Lesson 12: *Evolution Strategies*)
- Lässig et al. [42, 43] show that this selection strategy is optimal!
- However, the right mating pool size mps is not known...

Truncation Selection

matePool $\longleftarrow$ truncationSelection(μ, pop)

Input: pop: the list of individuals to select from (length λ or $\mu + \lambda$)
Input: μ: the number of individuals to be placed into the mating pool matePool
Output: matePool: the survivors of the truncation which now form the mating pool

begin
    sort the pop according to fitness (best first)
    return first μ individuals from pop

Truncation Selection

Listing: The Truncation Selection Algorithm

```
public class TruncationSelection implements ISelectionAlgorithm {
  public void select(final Individual<?, ?>[] pop, final Individual<?, ?>[]
      mate, final Random r) {
    Arrays.sort(pop);
    System.arraycopy(pop, 0, mate, 0, mate.length);
  }
}
```

Population Treatment

- Three different ways of population treatment

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  3. Elitism: Either steady-state OR generationals PLUS the best solutions survive always

Section Outline

Crossover

- Genetic Algorithms: crossover is a binary search operation

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- Idea:
  - two individuals have been selected (as parents)

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- Goal:
  - Combine these different (good) features...
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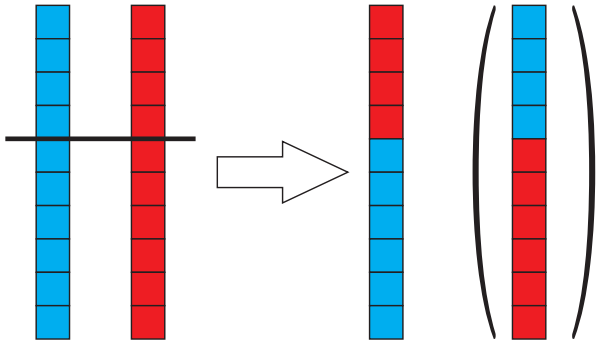
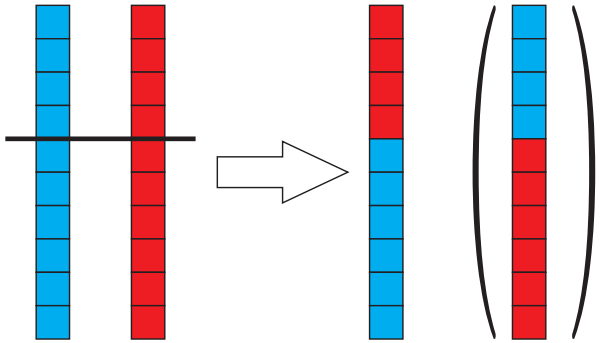
- There exist different crossover operators
- Building Block Hypothesis: Good genes/features will aggregate [16, 19, 20]

Crossover: SPX



Single-Point (SPX)

Crossover: TPX



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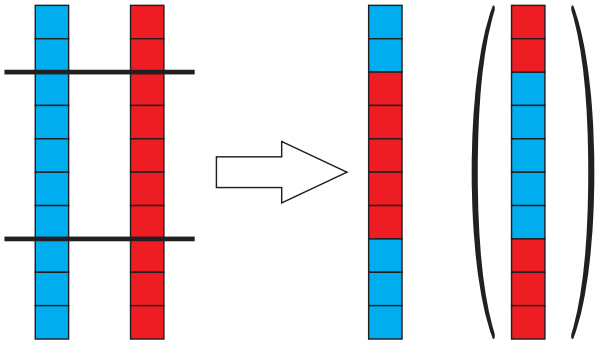
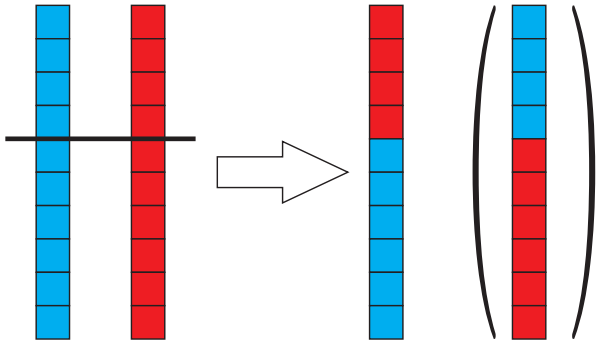


