Evolutionary Algorithms and its applications

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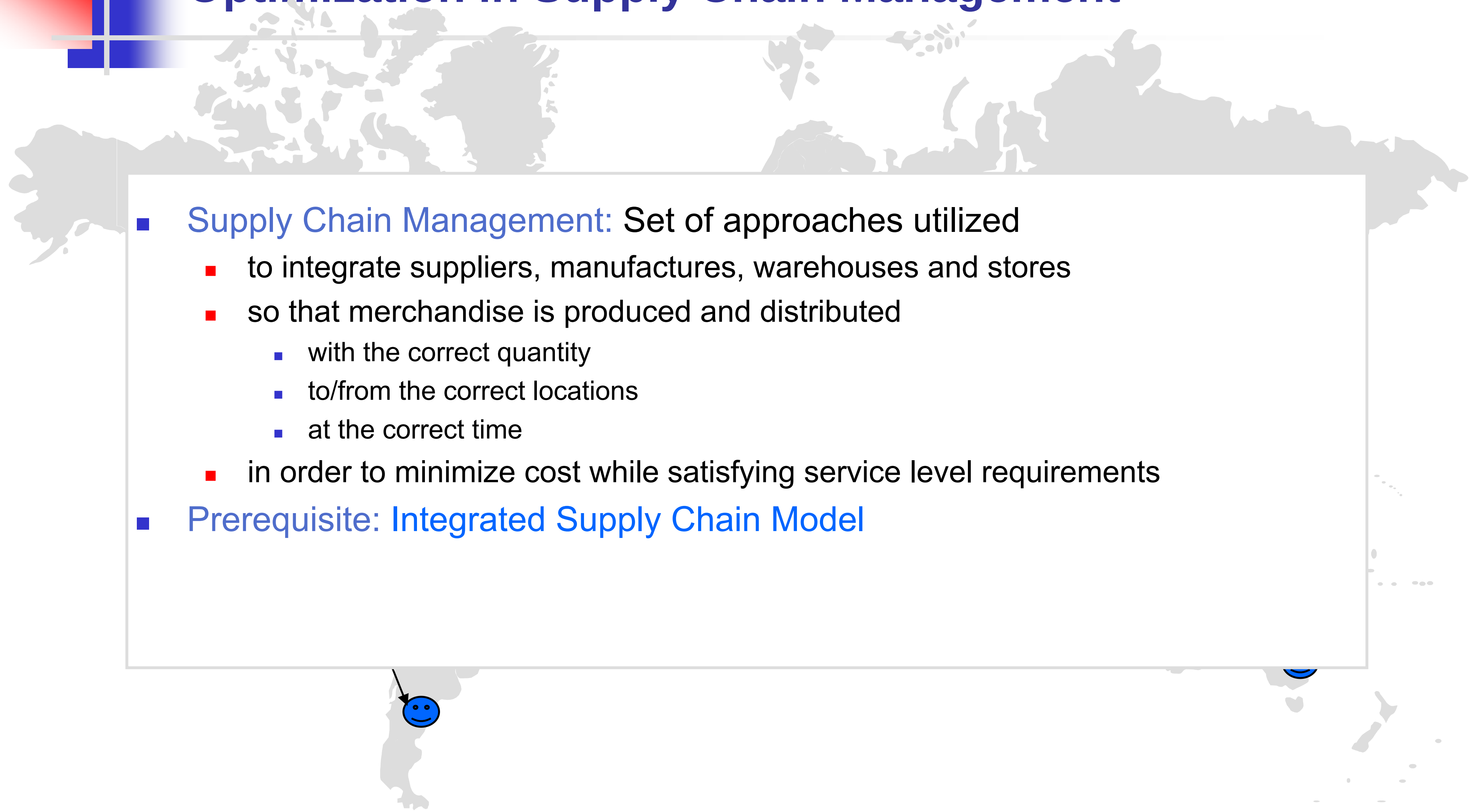
BA Karlsruhe

Overview

- Introduction
- Overview Optimization Methods
- Evolutionary Algorithms

Optimization in Supply Chain Management

- Supply Chain Management: Set of approaches utilized
  - to integrate suppliers, manufactures, warehouses and stores
  - so that merchandise is produced and distributed
    - with the correct quantity
    - to/from the correct locations
    - at the correct time
  - in order to minimize cost while satisfying service level requirements
- Prerequisite: Integrated Supply Chain Model

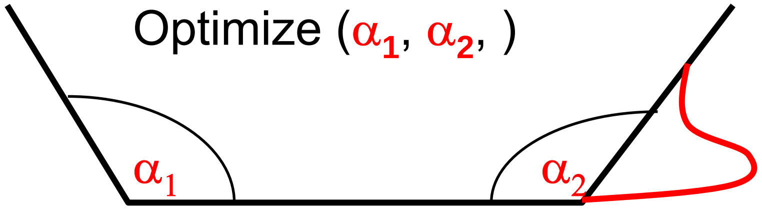


Supplier Plant DC ☺ Customer

Introduction: Nature versus Engineers

- Typical Engineering Approach for Optimization
  - Specify
    - Model of the real world problem
    - Objective Function for evaluating alternative solutions
  - Optimize the free parameters of the model
- Typical Failure
  - Model is simple enough to optimize
  - But too simple for good solutions

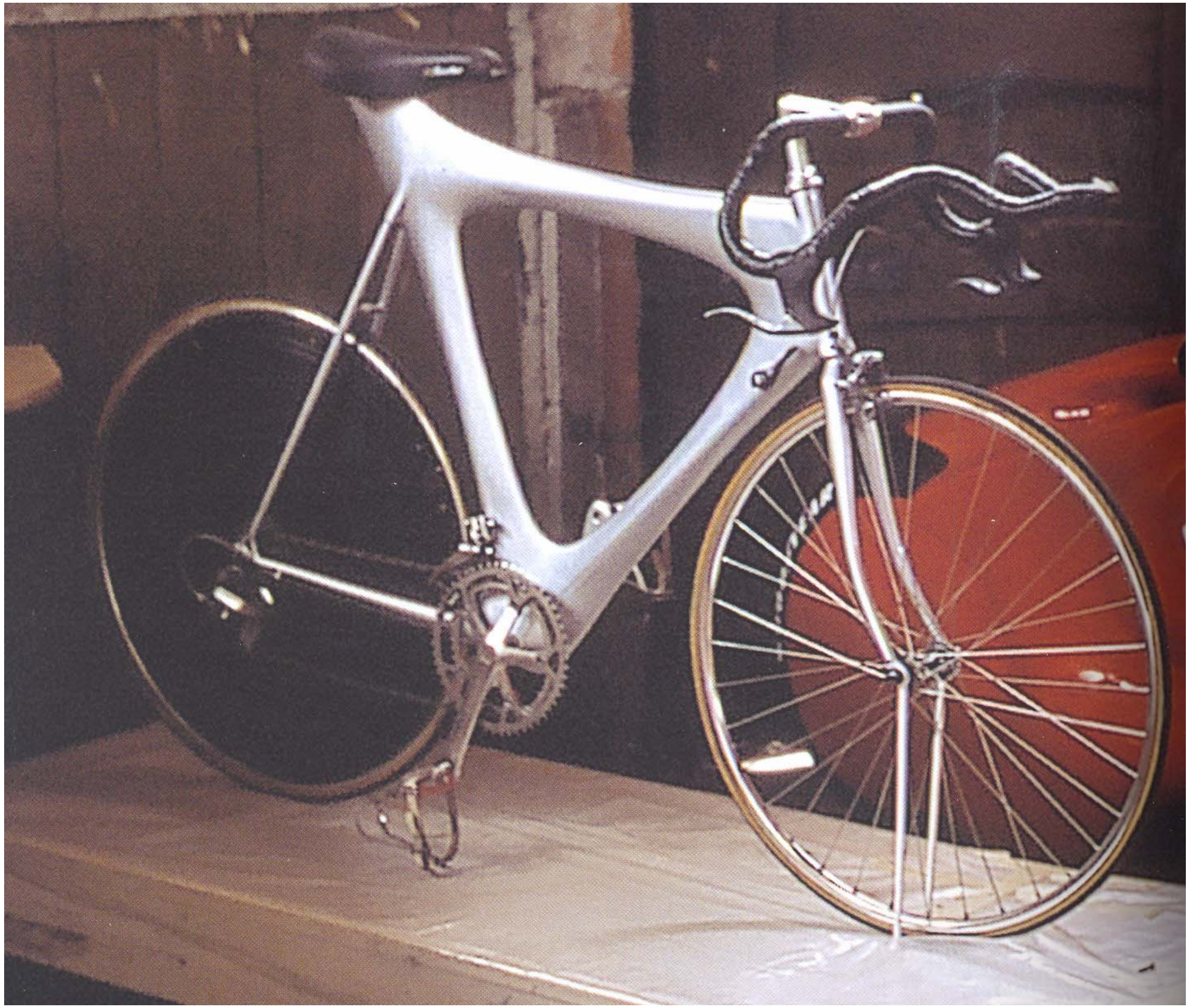
Ship Design



Optimize (α_1, α_2,)

- Mind the difference
  - Engineers model with simple geometric: Straight lines, circles
  - Nature is not so simple minded!!

Natural Design by famous Designer Colani (Karlsruhe)



Natural Design by famous Designer Colani (Karlsruhe)

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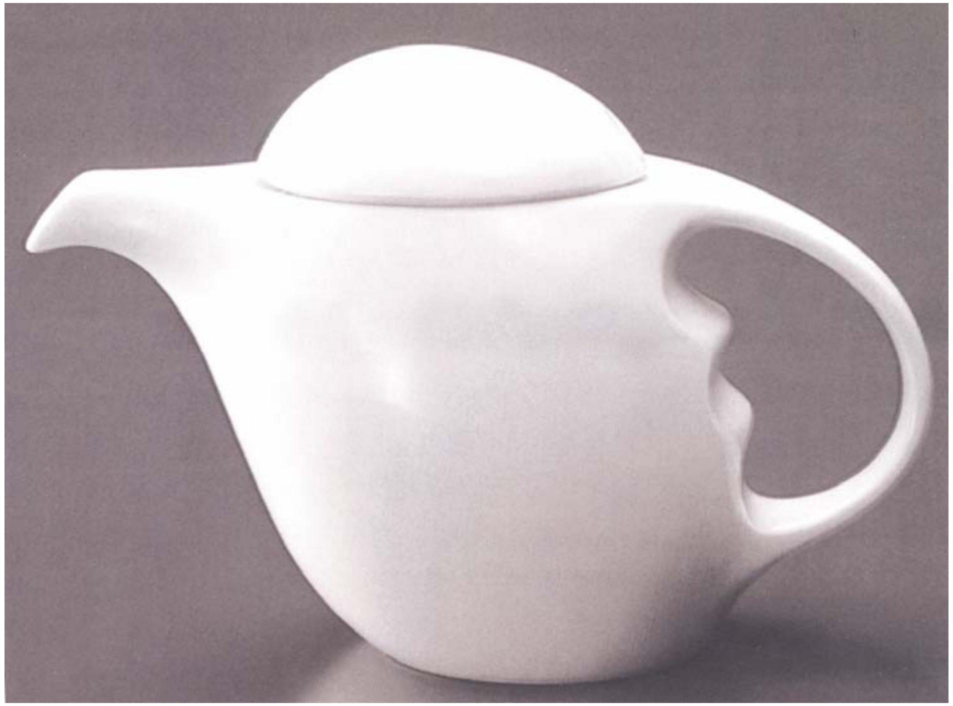
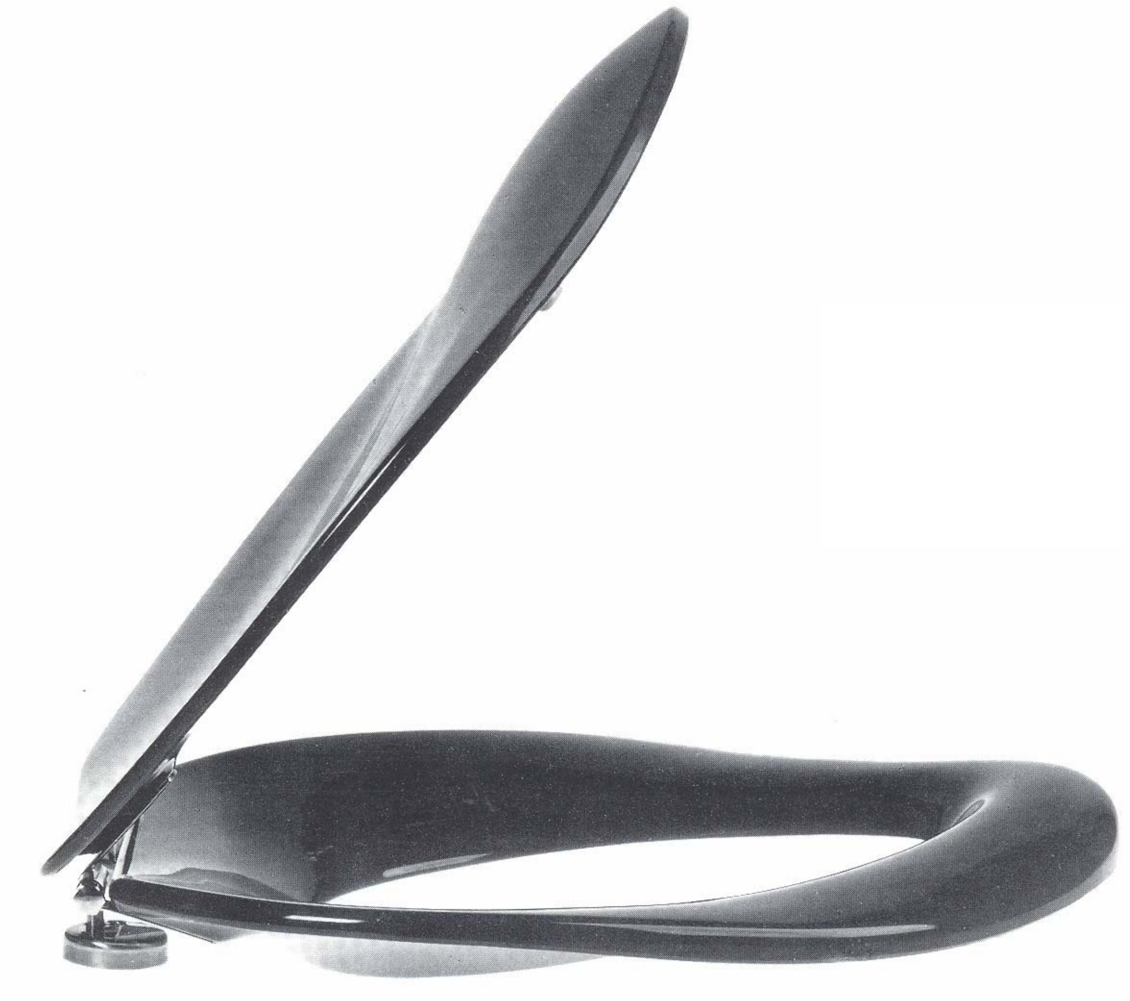
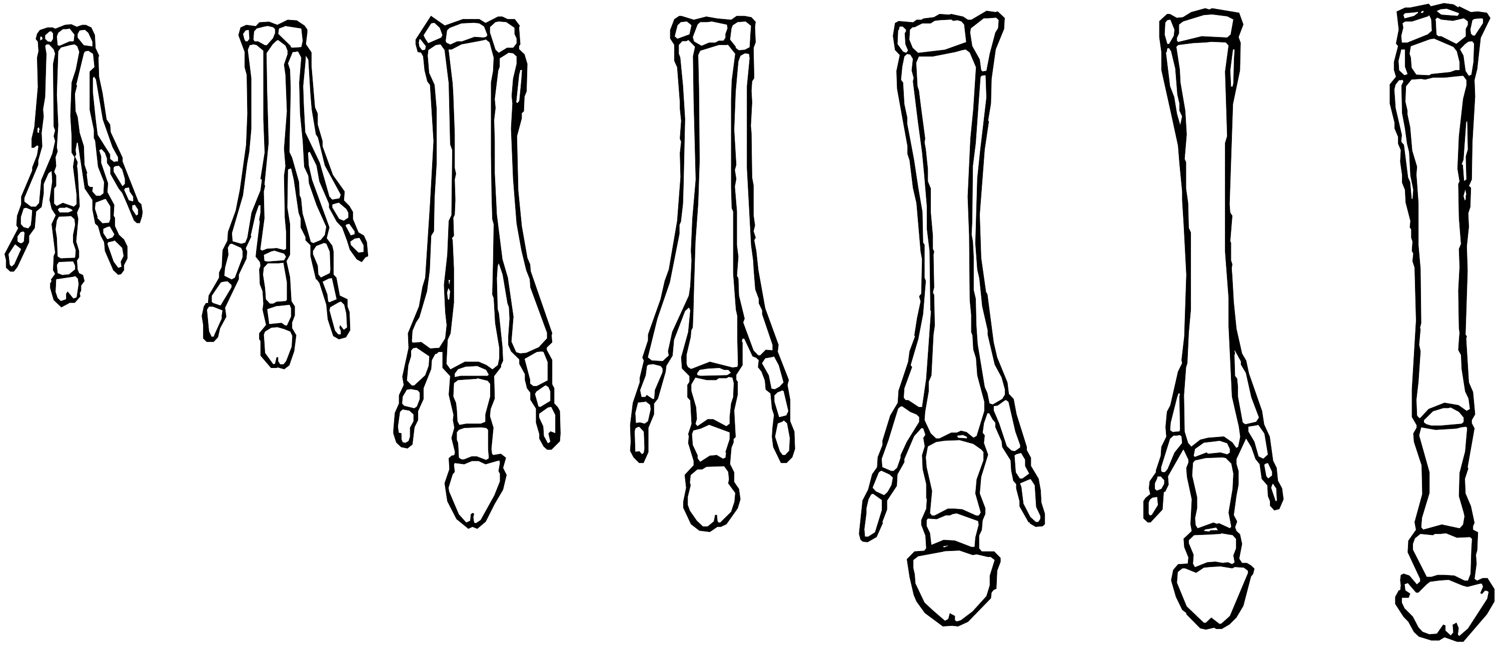


