# Intelligent and Adaptable Software Systems

## Advanced Algorithms: Optimization and Search Methods

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12/13



# Course organization

course notes

- Homepage:
  http://trevinca.ei.uvigo.es/~formella/doc/ssia12
- whiteboard
  (illustrations, notations, ideas for proofs, algorithms etc.)
- very short introduction to certain aspects related to optimization and search methods, and some applications



# Course organization

class room hours (preliminary)

Optimization and Search Methods
fridays, 16:00–18:00

| | | | | |
|---|---|---|---|---|
| 28.09. class | 05.10. class | 19.10. (no-class) | 26.10. class | 02.11. lab |
| 09.11. class | 16.11. class | 23.11. class | 30.11. lab | 07.12. lab |
| 14.12. class | 21.12. class | 11.01. class | 18.01. class | 25.01. eval |



# Course organization

class room hours

- Dr. Arno Formella
  office hours: tuesdays, 09:30-13:30 and 17-19

## Bibliography
books

- OUR 519.8.15, OUR 519.8/23, OUR 519.8/24, OUR 519.8/46, OUR 519/17, OUR 519/20



## Your work
homework, lab hours, presentations

- browse through the web pages provided in the following slides
- sort the information provided into the categories of optimization methods as mentioned below
- find a web service that allows you to compute the derivation of a function
- use the NEOS–server to find the minimum of the function

$$f(x) = a(x-b)^2 + c + d\cos(e(x-f)+g)$$

for some (different) values of the parameters (maybe you start with $d = e = f = g = 0$).



## Your work
more extensive research task I

1. form a group with at most one other student
2. select in accordance with Prof. Arno Formella one of the proposed algorithms on the next slide
3. elaborate a not too short and not too long article (6 to 10 pages) about the algorithm, including at least the aspects stated on the next but one slide.



## Your work
more extensive research task II, examples

- Nelder Mead algorithm
- Newton Raphson
- Rodríquez García-Palomares algorithm
- Levenberg Marquardt algorithm
- great deluge algorithm
- local unimodel sampling

## Your work

more extensive research task III

your article should treat the following issues

- description of the algorithm
- main field of application
- advantages and disadvantages compared to other algorithms
- available software/implementations
- critical discussion of their APIs
- references on the algorithm and its applications



## Bibliography I

links

(working in september 2012)

- http://www.neos-server.org
  online optimization project
- http://www.coin-or.org/index.html
  pperation research
- http://www.cs.sandia.gov/opt/survey
  global optimization
- http://www.mat.univie.ac.at/~neum/glopt.html
  global optimization



## Bibliography II

links

- http://www.stanford.edu/~boyd/index.html
  Stephen P. Boyd, Stanford
- http://iridia.ulb.ac.be/~mdorigo/ACO/
  ant colony optimization
- http://plato.asu.edu/gom.html
  continuous global optimization software
- http://www.swarmintelligence.org/index.php
  particle swarm optimization
- Rui Mendes. *Population topologies and their influence in particle swarm performance*. PhD Thesis, Universidad de Minho, 2004.
  http://www.di.uminho.pt/~rcm/



## Motivation

what is it?

Optimizing means

- search for (at least) one solution
- which is different from other possible solutions
- in the sense of being (sufficiently) extreme
- within an ordering
- possibly taking into account certain restrictions
- (within a certain limit of computing time).

Example: hiking in a mountain ridge (with fog).

## Motivation
### examples

Problems which one wants to solve:

- minimizing cost
- maximizing earnings
- maximizing occupation
- minimizing energy
- minimizing resources



## Basic concepts
### observations

the search space and/or the objective function can be

- discrete or continous
- total or partial
- simple or complex, especially in respect to evaluation time
- explicite, implicite, experimental
- linear or non-linear
- convex or non-convex
- differentiable or non–differentiable
- constrained or unconstrained
- static or dynamic

The objective function must be confined.



## Basic concepts
### objective functions

- Minimization
- Maximization
- Obviously any maximization problem can be converted to a minimization problem.



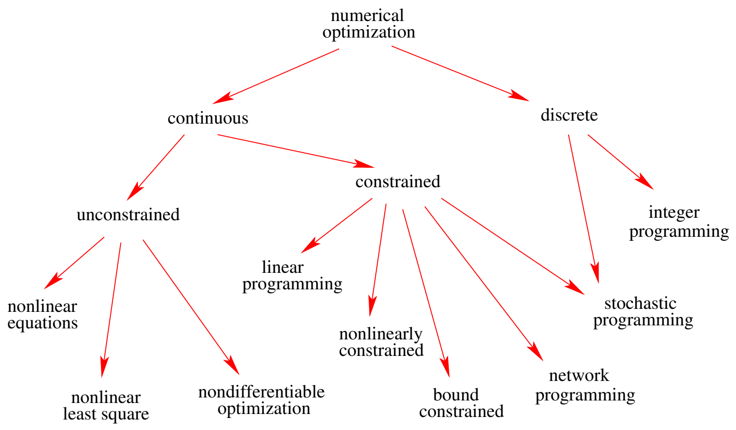
## Basic concepts
### conditions

- restrictions
- feasable solution (feasibility problem)
- coding of the solutions

# Basic concepts

## classification

(after NEOS server (almost), Argonne National Laboratory)






# Basic concepts

## types

to be distinguished

local optimization: usually one starts from an initial solution and stops when having found a local (close) minimum

global optimization: one tries to find the best solution globally (among all possible solutions)



# Basic concepts

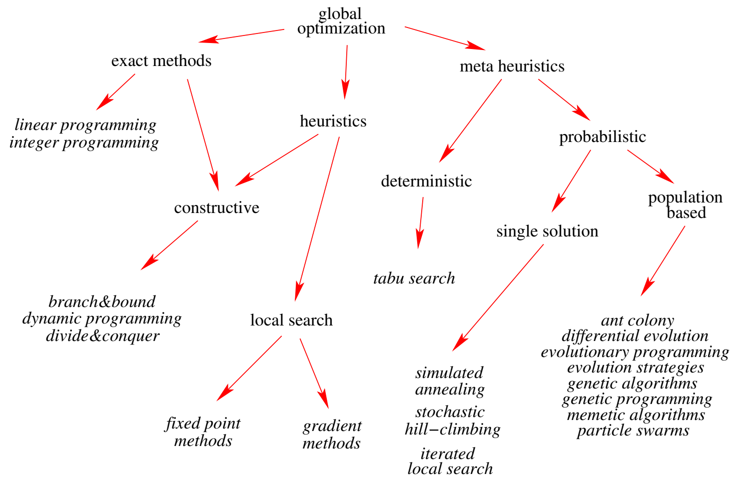
## problems

- The main problem of global optimization is: getting trapped in a local minimum (premature convergence)



# Basic concepts

## global optimization (incomplete intent)



## A real application
psm

approximate Point Set Match in 2D and 3D

An application where we need sophisticated search and optimization techniques.