Two-Point (TPX)

Crossover: MPX



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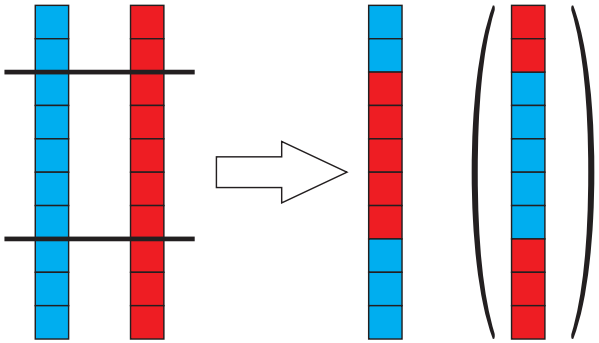

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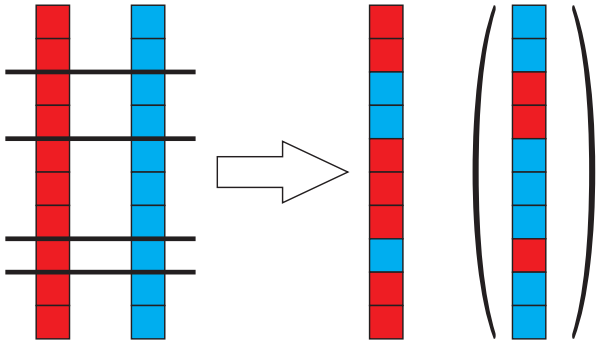
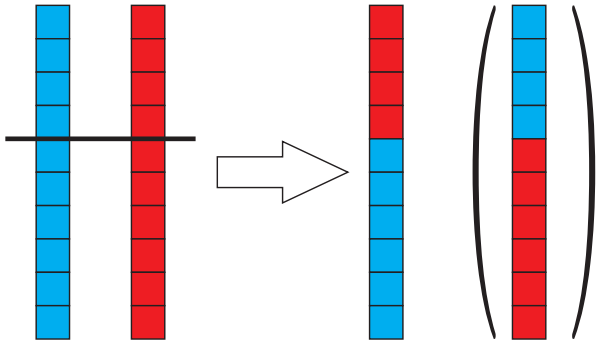


Multi-Point (MPX)



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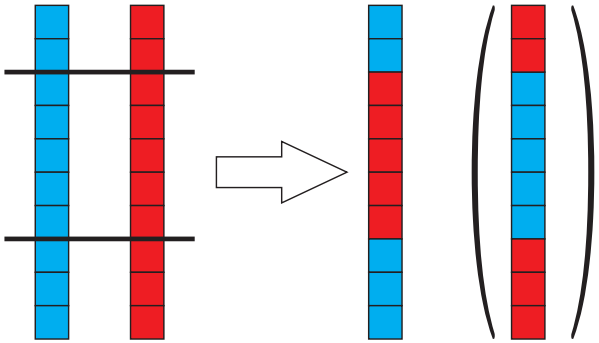

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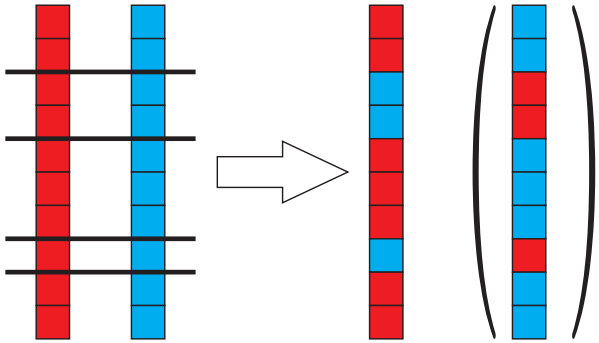

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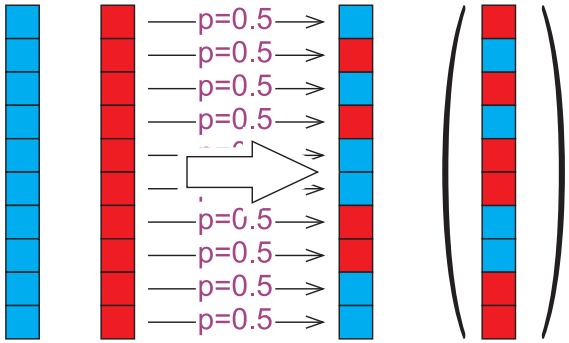