Natural Design by famous Designer Colani (Karlsruhe)

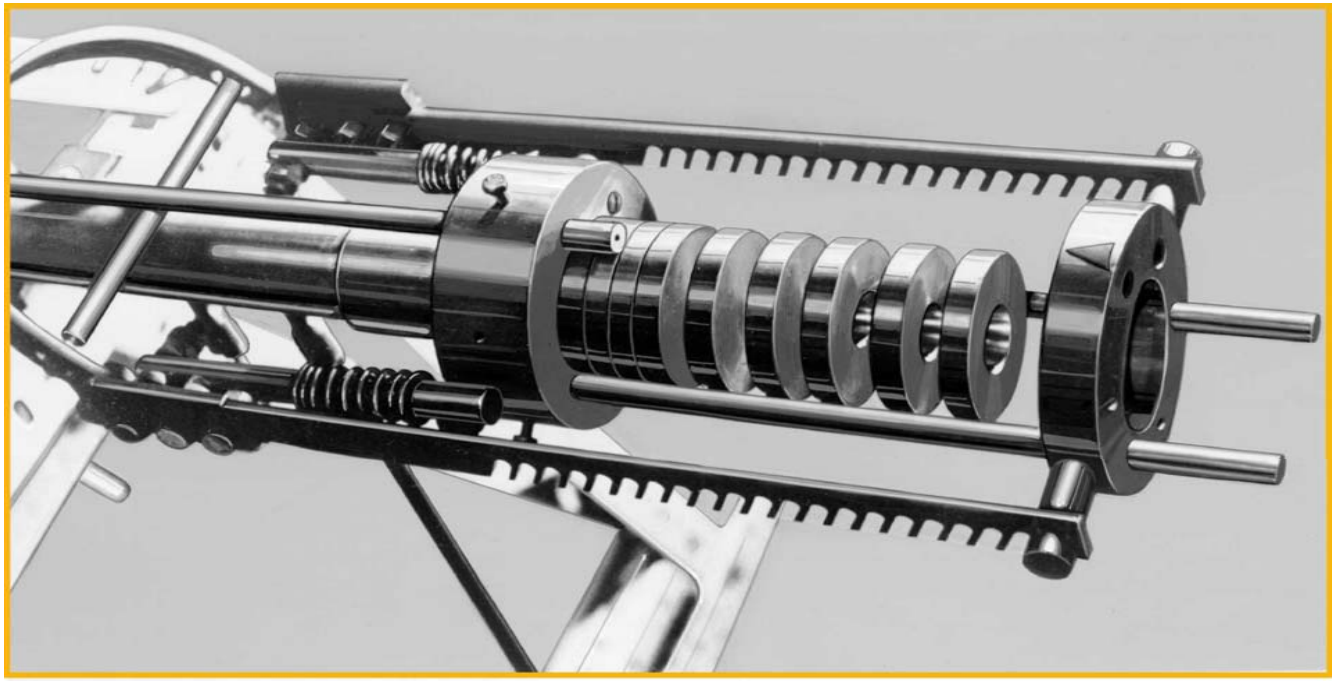


Evolution of the horse foot



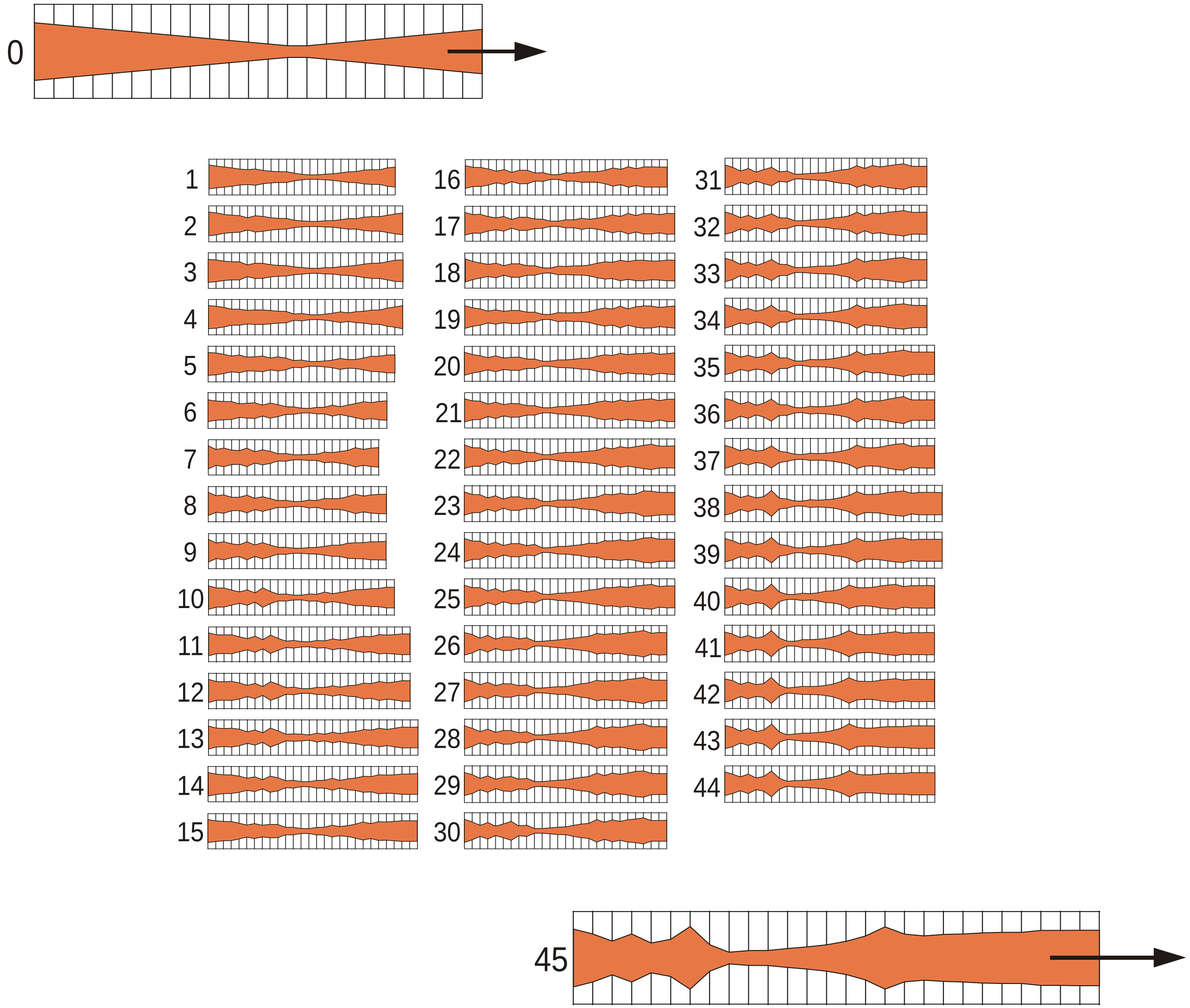
From Eohippus to Equus (60 Millionen Years)