## Dónde está Wally?



## Motivation
psm

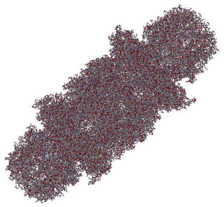
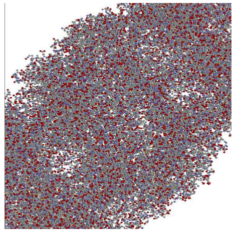
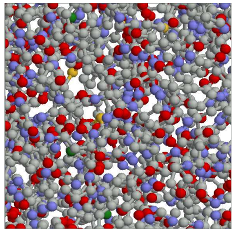
- searching of patterns
  (relatively small sets of two– or three–dimensional points),
  within search spaces
  (relatively large point sets)
- comparing point sets
- key words
  *geometric pattern matching*, *structure comparison*, *point set matching*, *structural alignment*, *object recognition*



## Joint work with

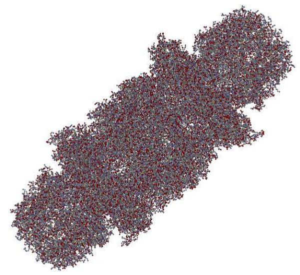
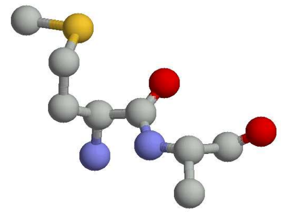
- Thorsten Pöschel
- some ideas from: Kristian Rother, Stefan Günther
- Humboldt Universität—Charité Berlin
  `http://www.charite.de/bioinf/people.html`
- `psm` is one of the algorithms available at
  `http://farnsworth.charite.de/superimpose-web`

## Search of a substructure in a protein
search space



## Search of a substructure in a protein
search pattern



## Dónde está Wally?



## Informal problem description

- given a search space and
- a search pattern,
- find the location within the space which represents best the pattern

## Extensions

- find the best part of the pattern which can be represented within the search space
- allow certain types of deformation of the pattern
- find similar parts within the same point set



## Formal problem description

- search space:
  $S = \{s_0, s_1, \ldots, s_{n-1}\} \subset \mathbb{R}^d, \qquad |S| = n$
- search pattern:
  $P = \{p_0, p_1, \ldots, p_{k-1}\} \subset \mathbb{R}^d, \qquad |P| = k \leq n$
- dimension $d = 2$ or $d = 3$



## Search and alignment

- the aligning process can be separated in two parts
  - find the matching points in the pattern and the search space
  - find the necessary transformation to *move* the pattern to its location
- an approximate alignment must be qualified



## Matching

- a matching is a function that assigns to each point of the search pattern a different point of the search space
- $\mu : P \longrightarrow S$ injective, i.e.,
- if $p_i \neq p_j$ then $\mu(p_i) \neq \mu(p_j)$
- let's write: $\mu(p_i) = s'_i$ and $\mu(P) = S'$

## Transformations

- transformations which maintain distances:
  translation, rotation and reflection
- transformations which maintain angles:
  translation, rotation, reflection and scaling
- deforming transformations:
  shearing, projection, and others (local deformations)



## Congruent and similar transformations

- rigid motion transformation
  (euclidean transformation or congruent transformation)
  only translation and rotation
- similar transformation
  rigid motion transformation with scaling
- we may allow reflections as well (L–matches)
- let $T$ be a transformation (normally congruent)
- we transform the pattern
- let's write: $T(p_i) = p'_i$ and $T(P) = P'$

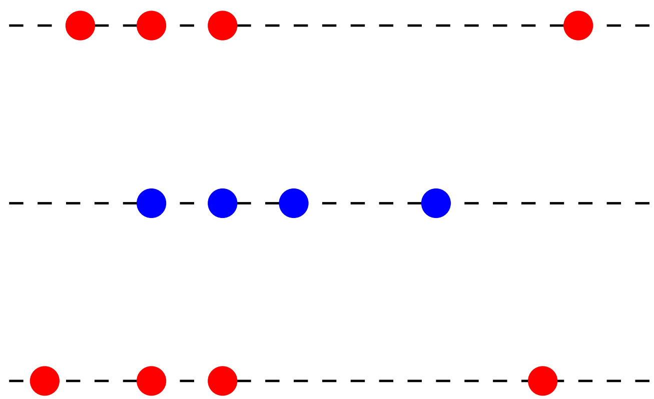


## Alignment

- a matching $\mu$ together with a transformation $T$ is an alignment $(\mu, T)$
- rigid motion transformation: congruent alignment
- with scaling: similar alignment
- with reflection: L–alignment



## One–dimensional example



## Distance of an alignment

- let $(\mu, T)$ be an alignment of $P$ in $S$
- we can measure the distances between transformed points of the pattern and their partners in the search space
- i.e., the distances

$$d_i = d(T(p_i), \mu(p_i)) = d(p_i', s_i')$$

- obviously, if $d_i = 0$ for all $i$
  then the alignment is perfect



## Examples of different distances of an alignment

- root mean square distance (RMS)

$$d = \sqrt{\frac{1}{n}\sum_i (p_i' - s_i')^2}$$

- average distance (AVG)

$$d = \frac{1}{n}\sum_i |p_i' - s_i'|$$

- maximum distance (MAX)

$$d = \max_i |p_i' - s_i'|$$



## Quality of an alignment

- there are many interesting distance measures
- a distance $d$ has its value in $[0, \infty[$
- we use the quality $Q$ of an alignment $Q = 1/(1+d)$
- (other possibility: $Q = \exp(-d)$)
- hence: $Q = 1$ perfect alignment, $Q \in ]0, 1]$
- and: $Q < 1$ approximate alignment



## Formal problem description

- given a search space $S$, and
- given a search pattern $P$
- given a distance measure
- find an alignment $(\mu, T)$ of $P$ in $S$
  with minimum distance $d$ (or maximum quality $Q$)