Uniform (UX)

Single-Point Crossover

Listing: Single-Point Crossover

```
public class BitsBinarySPX implements IBinarySearchOperation<boolean[]> {
  public boolean[] recombine(final boolean[] p1, final boolean[] p2, final
      Random r) {
    final boolean[] g;
    final int x;

    g = new boolean[p1.length]; // create empty bit string
    x = (1 + r.nextInt(g.length - 1)); // select crossover point
    System.arraycopy(p1, 0, g, 0, x); // copy from first parent
    System.arraycopy(p2, x, g, x, g.length - x);// copy from second parent

    return g; // return new bit string
  }
}
```

Crossover: MPX

$g \longleftarrow \text{recombinationMPX}(g_{p1}, g_{p2}, k)$

begin
- // find k crossover points from 0 to $n-1$
- $CP \longleftarrow$ new empty list
- **for** $i \longleftarrow 1$ **up to** k **do**
  - **repeat**
    - $cp \longleftarrow \{\text{randomly from } 0..n-1\} + 1$
  - **until** $cp \notin CP$
  - append cp to CP
- sort the list CP
- // perform the crossover by copying sub-strings
- $g \longleftarrow$ empty list
- $s \longleftarrow 0$
- $b \longleftarrow$ true
- $g_u \longleftarrow g_{p1}$
- **for** $i \longleftarrow 0$ **up to** k **do**
  - $e \longleftarrow CP[i]$
  - **if** b **then** $g_u \longleftarrow g_{p1}$
  - **else** $g_u \longleftarrow g_{p2}$
  - append sub-range $s..e-1$ of g_u to g
  - $b \longleftarrow \neg b$
  - $s \longleftarrow e$
- **return** g

Crossover: Uniform Crossover (UX)

$g \longleftarrow \text{recombinationUXX}(g_{p1}, g_{p2}, k)$

Input: $g_{p1}, g_{p2} \in \mathbb{G}$: the parental genotypes (n bits)
Data: i: a counter variable
Output: $g \in \mathbb{G}$: a new genotype (n bits)

begin
  $g \longleftarrow g_{p1}$
  for $i \longleftarrow 0$ **up to** $n-1$ **do**
    if $\{$randomly from $[0,1]\} < 0.5$ **then** $g[i] \longleftarrow g_{p2}[i]$
  return g

Uniform Crossover

Listing: Uniform Crossover

```
public class BitsBinaryUX implements IBinarySearchOperation<boolean[]> {
  public boolean[] recombine(final boolean[] p1, final boolean[] p2, final
      Random r) {
    final boolean[] g;

    g = p1.clone(); // copy first parent string
    for (int i = g.length; (--i) >= 0;) { // for all bits...
      if (r.nextBoolean()) {
        g[i] = p2[i];
      } // take value from p2 with probability 0.5
    }

    return g; // return new bit string
  }
}
```

Section Outline

Mutation

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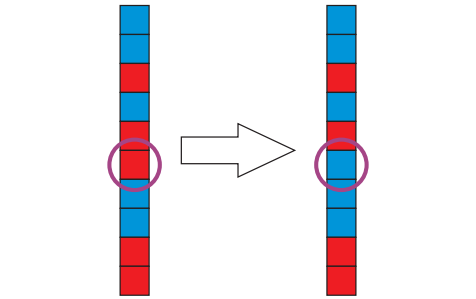
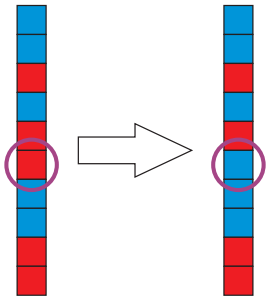
  - no now genetic material is created
  - crossover and selection alone may step by step make the population converge to one single genotype
- Mutation: introduce some randomnes (in from of new genetic material) into the population
- But: not too much, systems with too much and too powerful mutation cannot converge or exploit local optima sufficiently