Evolution of a water steam pipe in 1965

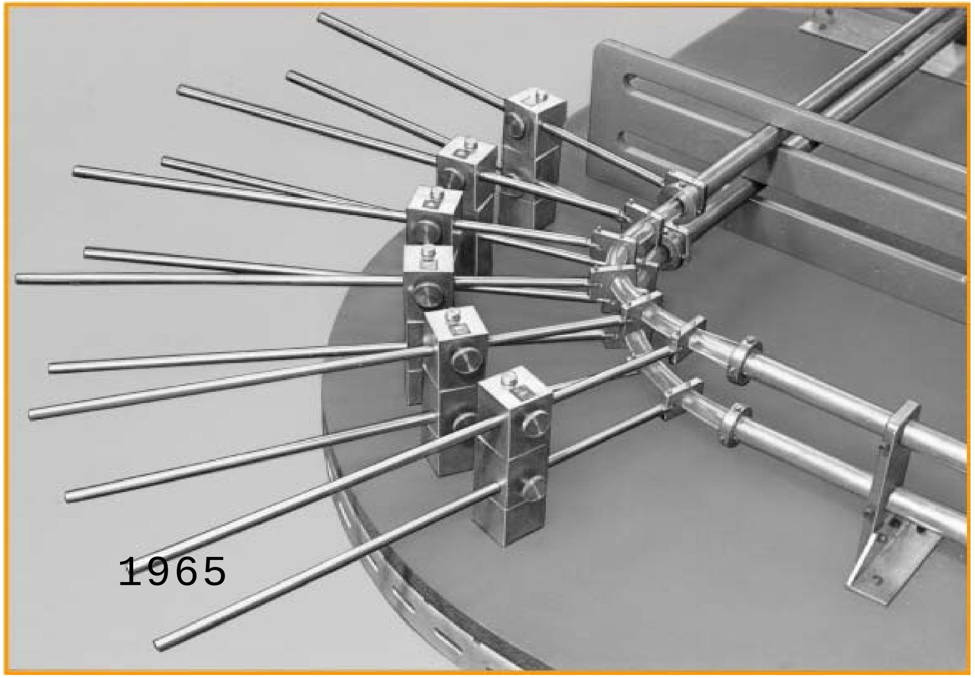


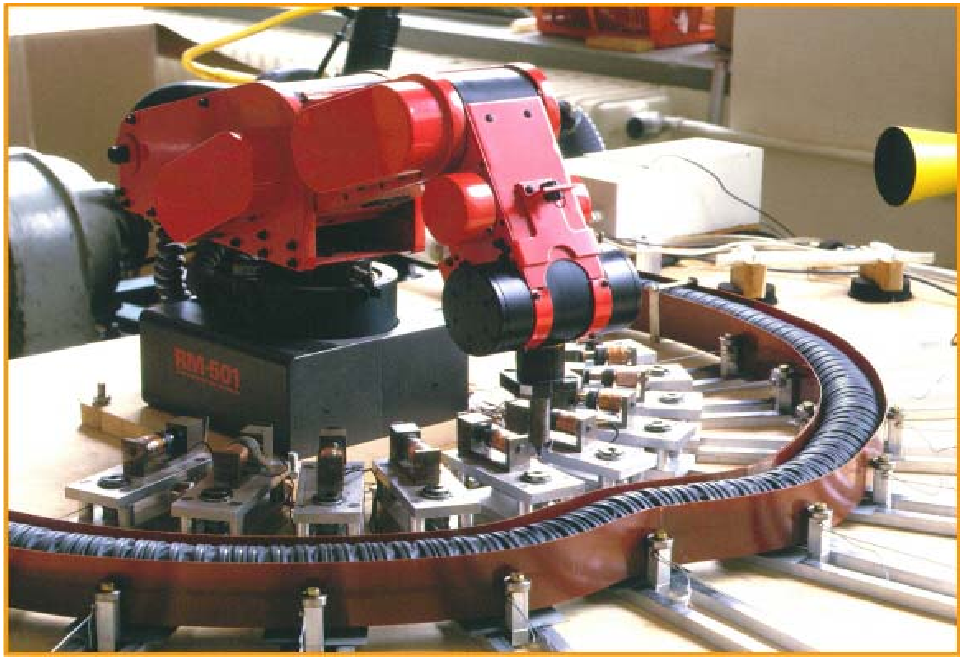
by Schwefel

Evolution of a steam pipe in 1965



Evolution of a curvature by Rechenberg





1980

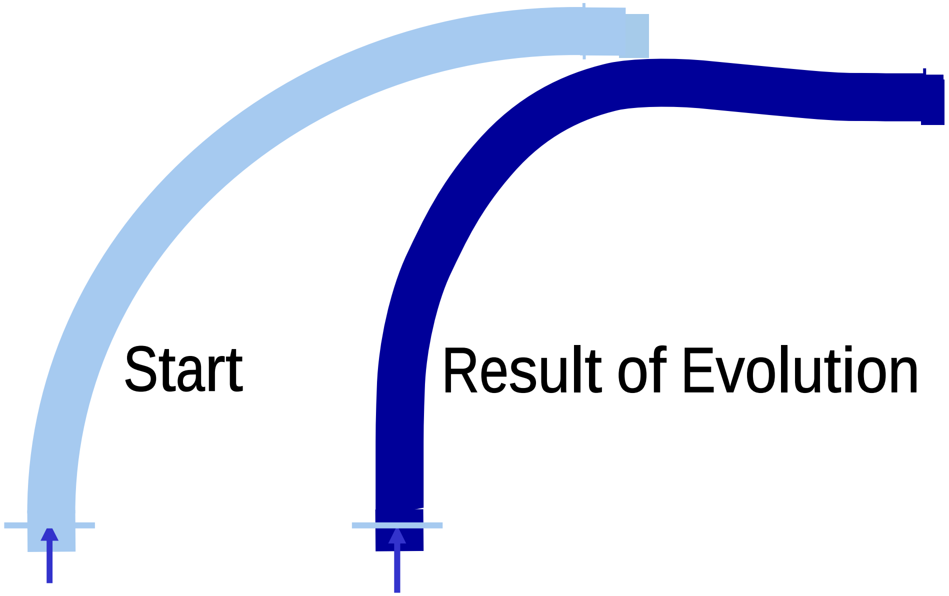
Manuel Adjustments

-> 6 hand driven contrals

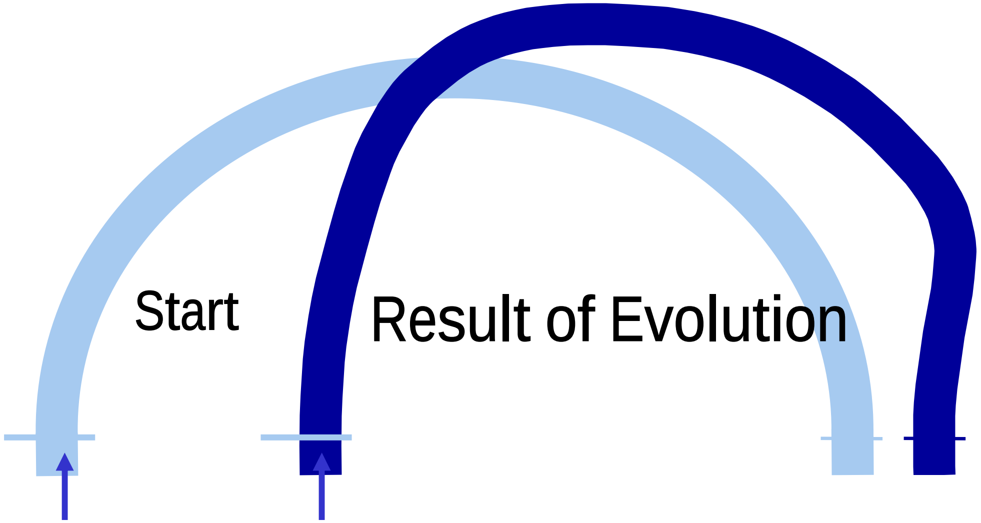
Automatic Adjustments

-> 10 robot driven controls

Evolution of a curvature by Rechenberg



Optimal 90°- solution



Optimal 180°- solution

Optimization Methods

model too simpel

exponential time

- Local Search
  - Deterministic
    - Hill Climbing
    - Gradient Descent
    - Tabu Search
  - Probabilistic
    - Simulated Annealing
    - Iterated local Search

- Global Search
  - Deterministic
    - Linear Optimization
    - Branch&Bound, Divide&Conquer
    - Dynamic Programming
  - Probabilistic
    - **Genetic algorithms**
    - **Evolution Strategies**

Production Planning

- **Decison Variables**
  - x_A = lot size for product A $\in |R^+$
  - x_B = lot size for product B $\in |R^+$

- **Objective Function**
  - Maximize $200x_A + 400x_B$ **Profit**

- **Constraints**
  - Assembling: $4x_A + 6x_B \leq 120$
  - Painting: $2x_A + 6x_B \leq 72$

Resource consumption

Resource capacity

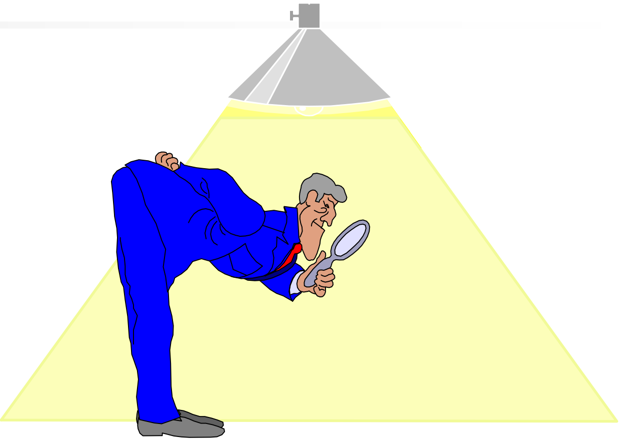
Problem

Linear model (objective function, constraints)

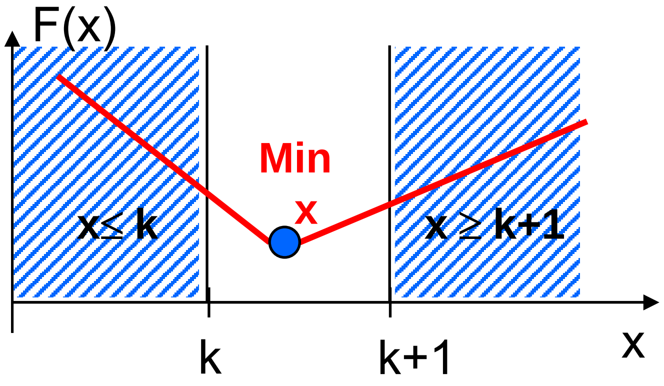
Integer solutions are NP-hard -> Branch&Bound

Classic Operations Research

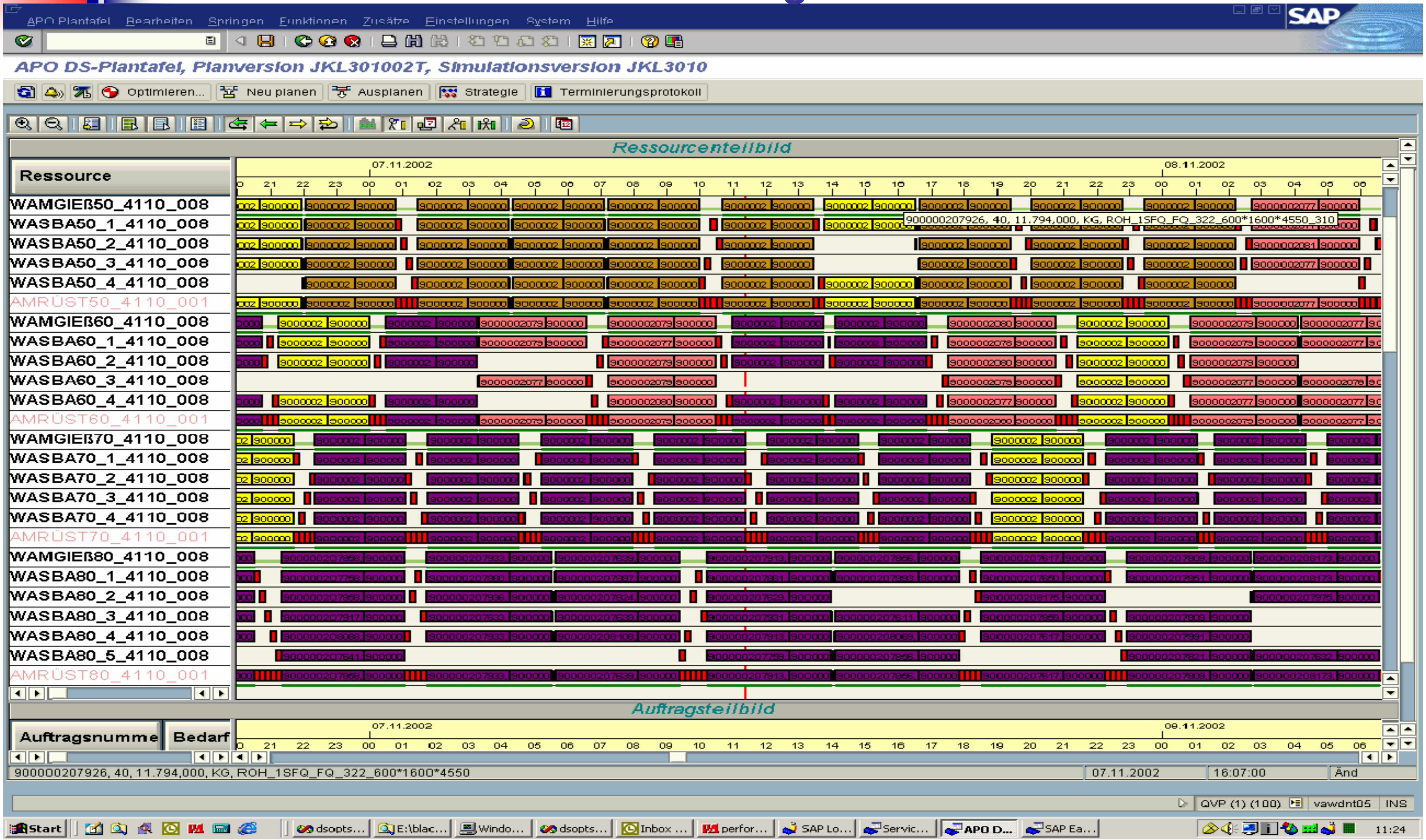
- **Linear Model**
  - Linear objective function
  - Linear constraint
  - Efficient algorithms (**Simplex Algorithm**)



- **Complex: modelling “integer” variables**
  - Optimize by relaxation
    - neglecting „integer“ constraint
    - Search optimum in both branches
  - **Branch&Bound method**
  - NP-hard



Detailed Production Planning



APO DS-Plantafel, Planversion JKL301002T, Simulationsversion JKL3010

Ressource

WAMGIEB50_4110_008
WASBA50_1_4110_008
WASBA50_2_4110_008
WASBA50_3_4110_008
WASBA50_4_4110_008
AMRÜST50_4110_001
WAMGIEB60_4110_008
WASBA60_1_4110_008
WASBA60_2_4110_008
WASBA60_3_4110_008
WASBA60_4_4110_008
AMRÜST60_4110_001
WAMGIEB70_4110_008
WASBA70_1_4110_008
WASBA70_2_4110_008
WASBA70_3_4110_008
WASBA70_4_4110_008
AMRÜST70_4110_001
WAMGIEB80_4110_008
WASBA80_1_4110_008
WASBA80_2_4110_008
WASBA80_3_4110_008
WASBA80_4_4110_008
WASBA80_5_4110_008
AMRÜST80_4110_001

900000207926, 40, 11.794,000, KG, ROH_1SFQ_FQ_322_600*1600*4550_310

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QVP (1) (100) | vawdnt05 | INS

Knappsack Problem

- **Decision Variables**
  - $x_{i,} \in \{0,1\}$
  - $x_{i,} = 1 \quad \Leftrightarrow$ take object i

- **Objective Function**
  - Maximize $120\,x_1 + 175x_2 + 200\,x_3 + 150\,x_4 + 30\,x_5 + 60\,x_6$

- **Constraint**
  - Limitation $20x_1 + 35x_2 + 50\,x_3 + 50\,x_4 + 15\,x_5 + 60x_6 \leq 100$

Truck Load Building

- **Decision Variables**
  - $x_{i,} \in \{0,1\}$
  - $x_{i,} = 1 \Leftrightarrow$ load order i on the truck

- **Objective function**
  - Maximize $10\,x_1 + 20x_2 + 50\,x_3 + 200\,x_4 + 150\,x_5 + 250\,x_6 + 150\,x_7$

- **Constraints**
  - Weight $0{,}4\,x_1 + 0{,}7x_2 + 0{,}2\,x_3 + 2\,x_4 + 2\,x_5 + x_6 + 3\,x_7 \leq 5$
  - Volumen $0{,}4\,x_1 + 0{,}2\,x_2 + 3\,x_3 + 4\,x_4 + 3\,x_5 + 5_6 + 0{,}9\,x_7 \leq 5$

Truck Load Building
= Multidimensional Knappsack Problem

- **Decision Variables**
  - $x_{i,} \in \{0,1\}$
  - $x_{i,} = 1 \Leftrightarrow$ load order i on the truck
- **Objective function**
  - Maximize $\sum_i w_i x_i$
- **Constraints**
  - Weight $\sum_i G_i x_i \leq G$
  - Volumen $\sum_i V_i x_i \leq V$

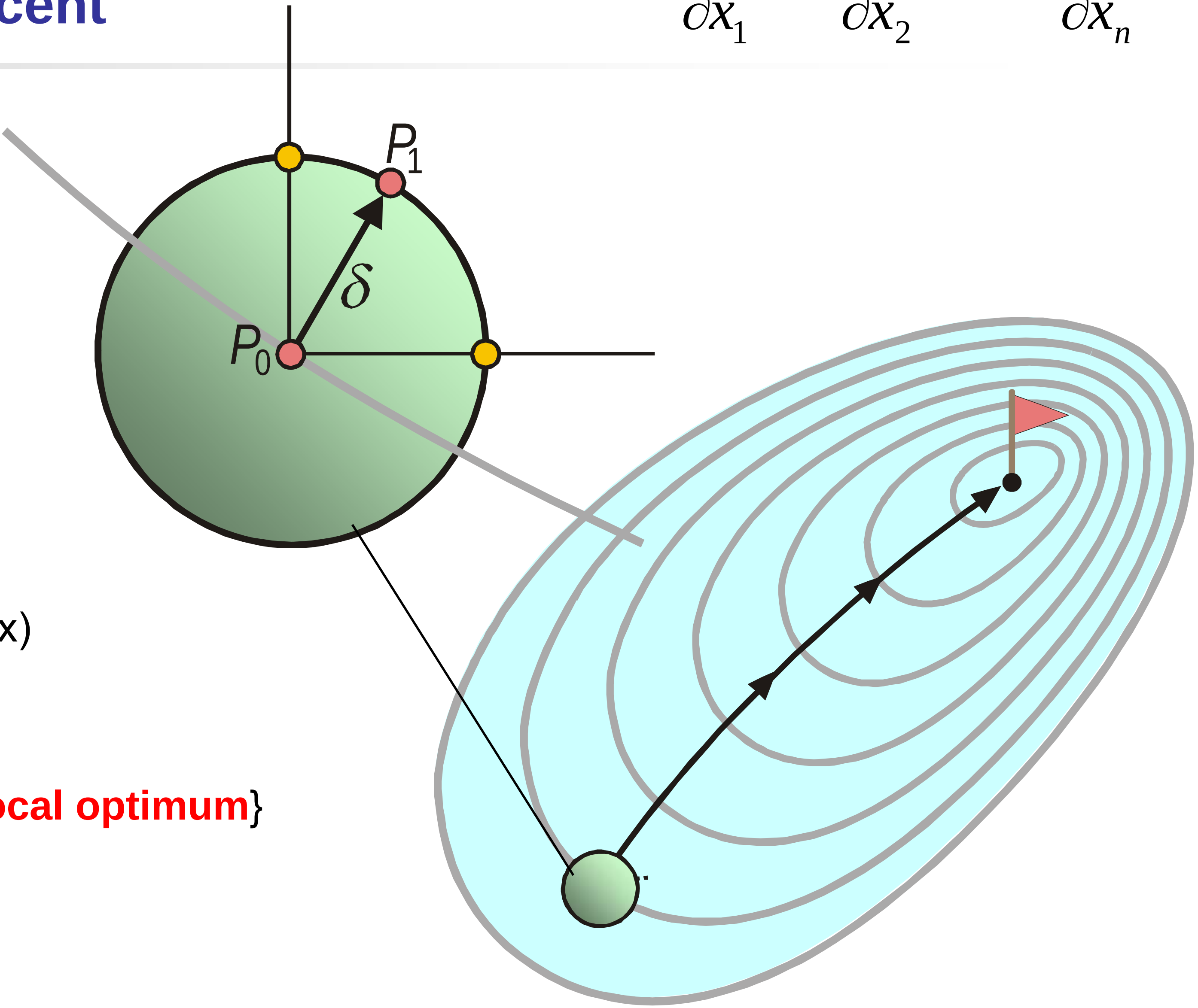
Optimization Methods

- Local Search
  - Deterministic
    - **Hill Climbing**
    - **Gradient Descent**
    - Tabu Search
  - Probabilistic
    - Simulated Annealing
    - **Iterated local Search**