## Perfect congruent alignments

- congruent alignments in $\mathbb{R}^3$ (Boxer 1999):

$$O(n^{2,5}\sqrt[4]{\log^* n} + \underbrace{kn^{1,8}(\log^* n)^{O(1)}}_{\text{output}}\log n)$$

- for small $k$ the first term is dominant
- $\log^* n$ is smallest $l$ such that

$$\left.2^{2^{\cdots^{2}}}\right\} l\text{−veces} \geq n \qquad \log^* n = 5 \implies n \approx 2^{65000}$$



## Perfect similar alignments

- similar alignments in $\mathbb{R}^3$ (Boxer 1999):

$$O(n^3 + \underbrace{kn^{2,2}}_{\text{output}}\log n)$$

- searching approximate alignments and/or partial alignments is a much more complex problem



## Perfect alignments
ideas

- choose one triangle, e.g. $(p_0, p_1, p_2)$, of $P$
- search for all congruent triangles in $S$ (and their corresponding transformations)
- verify the rest of the points of $P$ (after having applied the transformation)
- the run time is not proportional to $n^3$ (in case of congruence) because we can enumerate the triangles of $S$ in a sophisticated manner and there are not as many possibilities



## Approximate alignments

- as stated, we work in two steps
  - we search for adequate matchings $\mu$ (according to a certain tolerance)
  - we calculate the optimal transformations $T$ (according to a certain distance measure)
- we select the best alignment(s)

## Optimal Transformation

- let $S' = \mu(P)$ be a matching
- let $d$ be a distance measure
- we look for the optimal rigid motion transformation $T$, (only translation and rotation), such that
- $d(T(P), \mu(P)) = d(P', S')$ is minimal



## Root mean square distance

$$d = \sqrt{\frac{1}{n}\sum_i d(p_i', s_i')^2}$$
$$= \sqrt{\frac{1}{n}\sum_i (U \cdot p_i + t - s_i')^2}$$

- $U$ 3x3 rotation matrix, i.e., orthonormal
- $t$ translation vector

Objective: find $U$ and $t$ such that $d$ is minimal



## A little bit of math

we observe: $t$ and $U$ are independent

- with the partial derivative of $d$ according $t$

$$\frac{\partial d}{\partial t} = 2 \cdot \sum_i (U \cdot p_i + t - s_i') = 2U\sum_i p_i + 2nt - 2\sum_i s_i'$$

we obtain

$$t = -U\frac{1}{n}\sum_i p_i + \frac{1}{n}\sum_i s_i'$$
$$= -U \cdot p_c + s_c'$$

- where $p_c$ and $s_c'$ are the centroids of both sets



## Optimal Rotation

- with the above, $d$ can be written as

$$d = \sqrt{\frac{1}{n}\sum_i (U \cdot p_i + t - s_i')^2}$$
$$= \sqrt{\frac{1}{n}\sum_i (U \cdot (p_i - p_c) - (s_i' - s_c'))^2}$$

- where $U$ is a matrix with restrictions (has to be orthonormal)

## Extremal points of functions with restrictions

- one converts the problem with restrictions
- with the help of LAGRANGE multiplies into
- a problem without restrictions
- which exhibits the same extremal points



## Let's skip the details

- basically, we calculate first and second derivative according to the entries $u_{ij}$ of $U$
- we search for the extremal points
- KABSCH algorithm 1976, 1978
- open source code at my home page



## KABSCH algorithm

- let $\mathbf{S}$ be the matrix of rows containing the $s_i'$
- let $\mathbf{P}$ be the matrix of rows containing the $p_i$
- we compute $\mathbf{R} = \mathbf{S} \cdot \mathbf{P}^\top$
- we set $\mathbf{A} = [\mathrm{a}_0\ \mathrm{a}_1\ \mathrm{a}_2]$ with $\mathrm{a}_k$ being the eigenvectors of $\mathbf{R}^\top \mathbf{R}$
- we compute $\mathbf{B} = [\|\mathbf{R}\mathrm{a}_0\|\ \|\mathbf{R}\mathrm{a}_1\|\ \|\mathbf{R}\mathrm{a}_2\|]$
- and finally, we get $U = \mathbf{B} \cdot \mathbf{A}^\top$



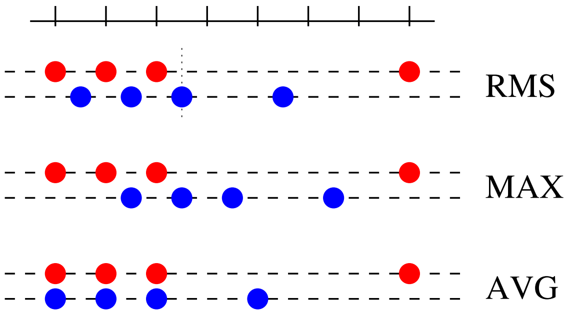
## Introduction of scaling

- let us introduce a scaling value $\sigma \in \mathbb{R}$

$$d = \sqrt{\frac{1}{n}\sum_i (\sigma U \cdot (p_i - p_c) - (s_i' - s_c'))^2}$$

- let $p_i'' = U \cdot (p_i - p_c)$ be the translated and rotated point $p_i$
- let $s_i'' = s_i' - s_c'$ be the centralized point $s_i'$
- the solution for the optimal $\sigma$: $\sigma = \dfrac{\sum_i \langle s_i'', p_i'' \rangle}{\sum_i \langle p_i'', p_i'' \rangle}$

## Different distance measures—different alignments






## Optimal transformations for non–derivable distance measures

- if the function for $d$ is not derivable, e.g., the average
- we use a gradient free optimization method (only with evaluations of the function)
- recently developed iterative method that is guaranteed to converge towards a local minimum
- algorithm of RODRÍGUEZ/GARCÍA–PALOMARES (2002)



## Idea behind RODRIGUEZ/GARCIA–PALOMARES

- let $f(\mathbf{x})$ be the function to be minimized
- we iterate contracting and expanding adequately parameters $h^k > 0$ and $\tau > 0$ such that
- $f(\mathbf{x}_{i+1}) = f(\mathbf{x}_i \pm h^k \mathbf{d}_k) \leq f(\mathbf{x}_i) - \tau^2$
- where $\mathbf{d}_k$ is a direction taken from a finite set of directions (which depends on the point $\mathbf{x}_i$)
- with $\tau \longrightarrow 0$, $\mathbf{x}_i$ converges to local optimum (while there are no constraints)