Mutation: Single Bit

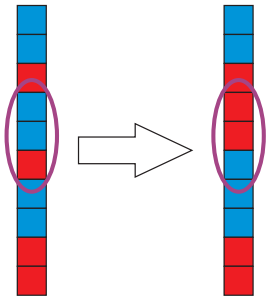


Single Bit Flip Mutation

Mutation: Multi Bit 1

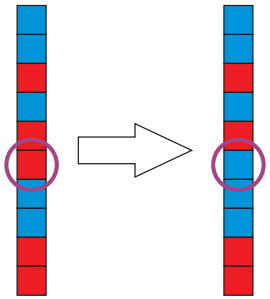


Single Bit Flip Mutation



Multi Bit Flip Mutation
(consecutive)

Mutation: Multi Bit 2



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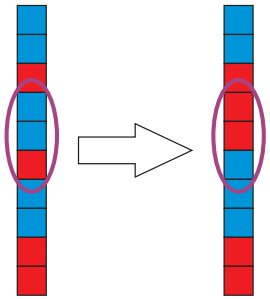

Multi Bit Flip Mutation
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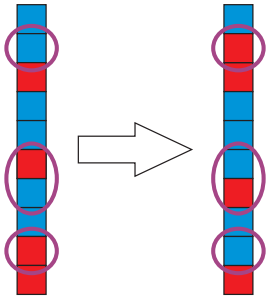
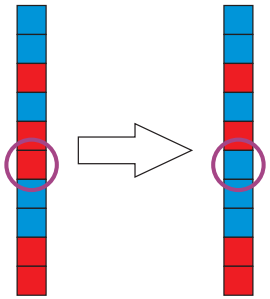


Multi Bit Flip Mutation
(random location)

Mutation: Complete



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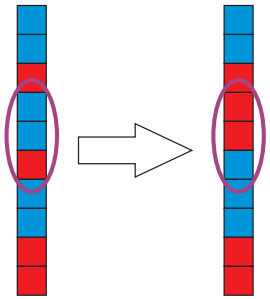

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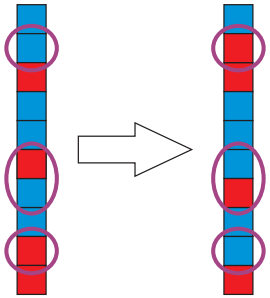

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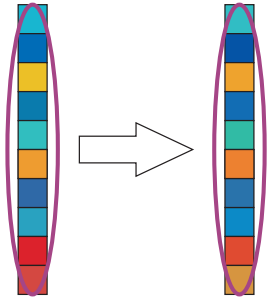

Complete Mutation
($\mathbb{G} \subseteq \mathbb{R}$)

Multi Bit Mutation

$g \longleftarrow \text{multiBitFlip}(g_p, \eta)$

Input: g_p: the parent individual
Output: g: the new random permutation of the numbers $0 \ldots n-1$

begin
  $g \longleftarrow g_p$
  repeat
    $i \longleftarrow \{\text{randomly from } 0..n-1\}$
    $g[i] \longleftarrow \neg g[i]$
  until $\{\text{randomly from } [0,1]\} < \eta$
  return g

Single-Bit Flip Mutation

Listing: The Single-Bit Flip Mutation

```
public class BitsUnarySingleFlip implements IUnarySearchOperation<boolean[]>
      {
  public boolean[] mutate(final boolean[] p, final Random r) {
    final boolean[] g;

    g = p.clone(); // copy parent string
    g[r.nextInt(g.length)] ^= true; // flip the bit
    return g; // return new bit string
  }
}
```

Multi-Bit Flip Mutation

Listing: The Multi-Bit Flip Mutation

```
public class BitsUnaryFlip implements IUnarySearchOperation<boolean[]> {
  public boolean[] mutate(final boolean[] p, final Random r) {
    final boolean[] g;

    g = p.clone();                          // copy parent string
    do {                                    // at least once, but maybe more often
      g[r.nextInt(g.length)] ^= true;       // flip the bit
    } while (r.nextBoolean());              // maybe repeat (small chance for
        large changes
    return g;                               // return new bit string
  }
}
```

Flip a Fraction of the Bits

Listing: Flip a Fraction of the Bits

```
public class BitsUnaryFractionFlip implements
    IUnarySearchOperation<boolean[]> {
  /** the fraction to flip */
  public final double frac;
  public boolean[] mutate(final boolean[] p, final Random r) {
    final boolean[] g;
    int f;

    g = p.clone(); // copy parent string
    f = Math.max(1, Math.min(p.length, ((int) (p.length * this.frac))));
    for (; (--f) >= 0;) {// go through the bits
      g[r.nextInt(p.length)] ^= true; // flip
    }

    return g; // return new bit string
  }
}
```

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  - these different good parts may be in different individuals
  - but may be combined later by crossover (Building Block Hypothesis, see later)

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- the Schema Theorem roughly estimates how such schemas multiply, depending on their average fitness
- It tries to answer the question: "How and why does a GA work?"