- Global Search
  - Deterministic
    - Linear Optimization ✓
    - Branch&Bound, Divide&Conquer ✓
    - Dynamic Programming
  - Probabilistic
    - Genetic algorithms
    - Evolution Strategies

Gradient Descent

$$gradient\ f(x) = \left(\frac{\partial f(x)}{\partial x_1}, \frac{\partial f(x)}{\partial x_2}, \ldots, \frac{\partial f(x)}{\partial x_n}\right)$$



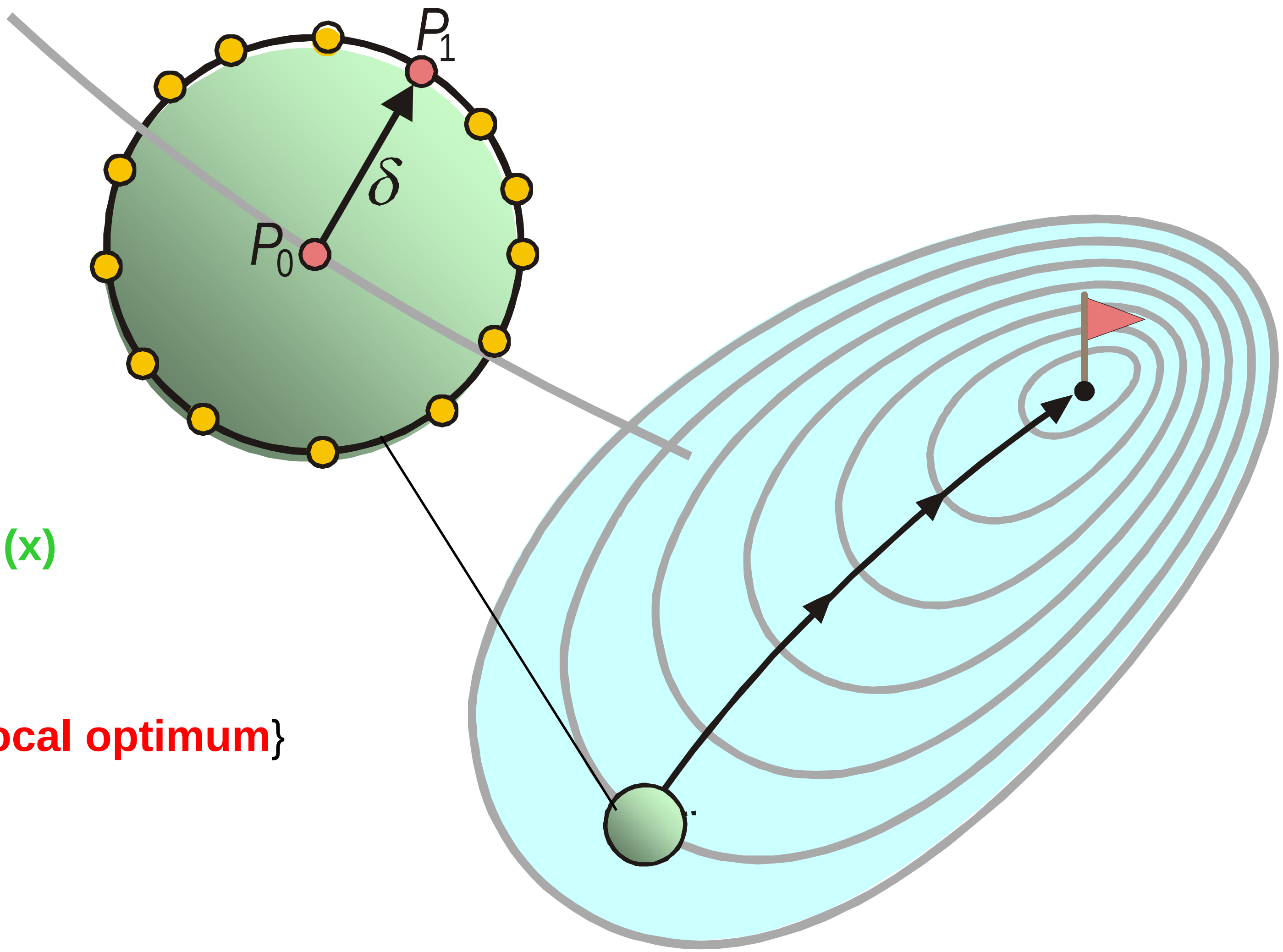
- **Initialization**

  X := random solution

- **Improvement Loop**

```
X´ := X +   δ* gradient f (x)
If f(X´) < f(X)
    Then      X:=X´
    Else      Stop     {local optimum}
```

Hill Climbing



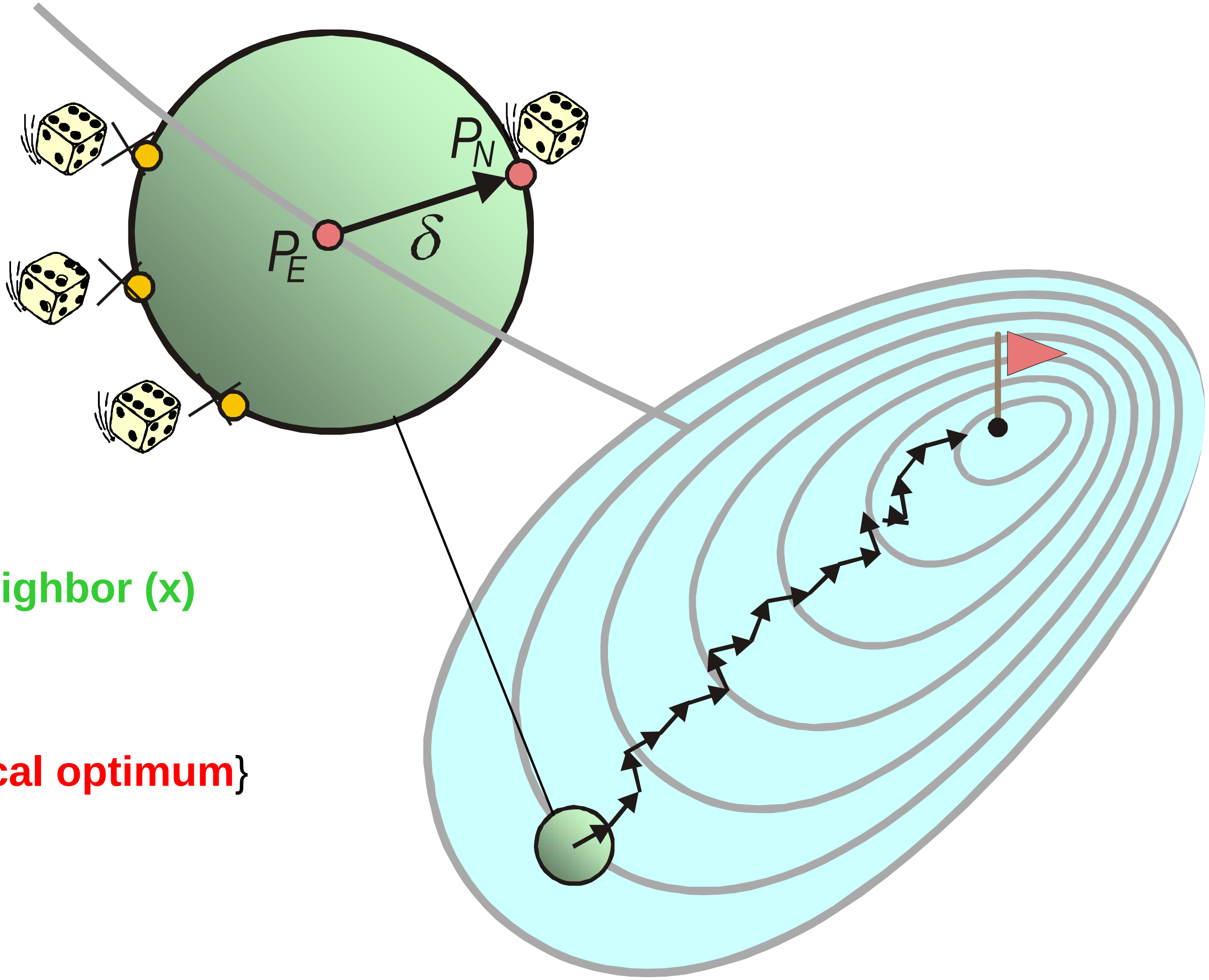
- **Initialization**

```
X := random solution
```

- **Improvement Loop**

```
X´ := Best of Neighbor (x)
If f(X´) < f(X)
    Then    X:=X´
    Else    Stop    {local optimum}
```

Probabilistic Hill Climbing



- **Initialization**

```
X := random solution
```

- **Improvement Loop**

```
X´ := Best of random Neighbor (x)
If f(X´) < f(X)
    Then    X:=X´
    Else    Stop    {local optimum}
```

Iterated Local Search

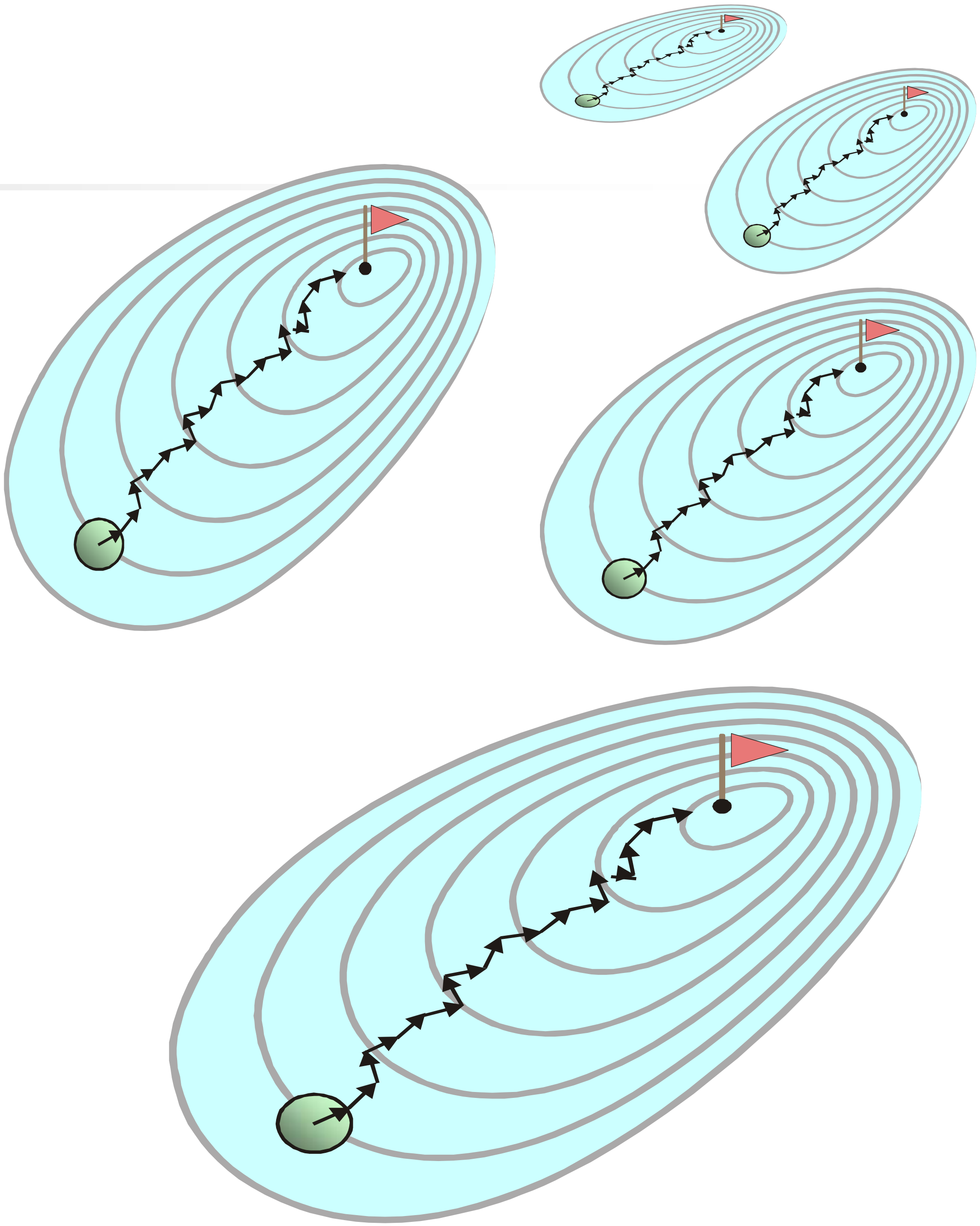
- **Iterate until time out:**

- **Initialization**

```
X := random solution
```

- **Improvement Loop**

```
X´ := Best of random Neighbor (x)
If f(X´) < f(X)
    Then    X:=X´
    Else    Stop    {local optimum}
```