## Rotation in *quaternion space*

- a rotation $U \cdot p$ of the point $p$ with the matrix $U$ can be expressed as
- $q \star \bar{p} \star q^{-1}$ in quaternion space $\mathbb{H}$ (HAMILTON formula, $\mathbb{C} \sim \mathbb{R}^2$, $\mathbb{H} \sim \mathbb{R}^4$)
- where $\bar{p} = (0, p)$ is the canonical quaternion of the point $p$
- and $q = (\sin(\varphi/2), \cos(\varphi/2)u)$ is the rotation quaternion (with $u \in \mathbb{R}^3$ being the axis and $\varphi$ the angle of rotation)
- instead of $U$ with 9 constraint variables we have $u$ and $\varphi$, i.e., 4 unconstraint variables

## Matching Algorithms

1. maximal clique detection within the graph of compatible distances
2. geometric hashing of the pattern
3. distance geometry



## Maximal clique detection

- we generate a graph $G = (V, E)$ (graph of compatible distances)
- vertices $v_{ij} \in V$ all pairs $(p_i, s_j)$
- edges $e = (v_{ij}, v_{kl}) \in E$, if $d(p_i, p_k) \approx d(s_j, s_l)$
- search for maximum cliques in $G$



## Properties of Clique Detection

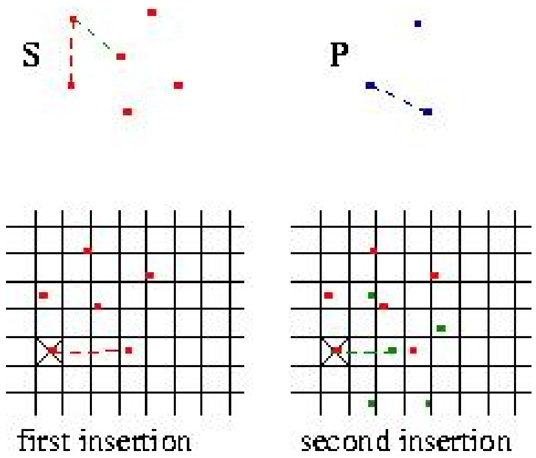
- the problem is NP–complete
  (however, we search only for *cliques* of size $\leq k$)
- fast algorithms need adjacency matrices
- if $n = |S| = 5000$ and $k = |P| = 100$ we need 30 GByte
  (counting only one bit per edge)



## Geometric hashing

- preprocessing of the search space
- let's describe the two–dimensional case
  - we align each pair $(s_i, s_j)$
    with $s_i$ at the origin and $s_j$ in direction $x$
  - we insert some information for each other point $s_k \in S$
    in a hashtable defined on a grid over $S$

## Example: geometric hashing






## Searching with geometric hashing

- we simulate an insertion of the points of $P$ into the hashtable
- but we count only the non–empty entries
- many votes reveal candidates for partial alignments
- e.g., if we encounter a pair $(p_i, p_j)$ such that
  for each other point of the pattern there is a non–empty cell in the hashtable
  we have found a perfect candidate



## Properties of geometric hashing

- grid size must be selected beforehand
- preprocessing time $O(n^{d+1})$
- searching time $O(k^{d+1})$
- works only for rigid motion transformations



## Distance geometry

- we represent both sets $S$ and $P$ as distance graphs
- the vertices of the graphs are the points of the sets
- the edges of the graphs hold the distances between the corresponding vertices
- e.g., $G_P = (P, P \times P)$ complete graph

## The ideas behind psm

- we define adequate distance graphs $G_P$ and $G_S$
- we search for subgraphs $G'_S$ of $G_S$ that are congruent to the graph $G_P$
  (allowing certain tolerances)
- we optimally align $G_P$ with the subgraphs of $G'_S$
- we select the best one among all hits

- we extend the search to work with subgraphs of $G_P$ as well
- we select a best subgraph as final solution



## The four main steps of psm

- construction of the graphs
  with: exploitation of locallity properties
- search of subgraphs
  with: sophisticated backtracking
- alignment
  with: minimization of cost functions
- search of partial patterns
  with: reactive tabu search



## Construction of the graphs

- let us assume that the pattern $P$ is small
- we construct $G_P$ as the complete graph
- we generate a dictionary $D$
  (ordered data structure)
  that contains all distances (intervals) between points in $P$
- we consider an edge between two vertices in $G_S$
  if the distance is present in the dictionary $D$



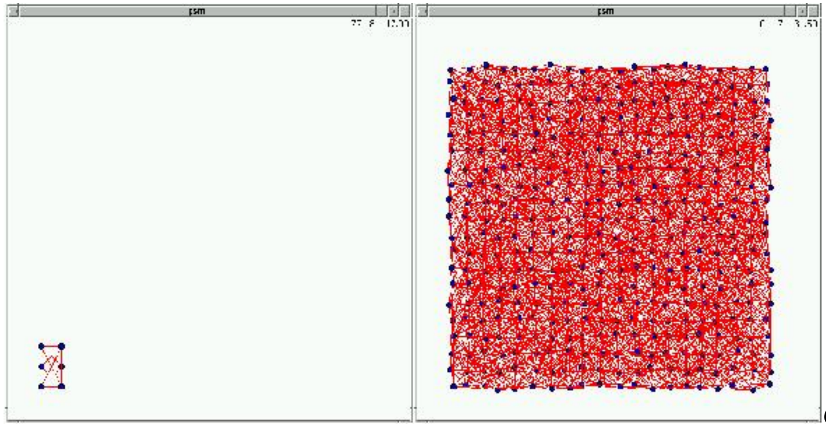
## Construction of the dictionary

- let $d_{ij} = d(p_i, p_j)$ be the distance between two points of $P$
- the dictionary will contain the interval

$$[\ (1-\varepsilon)\cdot d_{ij}\ ,\ (1+\varepsilon)/(1-\varepsilon)\cdot d_{ij}\ ]\ \in D$$

  where $0 \leq \varepsilon < 1$ is an appropriate tolerance
- the upper limit can be simplified to $(1+\varepsilon)$
  (but we loose the symmetry)
- we can join intervals in the dictionary $D$ if they intersect