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- A Schema H is an equivalence class concerning the values at specific loci (i.e., values of genotypes according to a mask): $H(j) \in \{0,1,*\} \forall j \in 0 \ldots n-1,\ H(j) = * \forall j \notin m$

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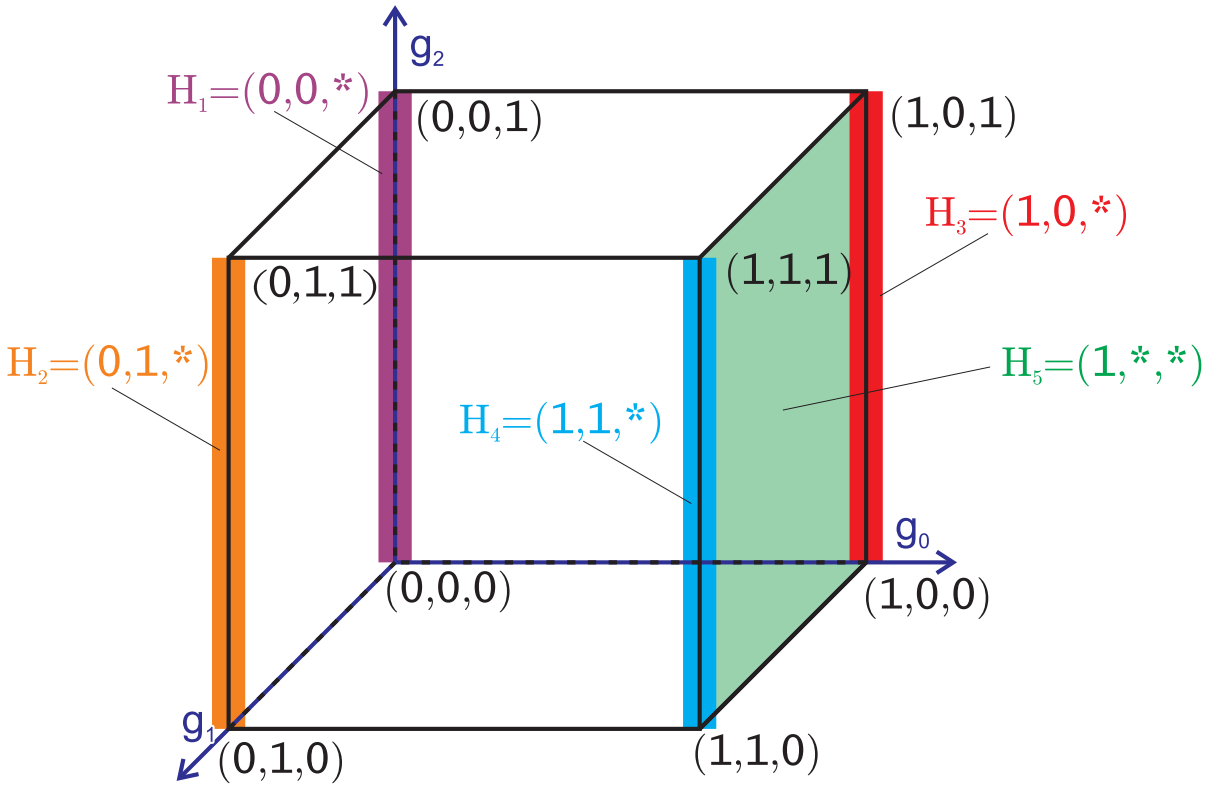

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$$P(\mathrm{select}(p)) = \frac{f(p.x)}{\sum_{\forall p' \in \mathrm{pop}} f(p'.x)} \tag{3}$$