Evolution

- **Iterate until time out:**

- **Initialization Population P**

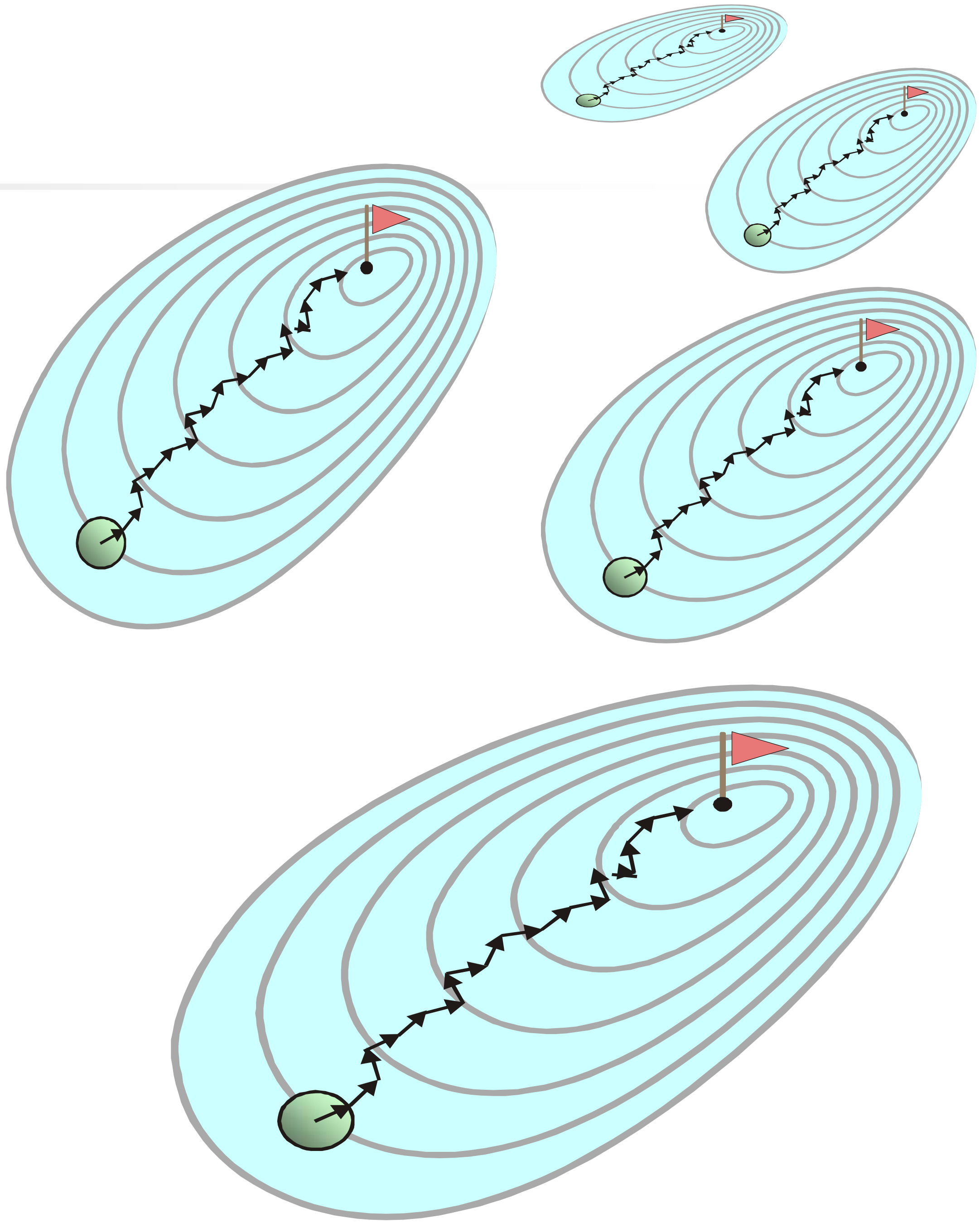
  P := random solutions

- **Improvement Loop**

  Generate **offsprings** (P)

  P := **select** **best** of offsprings (P)

  „survival of the fittest“



Optimization Methods

- Local Search
  - Deterministic
    - Hill Climbing ✓
    - Gradient Descent ✓
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- Global Search
  - Deterministic
    - Linear Optimization ✓
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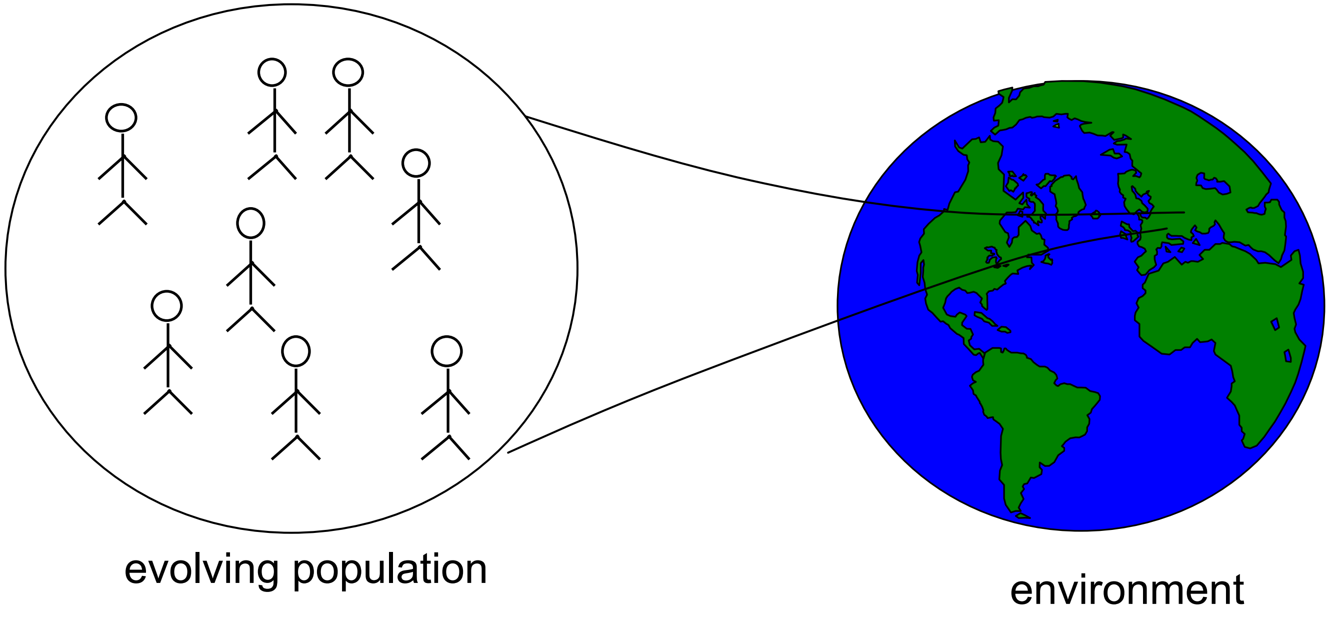
Inspiration from nature

Darwin’s prinziple of natural evolution:

survival of the fittest

in populations of individuals (plants, animals), the better the individual is adapted to the environment, the higher its chance for survival and reproduction.



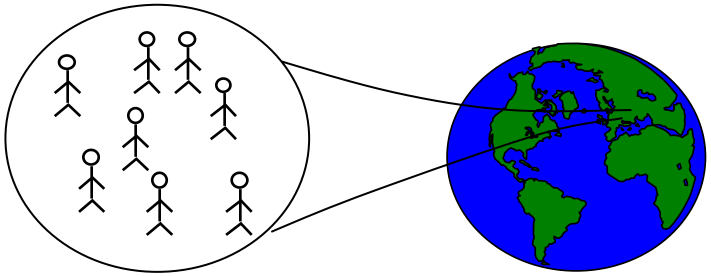
Analogies

Natural evolution

- individual
- environment
- fitness/how well adapted
- survival of the fittest
- mutation
- crossover

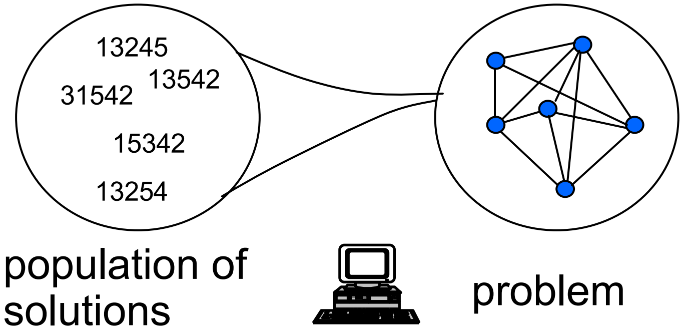
Evolutionary algorithms

- potential solution
- problem
- cost/quality of solution
- good solutions are kept
- small, random perturbations
- recombination of partial solutions



population of individuals

environment



population of solutions

problem

How are new individuals created?

- by **sexual reproduction**, i.e.
  - two individuals are selected
    (randomly, or actively through competition etc.,...),
  - a new individual is created based on the two parent‘s genetic material (recombination/crossover)
- by **mutation**, i.e. random change of
  - specific genes
  - the structure of chromosomes

Important principles in evolution

- Exploration: Increase diversity by
  - sexual reproduction (recombination/crossover)
  - mutation
- Exploitation: Reduce diversity by
  - selecting good parents
  - survival of the fittest

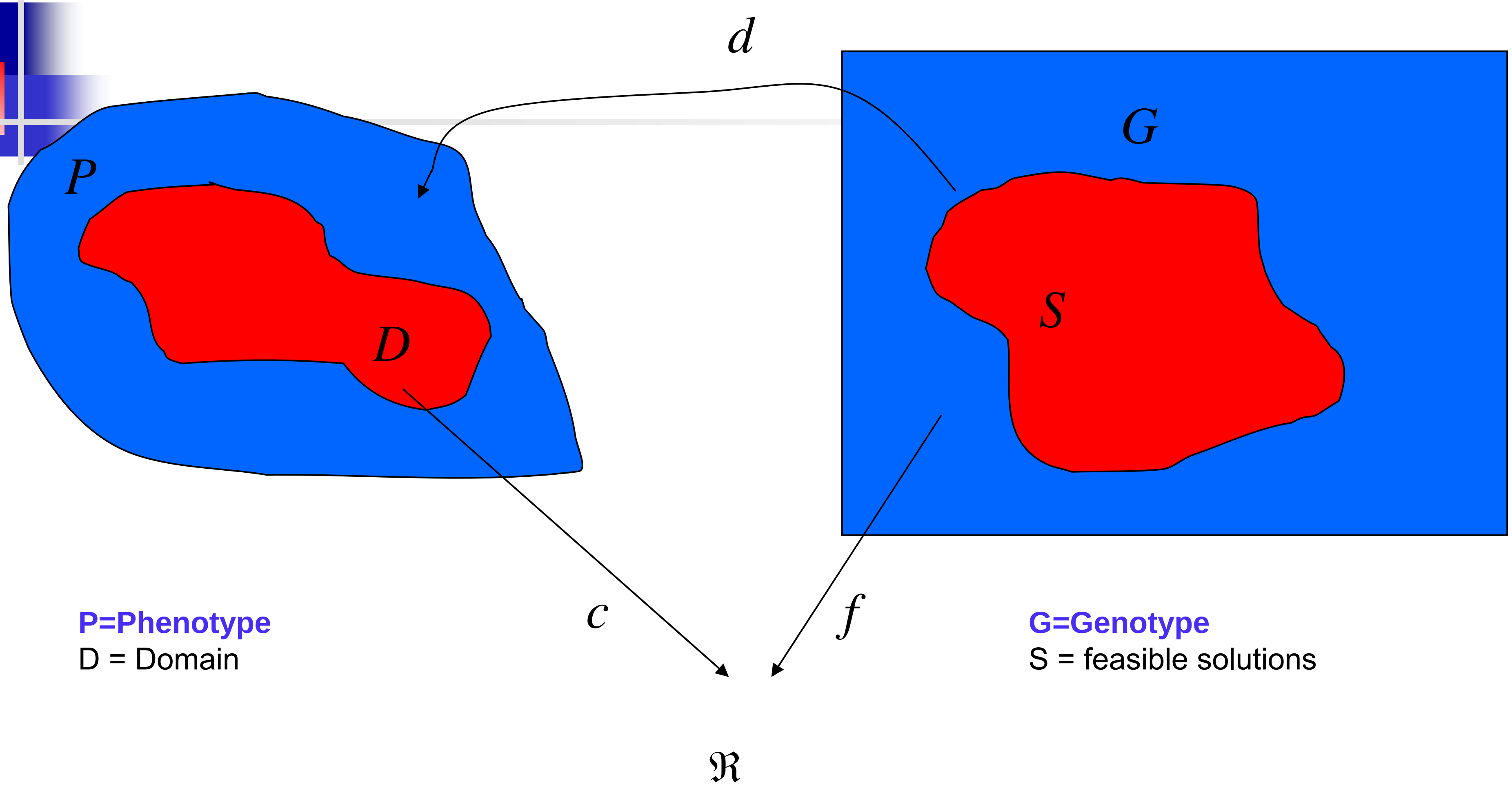
Major design decisions

- **representation**
- **fitness function**

- mutation operator
- crossover and mutation probabilities
- selection operator
- reproduction scheme
- crossover operator / recombination
- population size
- stopping criterion

Standard Representation

- Bit String
  - $x = b_1b_2\ldots b_n$ with $b_i \in \{0,1\}$
  - Similar to genetic representations
  - Difference: Chromosoms use an alphabet with 4 letters
- Real-valued Vector
  - $x = x_1x_2\ldots x_n$ with $x_i \in |R$
  - Favorable for engineering applications
- Universal Reprentations
  - Digital = Bit string
  - Analog = Real-valued Vector
  - Confer: MP3- Encoding