## Construction of the graphs that way

$G_P$  $G_S$

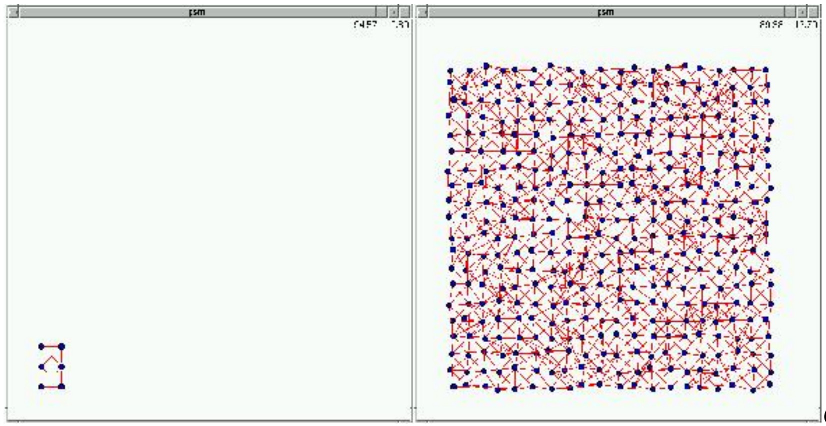


## Fast construction of the graphs

- we construct $G_P$ as a connected (and rigid) graph mantaining only the short edges
- we order the points of $S$ previously in a grid of size similar to the largest of the intervals



## Construction of the graphs that way

$G_P$  $G_S$



## Matching

- let us assume (at the beginning) that $G_P$ is a complete graph
- we order the points of $G_P$ according to any order e.g. $(p_0, \ldots, p_{k-1})$
- we apply a backtracking algorithm that tries to encounter for earch $p_i$ a partner $s_i$ following the established ordering
- hence:

## Backtracking for the search

- let us assume that we already found a subgraph $G_{s_0,\ldots,s_i}$ where the graph $G_{p_0,\ldots,p_i}$ can be matched
- we look for candidates $s_{i+1}$ for the next point $p_{i+1}$
  - that must be neighbors of the point $s_i$ within $G_S$
  - that must not be matched already and
  - that have similar distances to the $s_j$ ($j \leq i$) as the $p_{i+1}$ to the $p_j$ ($j \leq i$)
- while there is a candidate we advance with $i$
- if there are no more candidates for $s_{i+1}$, $s_i$ cannot be a partner for $p_i$ neither (i.e.: backtracking)



## Termination of the algorithm

- the algorithm *informs* each time a candidate for for $p_{k-1}$ has been found
- the algorithm terminates when
  - there are no more candidates for $p_0$ or
  - the first solution has been found



## Optimizations of the basic algorithm

- reduction of the edges in $G_P$ implies: reduction of the edges in $G_S$
- *good* ordering of the $p_i$ implies: reduction of the number of candidates
- consideration of the type of point (e.g. element type of the atom) implies: reduction of the number of candidates
- all heuristics imply: the backtracking advances faster



## Search for partial alignments

- find the subset of the points of the pattern that can be matched best to some points in the search space
- NP–complete
- there are $|\mathscr{P}(P)| = 2^k$ possibilities to choose a subset
- we apply:
  - genetic algorithm
  - reactive tabu search

## Genetic Algorithm

- maintain graph $G_S$ as complete graph
- genome: sequence of bits indicating if a point belongs to the actual pattern or not
- crossover: *two point crossover*
- mutation: *flip*
- selection: roulette wheel
- cost function: distance and size of alignment



## Termination of the GA

- it is not that easy
- once the first solution has been found
- once a sufficently good solution has been found
- after a certain number of iterations
- once diversity of population is too low



## Problems with GA

- $G_S$ must be a complete graph
  You know a crossover operation for non–complete graphs?
- more precisely:
  we need a crossover (and mutation) operation that maintains a specific property of the graphs (e.g., connectivity, rigidness)
- or some new idea...



## Reactive Tabu Search

- we start with an admissible solution
- we search for possibilities to improve the current solution
- if we can: we choose one randomly
- if we cannot:
  - we search for possibilities to reduce the current solution
  - if we can: we again try improvements
  - if we cannot: we jump to another admissible solution

## The Tabu criterion

- we avoid repetitive movements taking advantage of a memory that stores intermediate solutions
- i.e.: we mark certain movements as tabu for a certain number of iterations
- reactive means: we adapt the tabu period dynamically



## Quality of a partial alignment

- evaluation of the cost of a solution: number of aligned points plus quality of the alignment
- remember: quality $Q \in ]0,1]$, but we will use $Q \geq$ threshold
- hence, maximal quality: $|P| + 1$



## Reactive Tabu Search for `psm`

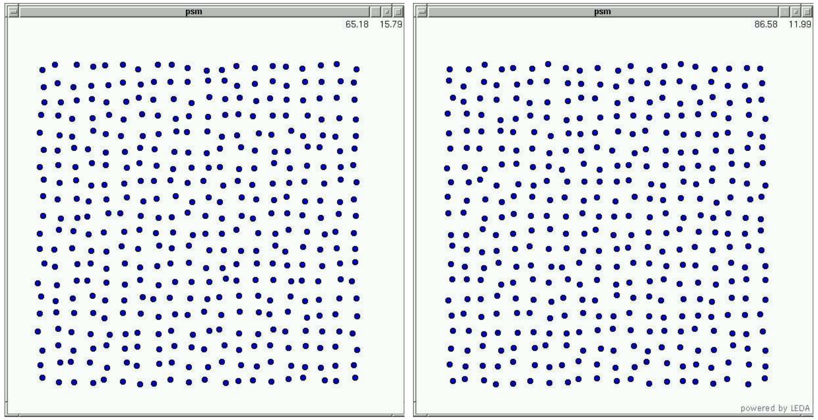
- representation of the problem: sets of indices of the matched points
- search for candidates to improve (*add*): (rigidly) connected neighbors within graph $G_S$
- search for candidates to reduce (*drop*): any point of the current solution that mantains the graph $G_S$ connected (and rigid)



## When do we terminate?

- not that simple
- once we found a sufficiently good solution
- once we have run a certain number of iterations