- But we do not look at a single individual $p \in (\mathrm{pop} \cap H)$, we look at *all the individuals* in population pop that fit to schema H

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- The chance $P(\text{select}(H))$ that one of them is chosen into the slot is[1]:

$$P(\text{select}(H)) = \sum_{\forall p \in (\text{pop} \cap H)} \left[\frac{f(p.x)}{\sum_{\forall p' \in \text{pop}} f(p'.x)} \right] \tag{4}$$

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$$P(\mathrm{select}(H)) = \frac{1}{\sum_{\forall p' \in \mathrm{pop}} f(p'.x)} \sum_{\forall p \in (\mathrm{pop} \cap H)} f(p.x) \tag{4}$$

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Schema Theorem: Selection + Mean Fitness

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- Consider the *mean fitness* $\overline{f}(\text{pop})$ of all individuals in the population and the mean fitness $\overline{f}(\text{pop} \cap H)$ of all instances of H in the population[2]:

$$\overline{f}(\text{pop}) = \frac{1}{ps} \sum_{\forall p' \in \text{pop}} f(p'.x) \qquad \overline{f}(\text{pop} \cap H) = \frac{1}{|\text{pop} \cap H|} \sum_{\forall p \in (\text{pop} \cap H)} f(p.x) \tag{6}$$

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- Now we put this into the first equation:

$$P(\text{select}(H)) = \frac{|\text{pop} \cap H| * \overline{f}(\text{pop} \cap H)}{ps * \overline{f}(\text{pop})} \tag{7}$$

Schema Theorem: Expected Selections

- Under Roulette-Wheel Selection, the chance $P(\text{select}(H))$ to select an instance of schema H from the population pop_t (at generation t) for one slot in the mating pool is

$$P(\text{select}(H)) = \frac{|\text{pop}_t \cap H| * \overline{f}(\text{pop}_t \cap H)}{ps * \overline{f}(\text{pop}_t)} \tag{8}$$

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- Holland assumes that the size mps of the mating pool is the same as the size ps of the population, so this is applied ps times
- The expected number of offspring of the schema's instances, i.e., its expected occurences $E(|\text{matePool}_t \cap H|)$ in the mating pool, are:

$$E(|\text{matePool}_t \cap H|) = \frac{|\text{pop}_t \cap H| * \overline{f}(\text{pop}_t \cap H)}{\overline{f}(\text{pop}_t)} \tag{9}$$

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- If $\overline{f}(\text{pop}_t \cap H) > \overline{f}(\text{pop}_t)$, then $E(|\text{matePool}_t \cap H|) > |\text{pop}_t \cap H|$

Schema Theorem: Expected Selections

- Under Roulette-Wheel Selection, the chance $P(\text{select}(H))$ to select an instance of schema H from the population pop_t (at generation t) for one slot in the mating pool is

$$P(\text{select}(H)) = \frac{|\text{pop}_t \cap H| * \overline{f}(\text{pop}_t \cap H)}{ps * \overline{f}(\text{pop}_t)} \tag{8}$$

- The expected number of offspring of the schema's instances, i.e., its expected occurences $E(|\text{matePool}_t \cap H|)$ in the mating pool

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- ξ be the probability that an instance of H is destroyed during reproduction, so we get:

$$E(|\text{pop}_{t+1} \cap H|) = (1-\xi)E(|\text{matePool}_t \cap H|) = \frac{|\text{pop}_t \cap H| * \overline{f}(\text{pop}_t \cap H)}{\overline{f}(\text{pop}_t)}(1-\xi) \tag{10}$$

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- Hence:

$$E(|\text{pop}_{t+1} \cap H|) = \frac{|\text{pop}_t \cap H| * \overline{f}(\text{pop}_t \cap H)}{f_t(\text{pop}_t)}\left(1 - cr\frac{\delta(m)}{n-1} + mr\frac{\text{order}(m)}{n}\right) \quad (14)$$

- Let's go back to:

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  3. actually, only $\overline{f}(\text{pop}_t \cap H)$ is not known (samples of H), not $\overline{f}(H)$
     $\Longrightarrow$ new instances of H may actually be very bad

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- useful gene sequences which step-by-step are built by mutation

Section Outline

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  - Why not including a local search (such as Hill Climbers) to refine the results? (MAs) [73, 74]

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- Many extensions

谢谢

Thank you

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