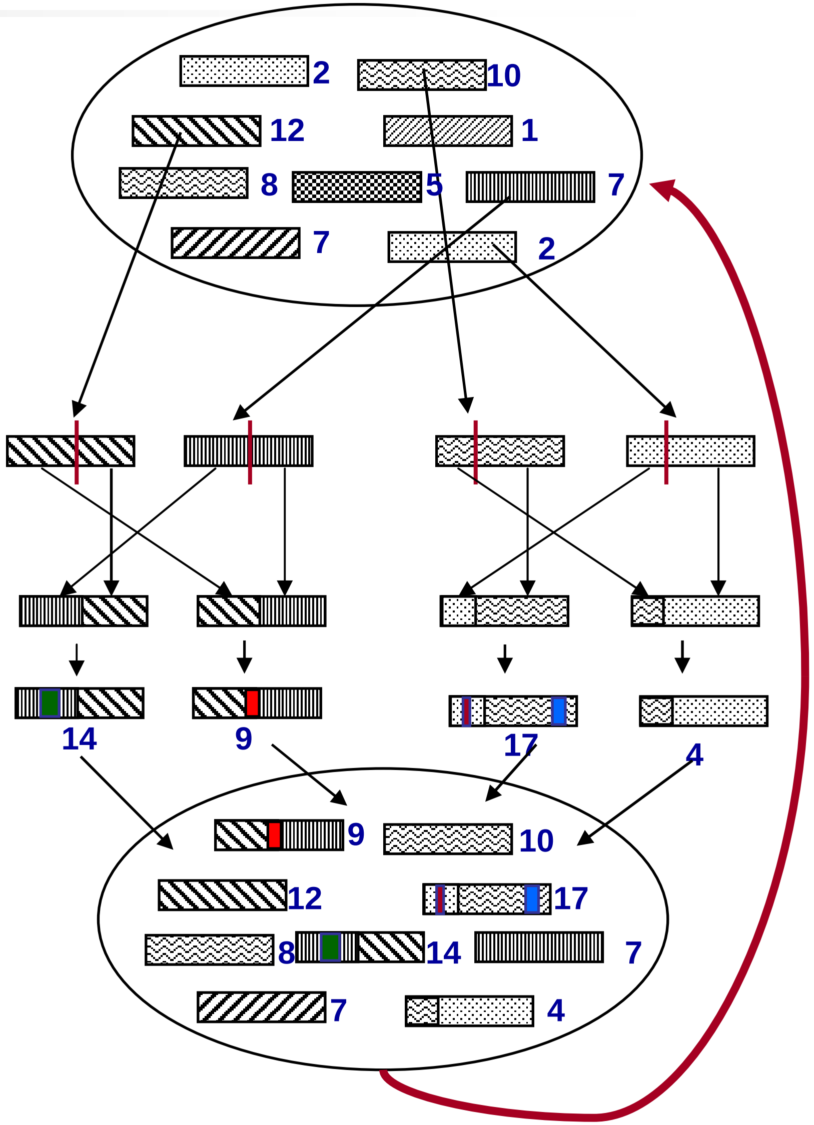
P=Phenotype
D = Domain

G=Genotype
S = feasible solutions

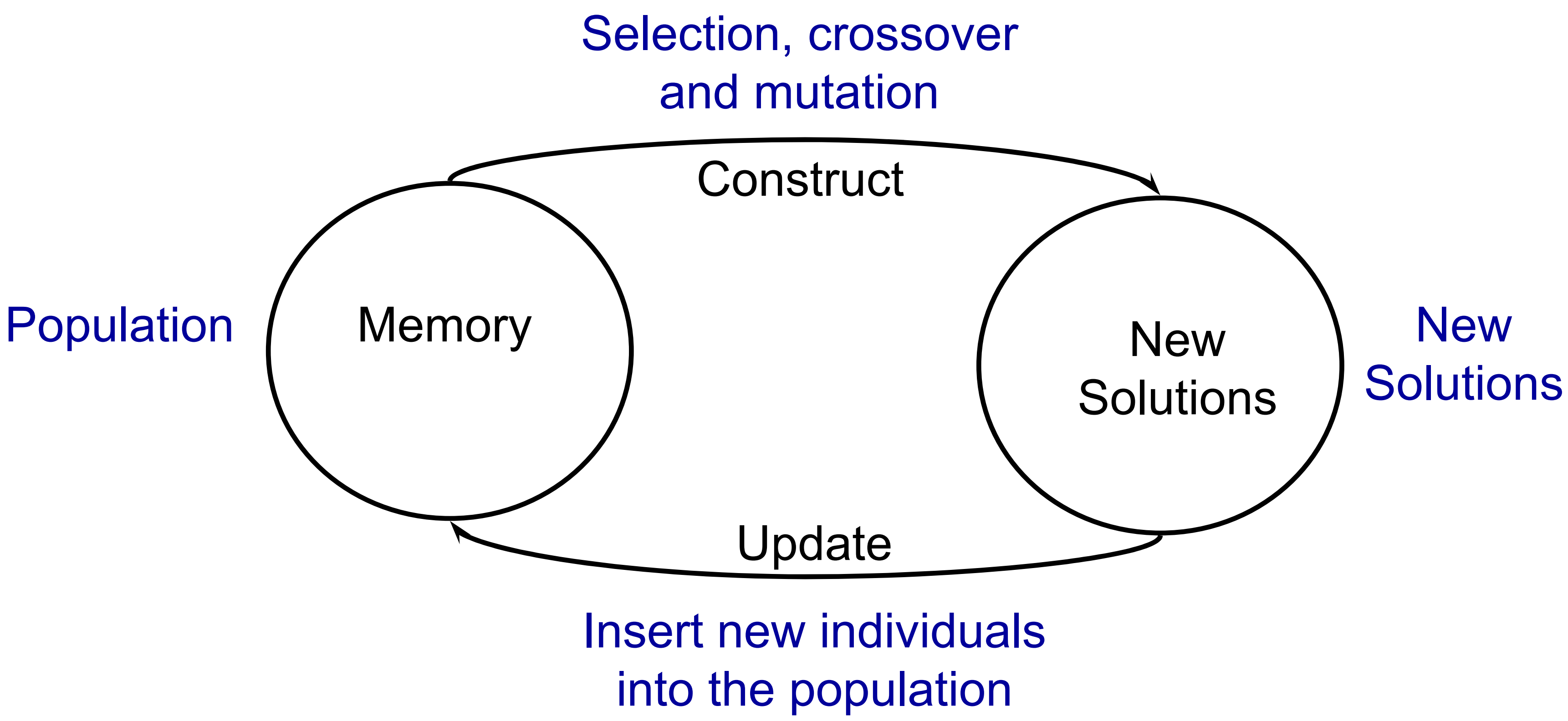
$$S = d^{-1}(D) \text{ und } f = c \circ d = fitness$$

Evolutionary Algorithm

```
INITIALIZE population
        (set of solutions)

  EVALUATE Individuals
        according to goal ("fitness")

  REPEAT

    SELECT parents

    RECOMBINE parents (CROSSOVER)

    MUTATE offspring

    EVALUATE offspring

   FORM next population

  UNTIL   termination-condition
```



Unified Model



Mutation - one parent

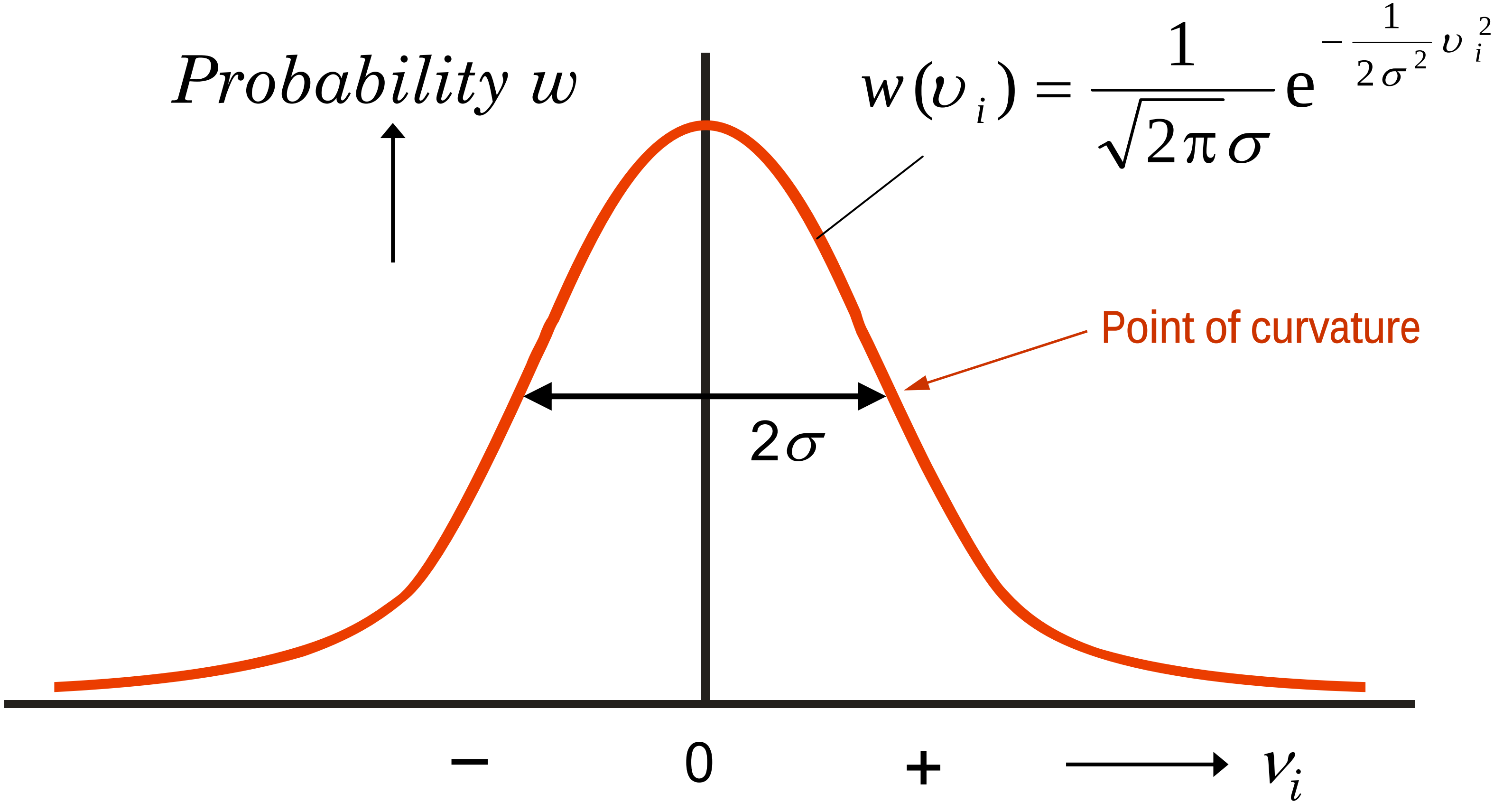
- Standard mutation operators
  - Bit string (e.g. x = $b_1 b_2 \ldots b_n$ with $b_i \in \{0,1\}$)
    flip each bit with probability p_m,
    i.e.

$$y_i = \begin{cases} 1 - x_i & \text{with probability } p_m \\ x_i & \text{otherwise} \end{cases}$$

  - Real-valued vector (e.g. x = $x_1 x_2 \ldots x_n$ with $x_i \in$ |R)
  - Input: $\vec{x}$
  - Output: $\vec{y}$ with

$$y_i = \begin{cases} x_i + v_i, \; v_i \in N(0, \sigma^2) & \text{with probability } p_m \\ x_i & \text{otherwise} \end{cases}$$

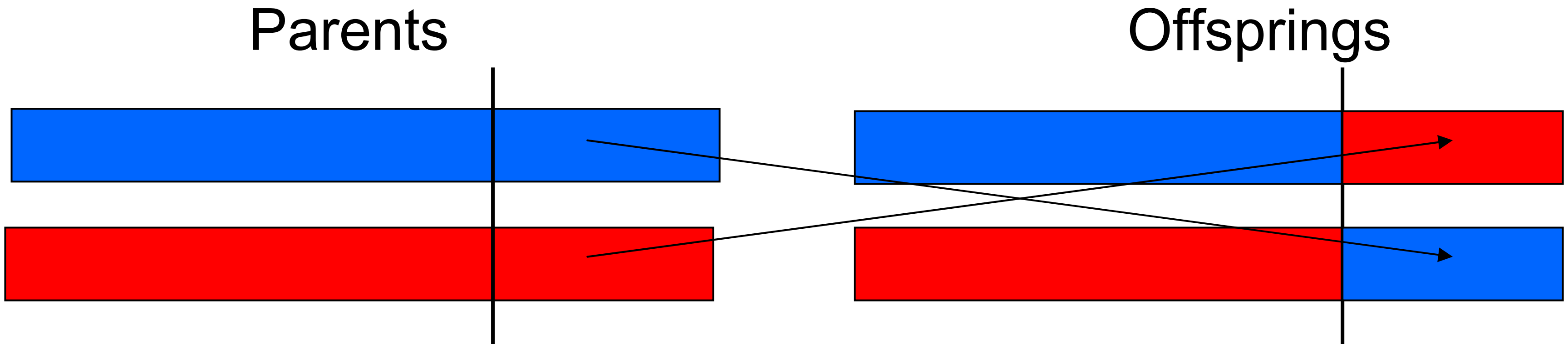
- Difficulty: how to select mutation probability p_m and mutation step size σ?



Gaussian random number v_i for mutation of variable x_i

Crossover - Two Parents

Exchange genes of the genotypes



Variants of evolutionary algorithms

- Genetic algorithms (Holland 1965 and Goldberg 1989)
  - binary representations
  - main focus on crossover, mutation only with minor role
- Evolution strategies (Rechenberg and Schwefel 1965)
  - real-valued representation
  - mutation as primary operator
  - self-adaptive mutation

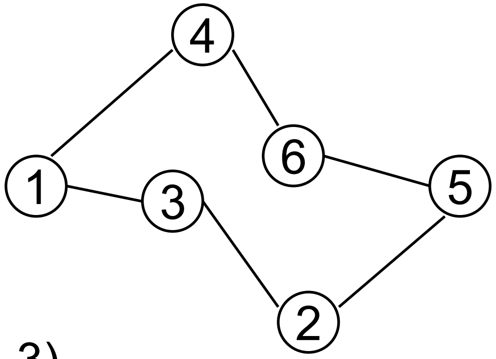
Example: Traveling Salesperson Problem (TSP)

- Given: a set of cities $C = \{c_1,..c_N\}$ and a distance function $d(c_1,c_2)$ that defines the distance for all possible paths from city c_i to city c_j.

- Goal: find a permutation of cities π which minimizes the

  total tour length

$$\sum_{i=1}^{N-1} d(c_{\pi(i)},c_{\pi(i+1)}) + d(c_{\pi(N)},c_{\pi(1)})$$



- Representation
  - Digital: Permutation, e.g. (1 – 4 – 6 – 5 – 2 – 3)
  - Analog: Preferences, e.g. (~~1.~~8, ~~0.~~3, ~~0.~~2, ~~1.~~2, ~~0.~~5, ~~0.~~7)

Special mutation for Traveling Salesman Problem

- Permutation Representation
  - $\pi(1)\ \pi(2)\ \pi(3)\ \ldots\ \pi(n)$ $\pi(i)$ = city visited in position i
  - e.g. 1-4-6-5-2-3

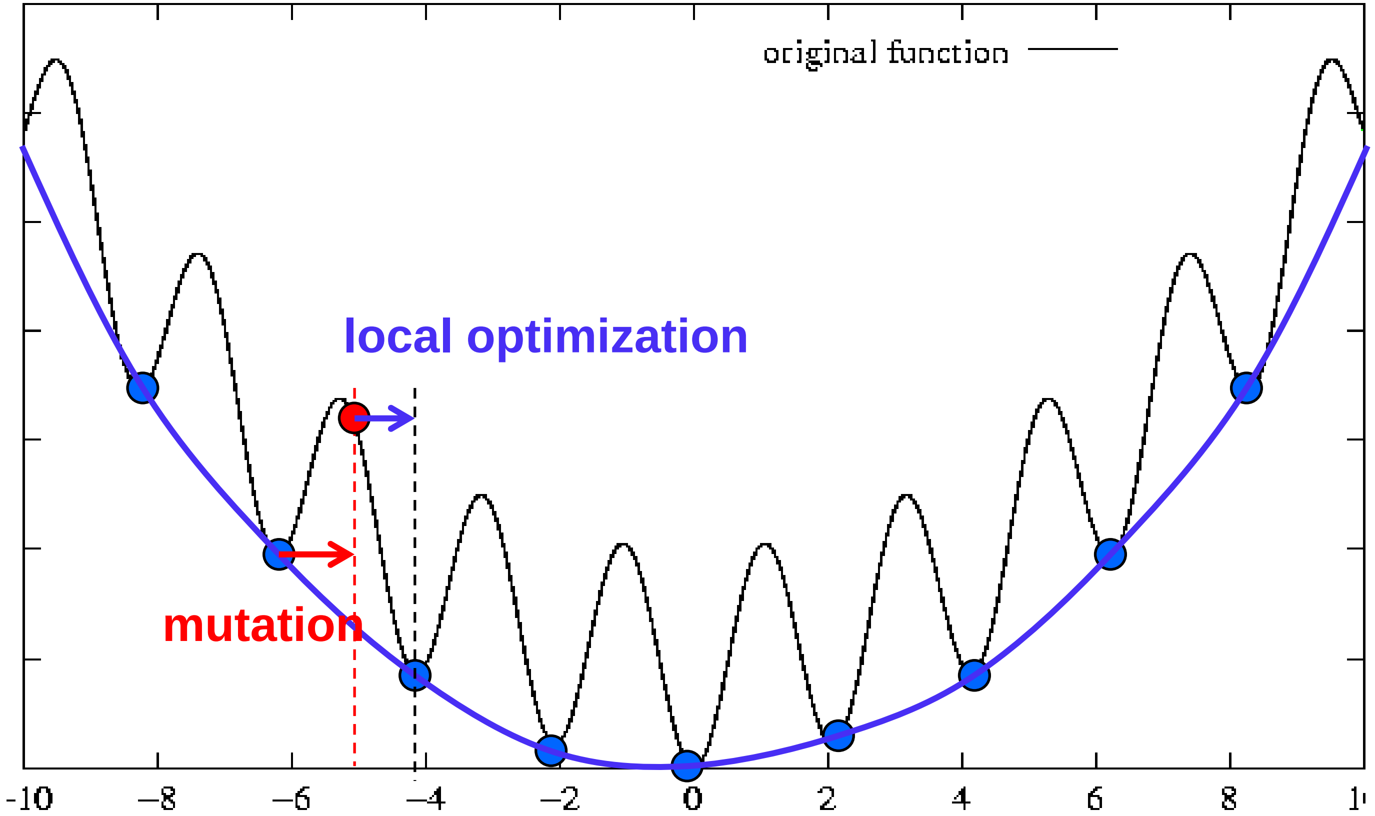
- Mutation Operators
  - Swap
    - exchange two cities
    - e.g. 1-**2**-6-5-**4**-3
  - Insert
    - remove one city and insert it at another position
    - e.g. 1-6-5-2-**4**-3
  - Inversion
    - select a random subtour and inverse the order of these cities
    - e.g. 1-4-**2-5-6**-3