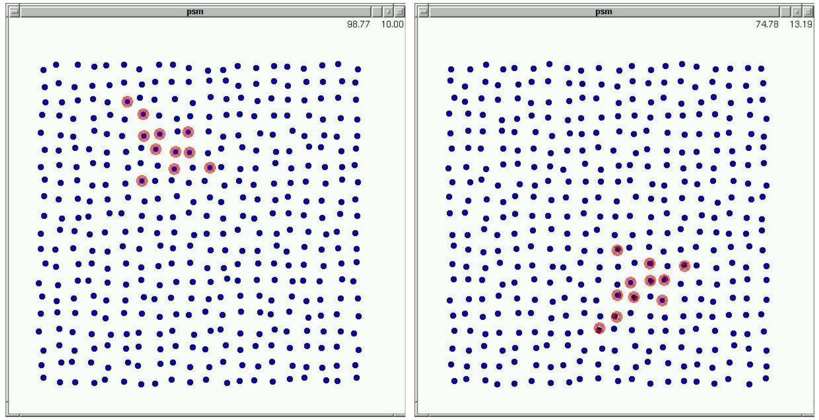
# Search for the largest common pattern




*P* *S*



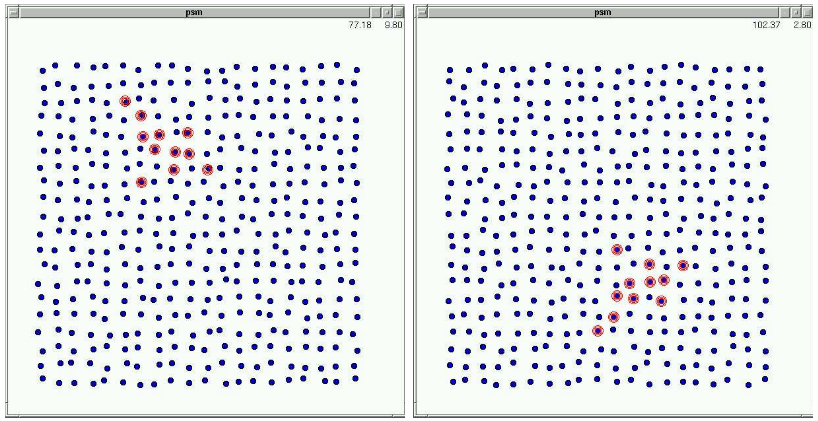
# Search for the largest common pattern




$p/P$ $p/S$



# Search for the largest common pattern




$s/P$ $s/S$



# Search for pattern with deformation

- instead of the complete graph use a connected sparse graph
- parts of the graph could be rigid
- the graph may specify hinges or torsion axis

## psm

- command line tool with configuration file
- GUI
- web–site to perform searches



## Possible extensions

- enumerate more rigorously all locations
  (up to now we have concentrated on the best solution)
- extend the properties of the graphs defining deformations of the pattern (e.g. torsion of parts, restriction of angles)
- allow local tolerances (e.g. per edge), especially with preknowledge of the biochemical properties
- improve heuristics with statistical analysis of distributions of distances (*look for the unusual first*)
- improve the user interface
- more applications



## No free lunch theorem

### theory

Basically states:

*The performance of all optimization algorithms amortized over all objective functions is always equal (in discrete spaces).*

With consequence: no algorithm can outperform (in general) exhaustive search (or even random search).



## No free lunch theorem

### reality

Fortunely, we are not interested in optimizing *some* function, rather we like to optimize a *specific* one, i.e., an optimization algorithm is only useful in *his field* (because necessarily there are fields where its performance is very poor).

# optimUMTS

`optimUMTS`

Optimization of wireless UMTS networks



# Joint work with

- Fernando Aguado
  Departamento de Teoría de la Señal
  Universidad de Vigo
- Luis Mendo
  Universidad Politécnica de Madrid



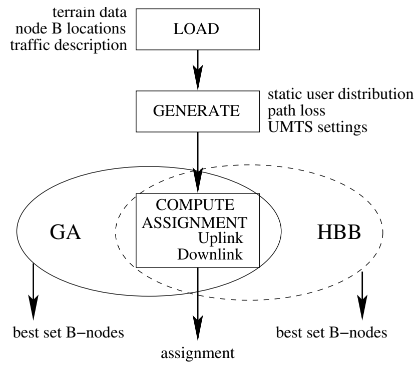
# Objectives

- given a set of possible nodes B (base stations)
- find optimal subset
- to guarantee certain services (bandwidth)
- to an estimated user distribution

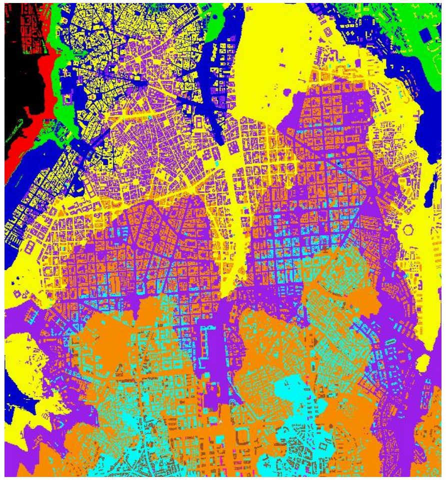


# Principal algorithm

## evolutionary and exact



## Cartography of Madrid
input data





## Calculation of attenuation matrix $\alpha$
indirect input data

- simple logarithmic decay

$$L(m,k) = 10^{0{,}1\cdot(32{,}2+35{,}1\cdot\log(d(m,k)))}$$
$$\alpha(m,k) = \frac{G_{\text{eff}}(m)\cdot G_{\text{eff}}(k)}{L(m,k)}$$

- simplied Xia model
- mixed model: close—Xia, far—simple



## Coverage around a node B
computed input data



## Traffic distribution
stochastic input data

- static distribution
- grid of estimated user with activation percentage
- polygons with Poisson process per service
- uniform distibution everywhere or only on streets

## Calculation of SIR
objective function, part I

- uplink SIR $\gamma_{UL}$:

$$\gamma_{UL}(m,k) = (E_b/N_0)_{UL} \cdot b_0(k)/B_0$$

- downlink SIR $\gamma_{DL}$:

$$\gamma_{DL}(m,k) = (E_b/N_0)_{DL} \cdot b_0(k)/B_0$$



## Calculation of noise
objective function, part II

- uplink noise $N_T(m)$ at transmitter $m$:

$$\begin{aligned} F(m) &= 10^{0{,}1 \cdot N^F(m)} \\ N(m) &= k_B \cdot T_{\text{amb}} \cdot B_0 \cdot F(m) \end{aligned}$$

- downlink noise $N_R(k)$ at receiver $k$:

$$\begin{aligned} F(k) &= 10^{0{,}1 \cdot N^F(k)} \\ N(k) &= k_B \cdot T_{\text{amb}} \cdot B_0 \cdot F(k) \end{aligned}$$



## Calculation of power (Hanly and Mendo)
objective function, part IVa, iterative method

- initial power $P_0(k)$ for receiver $k$:

$$t_0(m,k) = \frac{\gamma_{UL}(m,k)}{\alpha(m,k)} \cdot N(m) \qquad P_0(k) = \min_m\{t(m,k)\}$$

- power $P_i(k)$ for receiver $k$ in iteration $i$:

$$\begin{aligned} s_i &= P_{i-1} \cdot \alpha(m) \\ t_i(m,k) &= \frac{\gamma_{UL}(m,k)}{\alpha(m,k)} \cdot ((s_i - P_{i-1}(k) \cdot \alpha(m,k)) \cdot a(k) + N(m)) \\ P_i(k) &= \min_m\{t_i(m,k)\} \end{aligned}$$



## Termination criteria for iteration
objective function, part IVb, iterative method

$$\begin{aligned} \exists k \text{ with } P(k) > P_{\max}(k) &\implies \text{no assignment} \\ i > I_{\max} &\implies \text{no assignment} \\ \max_k \left\{ \frac{P_i(k)}{P_{i-1}(k)}, \frac{P_{i-1}(k)}{P_i(k)} \right\} \leq \Delta &\implies \text{assignment possible} \end{aligned}$$

## Calculation of assignment

objective function, part V

$$A(k) = m \text{ with } t(m,k) = \min_m \{t(m,k)\}$$
$$P(k) = \min_m \{t(m,k)\}$$



## Validation of assignment

objective function, part VI

- uplink:

$$P_{\min}(k) \leq P(k) \leq P_{\max}(k)$$



## Direct solution

objective function, part VII

- downlink:

$$\beta(n,k,m) = \begin{cases} \rho(m,k) & \text{if } m=n \\ 1 & \text{otherwise} \end{cases}$$

calculation of SSIR $\tilde{\gamma}$:

$$\tilde{\gamma}(m,k) = \frac{\gamma_{DL}(m,k)}{1+\rho(m,k)\cdot\gamma_{DL}(m,k)}$$



## System to solve for transmitter power calculation

objective function, part VIII

$$H(m,n) = \delta_{m,n} - \sum_{k\in\mathscr{A}^{-1}(m)} \frac{\alpha(n,k)\cdot\beta(n,k,m)\cdot\tilde{\gamma}(m,k)}{\alpha(m,k)}$$
$$v(m) = P_{\mathrm{plt}}(m) + \sum_{k\in\mathscr{A}^{-1}(m)} \frac{\tilde{\gamma}(m,k)\cdot N(k)}{\alpha(m,k)}$$
$$H\cdot T = v$$

## Validation of power restrictions
restrictions I

- validation of maximum power of transmitter $m$:

$$0 < T(m) \leq T_{\max}(m)$$



## Validation of power restrictions
restrictions II

- calculation of downlink power of receiver $k$:

$$P(k) = \frac{\tilde{\gamma}(m,k)}{\alpha(A(k),k)} \left( \sum_{m=1}^{M} \alpha(m,k) \cdot \beta(m,k,A(k)) \cdot T(m) + N(k) \right)$$

- validation of transmitter maximum channel power:

$$P(k) \leq P_{\text{chn}}$$



## Optimization with heuristic backtracking
exact method

Observation:

- if there is no assignment with certain $m$ nodes B
- then there is no assignment with less nodes B

hence

- start with all nodes B
- eliminate nodes B til optimum found with heuristic backtracking



## Termination with heuristic backtracking

- stop if stagnation occurs
  (if within a subtree all minimum solutions are at the same depth)
- finds optimum solution

## Heuristics
how to be fast at the beginning

- ordering of nodes B plays an important role in finding fast good solutions
- reorder nodes B for backtracking according to heuristics
- for instance: eccentricity, random, number of initial connections, etc.



## Optimization with genetic algorithm (GA)
evolutionary method

- steady-state incremental evolution
  (in each iteration two new decendents are generated)
- selection: roulette wheel
- mutation: flip
- crossover: two–point–cyclic
- quality: number of nodes B plus power as tiebreak

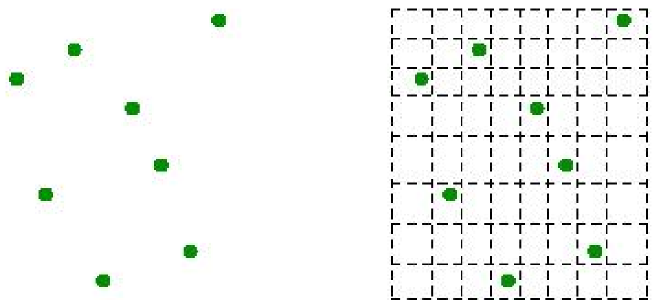


## Genom generation I

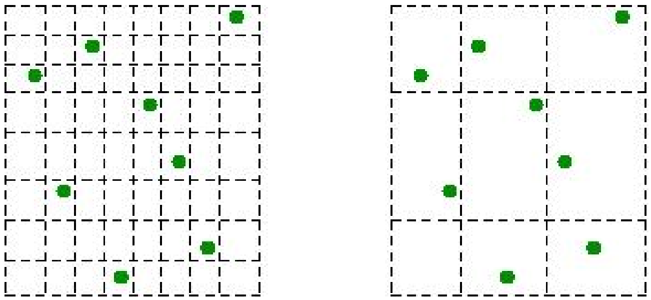
- matrix representation of nodes B
- exploiting locality properties
- using allele: usable, unusable, used, fixed