Neighborhood Idea for mutation

- Focus mutation on promising changes
  - Exchange similar partners (neighbors)
  - No disruptive changes
- Example
  - Traveling Salesman Problem
  - Magic Square
- Mutation Operators
  - Swap (Magic Square)
    - exchange **two neighboring numbers**
    - e.g. 1-**2**-6-5-**4**-3
  - Insert (TSP)
    - remove one city and insert it at another position **of a neighboring city**
    - e.g. 1-6-5-2-**4**-3
  - Inversion (TSP)
    - select a random subtour **with neighboring ends** and inverse the order of these cities
    - e.g. 1-4-**2-5-6**-3

Local optimization of each solution generated

- Domain Reduction: Search on local optimas
- Required: fast local optimizer
- removes “obvious” flaws from the offsprings
- Effect on the fitness landscape: smoothing



Local optimization of each solution generated

- Domain Reduction: Search on local optimas
- Required: fast local optimizer
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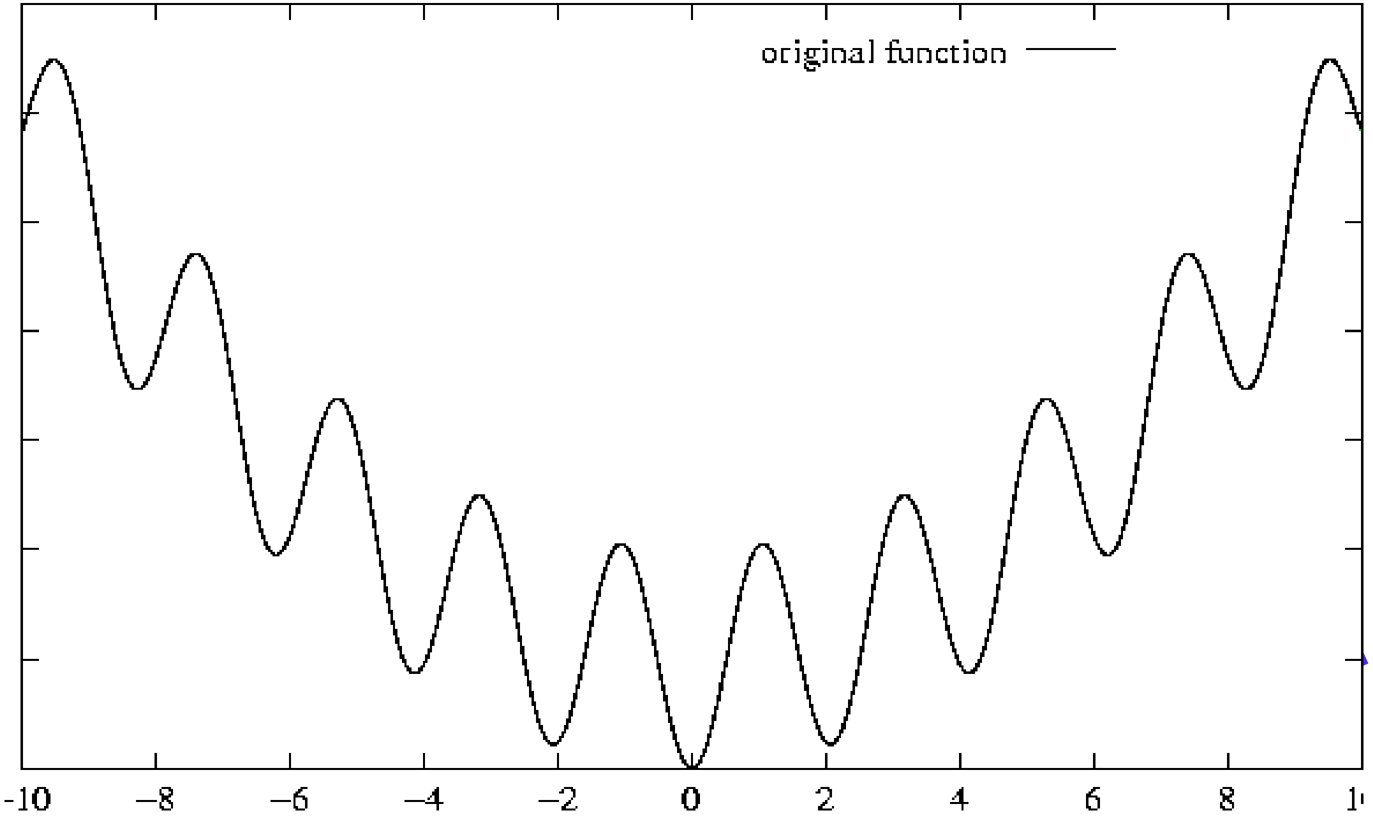
- Effect on the fitness landscape: smoothing
- **Cf. Hillclimbing in the Swiss alps or Spanish Pyrenees**



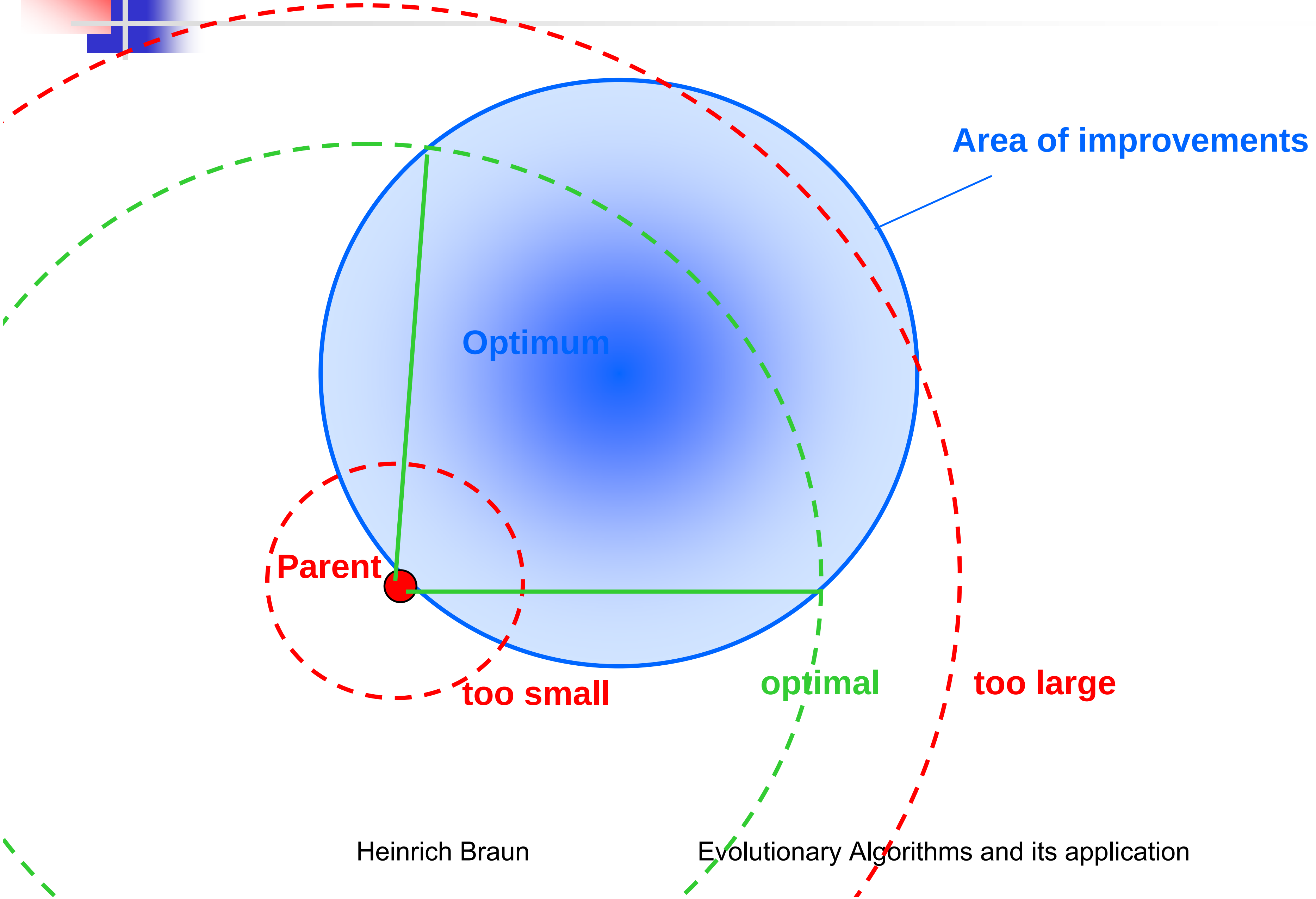
Mutation probability and step size

- For some simple problems
  - mutation rate of 1/n is optimal
  - n: chromosome length

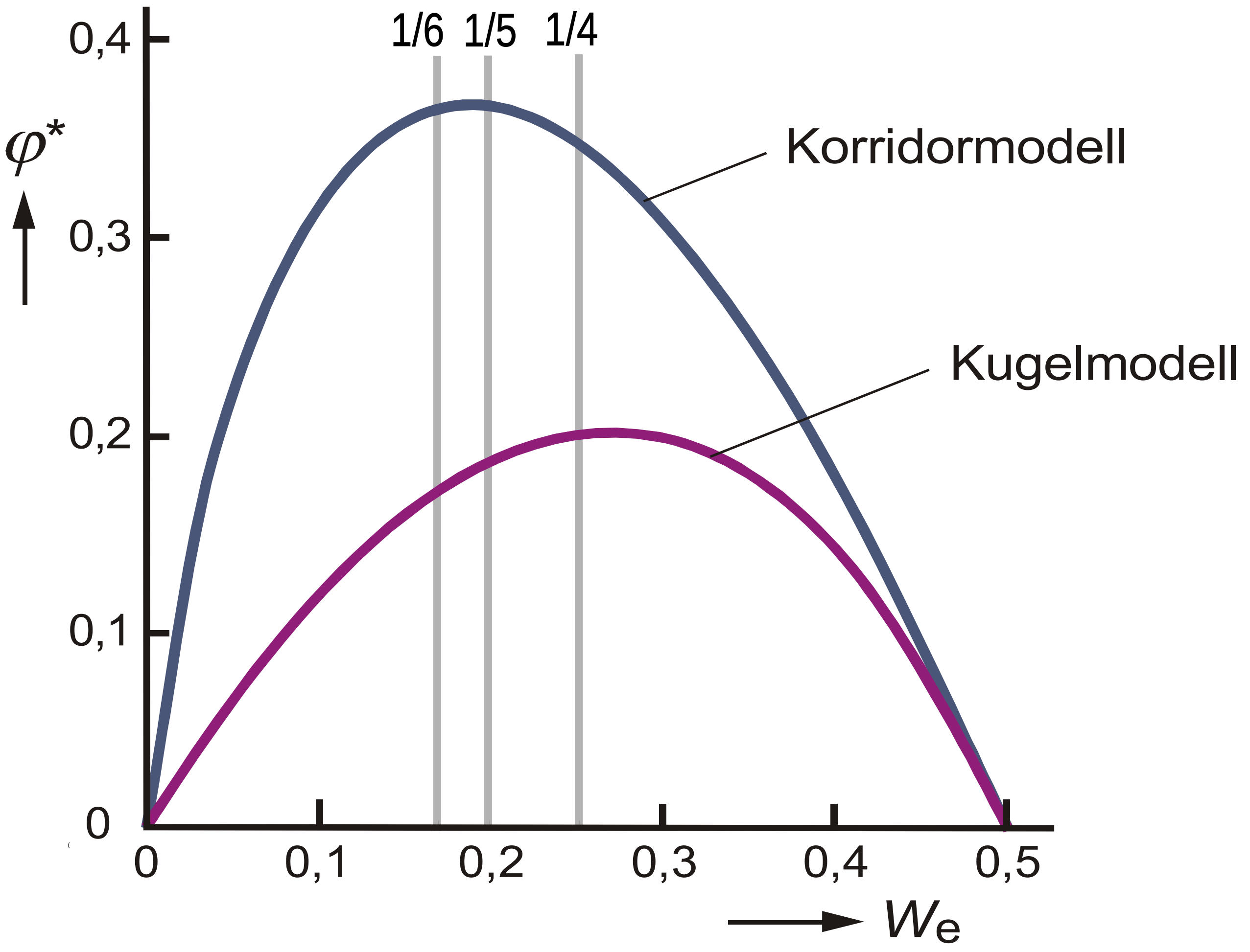
- 1/5 rule
  - 1/5 of mutations should be successful (generate a superior solution)
  - **increase** step size, If rate of successful offspring **>** 1/5,
  - **decrease** step size, If rate of successful offspring **<** 1/5,
  - danger of getting stuck in a local minimum, as mutation rate is decreased there

- self-adaptive mutation
  - expand genotype by control information
  - Step size

Mutation probability and step size – 1/5-rule



Berechnungder optimalen “Schrittweite” von Rechenberg



(**1**+1)-Evolutionsstrategie: 1/5-Erfolgsregel

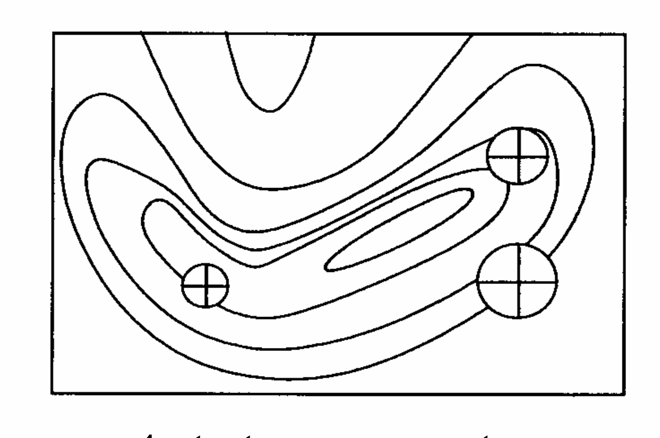
Self-adaptive mutation

- Extend genotype by **strategy parameters**
- These strategy parameters are also subject to evolution
- Simplest example: only one strategy parameter defining the mutation step size (same in every dimension)

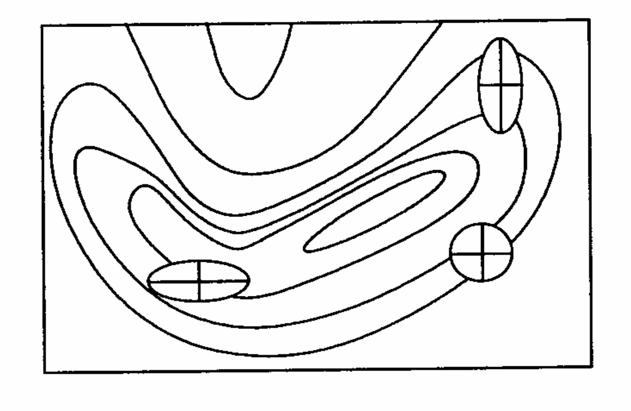
$x = (x_1, x_{2,} ..., x_n, \sigma)$ with $x_i \in \Re$

```
procedure self-adaptive mutation
Input: Individual   $x = (x_1, x_{2,} ..., x_n, \sigma_x)$
begin
    $\sigma_y \leftarrow \sigma_x \exp\left(u / \sqrt{n}\right)$ where u~N(0,1)
  for i=1 to n do
      $y_i \leftarrow x_i + N(0, \sigma_y^2)$
  end //for
  Output: Individual   $y = (y_1, y_{2,} ..., y_n, \sigma_y)$
end
```

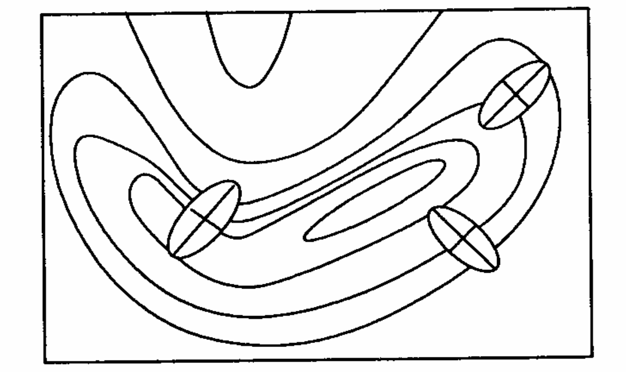
- Remark: it is possible to extend self-adaptation to allow independent mutation step sizes in every dimension. Note, however, that with an increasing number of strategy parameters, self-adaptation becomes slower and slower.



1 strategy parameter



d strategy parameters



d(d+1)/2 strategy parameters

Crossover

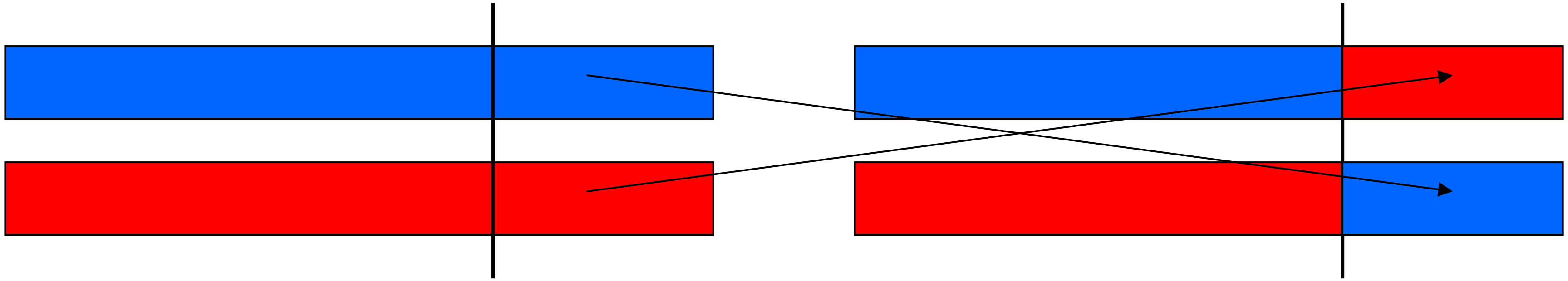
- Main idea
  - combine partial solutions of parents
  - to form new, promising solution

- Try to use as much information from the parents as possible

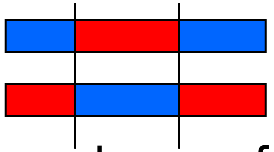
- Refinement
  - similar considerations as neighborhood move operator
  - rather problem specific

Standard crossover

- Exchange genes of the genotypes
- One point crossover:



- Assumption: closely related information should be encoded closely together on the genotype, since this reduces the probability of disruption (cf. Schema Theorem)
- Alternatives with smaller dependence on ordering of genes:
  - two point crossover



  - uniform crossover (decide for each gene from which parent it is chosen)

Special crossover for real values

Let x_i, y_i be the i-th gene of the two parent individuals x and y

- Arithmetic crossover: $z_i = \lambda_i x_i + (1 - \lambda_i) y_i, \quad \lambda_i \in [0 - \varepsilon, 1 + \varepsilon]$

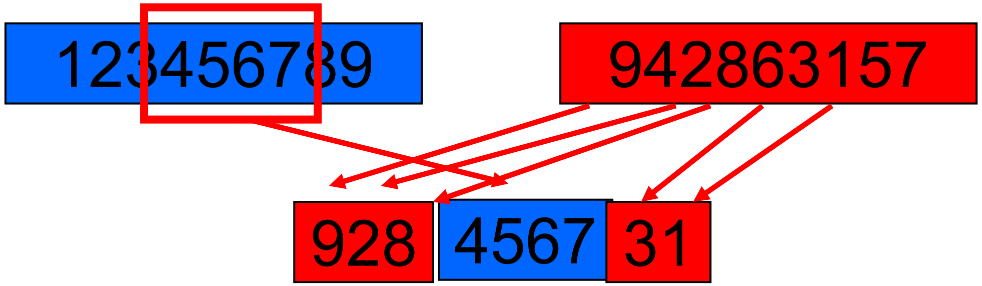
  ⇨

  - ε determines degree of extrapolation
  - if $\lambda_i = \lambda_j = \lambda \quad \forall i, j$ restricted to line between x and y

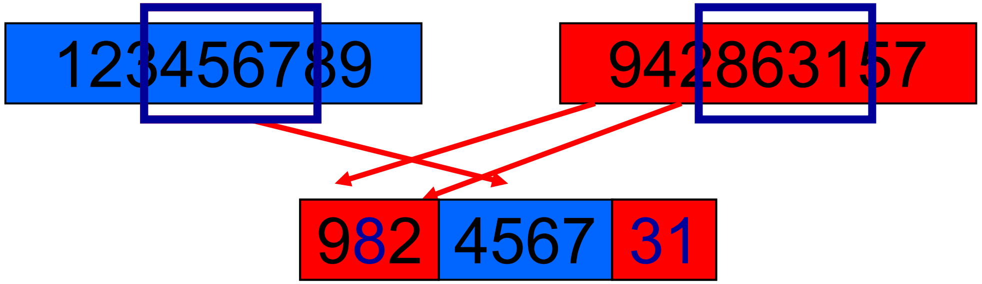
- Discrete Crossover
  - z_i = x_i or y_i
  - Random recombination of the parental genes

Special crossover for TSP

- Order crossover (OX)
  - select partial sequence from one parent, fill up in order of other parent



- Partially mapped crossover (PMX)
  - select partial sequence from one parent, fill up from other parent, resolve conflicts by mapping defined by partial sequence



move without conflict

mapping 4-8, 5-3, 7-1

- Edge recombination crossover (ERX)
  - idea: maintain as many edges from parents as possible (ERX achieves 95% usage of old edges)
  - computationally more expensive

```
procedure edge recombination crossover
$E_x$:= edges from parent x, $E_y$:= edges from parent y
$E_i$:= {e∈$E_x$∪$E_y$|e is incident to city i}
U:= {1,2,3,…,n} // list of all unvisited cities
begin
   select first city c(0) randomly from  $\{i \mid |E_i| = \min_j |E_j|\}$
   for t:=0 to n-2 do
      U ←U \{c(t)}
      if (|$E_{c(t)}$|>0)  // parental edge can be used
         select c(t+1) randomly from  $\{i \mid (|E_i| = \min_{j\in U} |E_j|) \wedge ((i,c(t)) \in E_{c(t)})\}$
      else
         select c(t+1) randomly from  $\{i \mid |E_i| = \min_{j\in U} |E_j|\}$
      end //if
      remove (c(t),i) from all edge sets $E_i$ if contained
   done
end
```

Preferring better individuals

- Necessary to advance the search
- Selection pressure
  - too high: loss of diversity, risk of getting stuck in local optimum
  - too low: no search focus, similar to random search
- Two aspects:
  - preferring better individuals when selecting the parents (usually termed selection step)
  - preferring better individuals when deciding who survives to the next generation (usually termed the reproduction scheme)

Reproduction schemes (who survives to next generation)

Evolutionsstrategien

- (μ,λ)-selection
  - from μ parents, generate λ children
  - the best μ out of the λ children forms the next parent generation
- $(\mu+\lambda)$-selection
  - from μ parents, generate λ children
  - the best μ out of the combined μ parent and λ child individuals form the next parent generation

Genetische Algorithmen

- Generational reproduction ($\cong$ (μ, μ)-selection)
  - generate n children, the children replaces the parent generation
  - usually with **elitism**, i.e. the best solution found so far survives
- Steady-state reproduction ($\cong$ $(\mu+1)$-selection)
  - in each iteration, select only two parents, generate one child
  - the child replaces the worst individual in the population.
- Hillclimbing ($\cong$ $(1+\lambda)$-selection)

Selection probabilities

Let p_i: probability of individual i to be selected as parent

f_i: fitness of individual i

- **Fitness proportional selection**

$$p_i = \frac{f_i}{\sum f_j}$$

  - most common selection scheme for early GAs
  - assumes maximization problem and positive fitness values
  - $f(x)$ und $f(x)+c$ are handled differently
  - if fitness values are all very large, basically no selection pressure
  - basically no selection pressure towards the end of the run (when all individuals are similar)
  - super-individual can take over population quickly (reduced diversity)
  - some pitfalls can be avoided by using normalized fitness values, e.g.
    - subtract minimum fitness value,
      but: influence of worst individual becomes very high

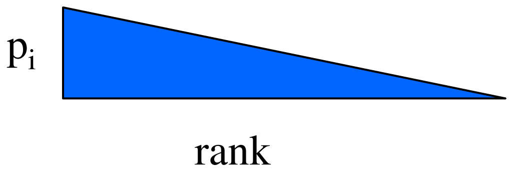
$$f'_i = \frac{f_i - f_{worst}}{f_{best} - f_{worst}}$$

Rank-based selection

Instead of considering fitness values, consider ranks

- Linear ranking selection
  - sort individuals
  - if $r_i \in [1 \ldots n]$ is the rank of individual i, select individuals according to

$$p_i = \frac{b}{n} - \left(\frac{2b-2}{n}\right)\left(\frac{r_i - 1}{n-1}\right)$$



  - constant selection pressure defined by b∈[1,2]

- Tournament selection
  - randomly choose t individuals from the population (usually t=2)
  - select the better one as parent
  - easy to implement, efficient to compute (no sorting)
  - same expected probabilities as linear ranking selection with b=2

Sampling

- Determining an individual’s selection probability, and actually choosing the parents (sampling) are two different things.
- When parents are sampled independently, variance may be high (it is possible that the worst individual is selected n times) high genetic drift

→

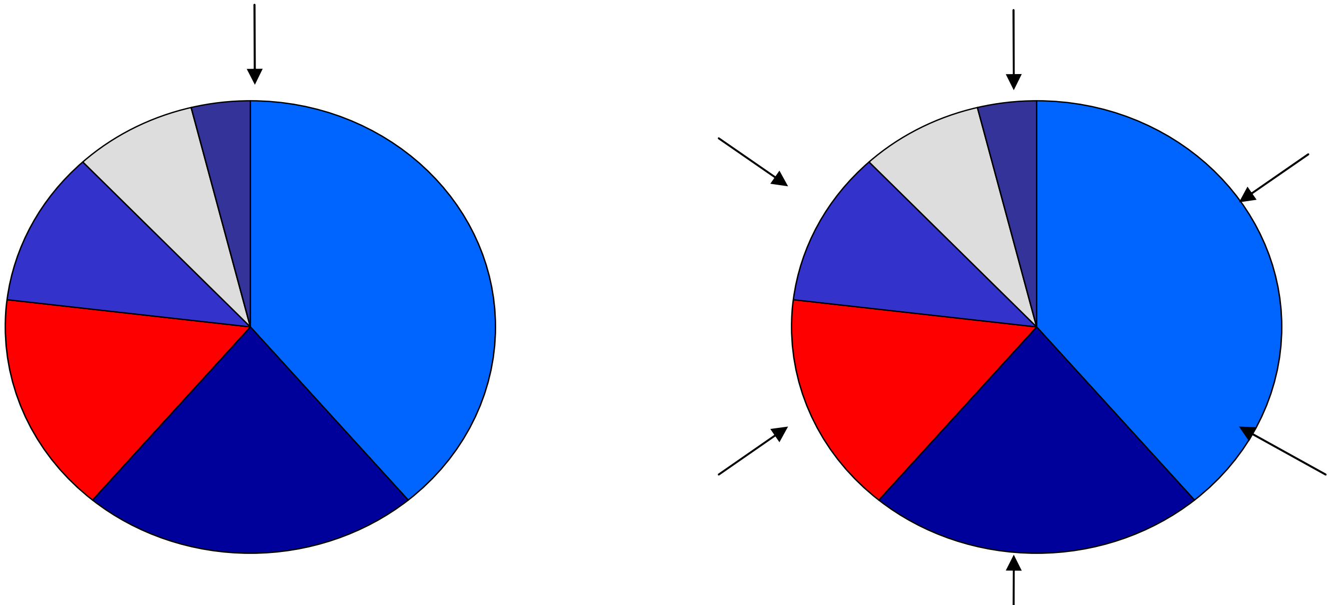
- Genetic Drift: Sampling error due to stochastic nature of selection and finite population size (decreases with increasing population size).

Ind.	f_i	p_i	a_i	$E_i=p_i*n$
1	6.0	0.39	1 0	2.34
2	3.4	0.22	1 0	1.32
3	2.5	0.16	2 0	0.96
4	1.7	0.11	1 0	0.66
5	1.2	0.08	0	0.48
6	0.6	0.04	1 6	0.24
	∑=15.4	∑=1.0	∑=6	∑=6.0

with probability $4.1*10^{-9}$

Stochastic Universal Sampling

- General idea:
  - generate one random variable $\nu\in[0,1]$,
  - select n individuals sequentially:
    for each $k\in\{0,1,..,n\}$ select the individual i, if: $\sum_{k=1}^{i} p_k \,{}_i\!\leq \nu+k/n - \lfloor \nu+k/n \rfloor < \sum_{k=1}^{i+1} p_k$



- each individual is selected at least $\lfloor np_i \rfloor$ and at most $\lceil np_i \rceil$ times
- only one random variable has to be generated to select n individuals

Population size

- If too small
  - not enough diversity in population for crossover to be useful
  - premature convergence
- If too large
  - slow convergence (in terms of fitness evaluations)
- Rule of thumb: 10 – 30

Stopping criteria

- low diversity in population (e.g. avg. fitness = best fitness)
- maximum number of iterations
- no improvement for k iterations