## Genom generation II

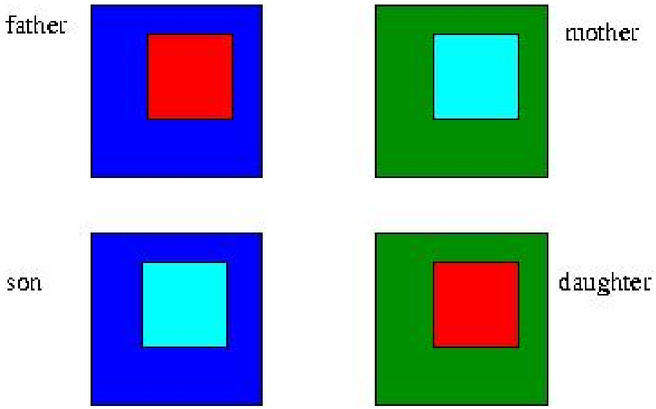


# Genom generation III



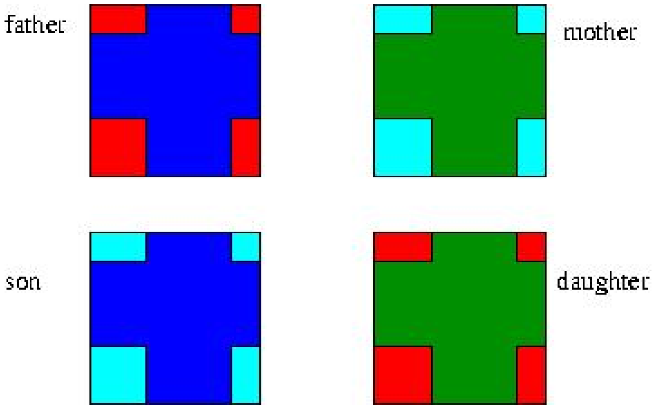


# Crossover I



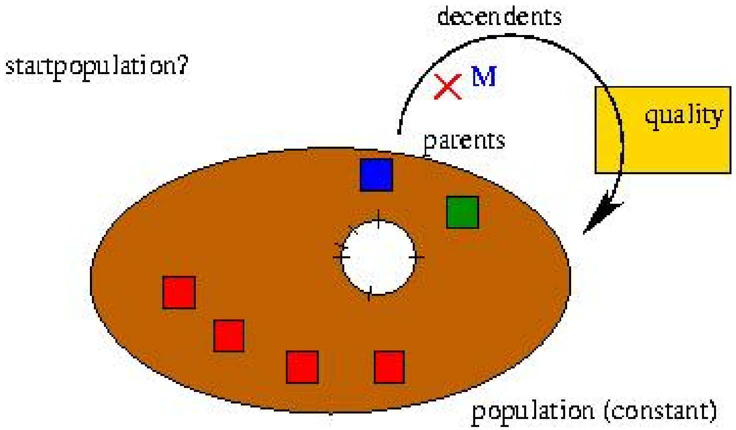



# Crossover II

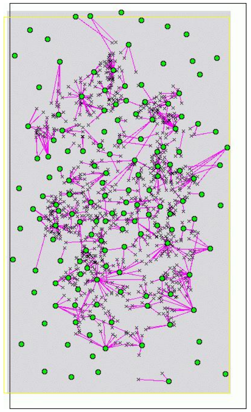


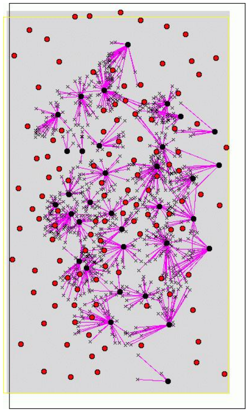



# Evolution



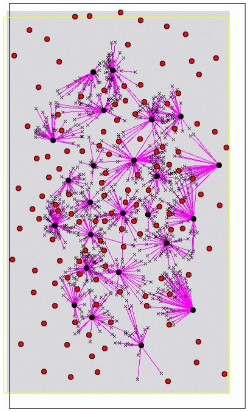
## Assignment and heuristic branch result

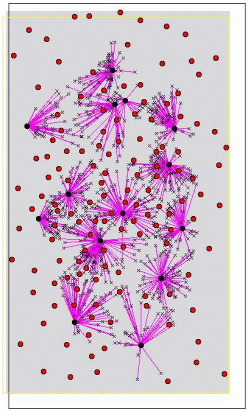






## GA results with and without downlink







## Further research and implementations

- use of MonteCarlo method
- to find best subset of nodes B
- for several user distributions
- i.e., find best subset to satisfy different scenarios



## `shaprox`

Approximation of point sets with shapes

## Informal problem description

- given a set of points in the plane
- construct a geometric figure interpolating the sample points
- that reasonably captures the shape of the point set

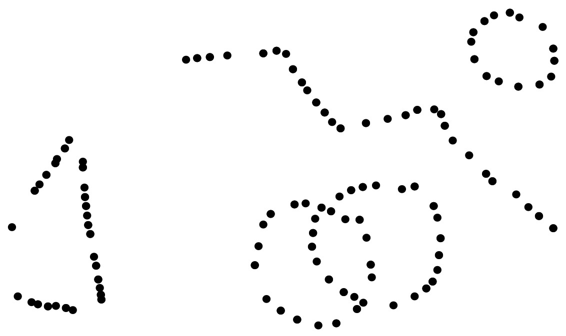


## Applications

- pattern recognition
- object definition in geographic information systems
- CAD/CAM services
- vectorization tasks
- curve reconstruction in image analysis
- single–computation pose estimation
- geometric indexing into pictorial databases
- shape tracking etc.

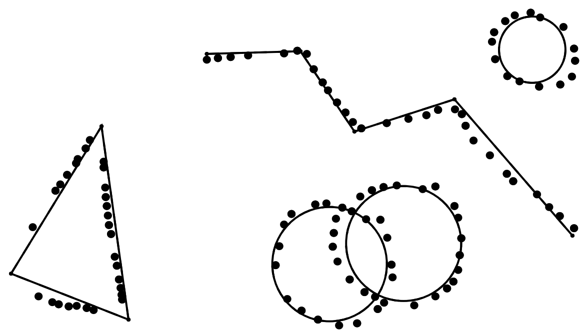


## Example
point set



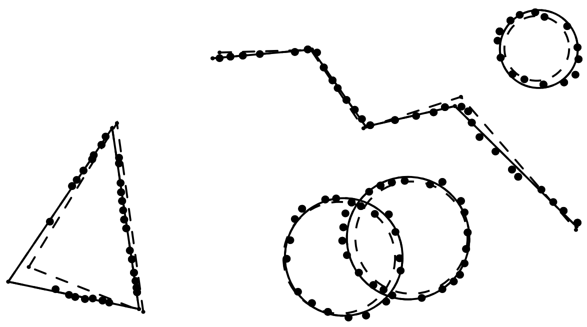


## Example
initial shapes



# Example

adapted shapes





# Approximation task

Three steps:

- clustering of the points to identify the individual parts of a set of shapes,
- generating of an initial guess of the individual shapes,
- adapting the individual shapes to the underlying point set according to some distance metric.



# Brain storming

distances, metrics, optimization, local and global minima, discrete–continuous, partially plain functions, multi–objetive optimization, local decisions, multi–scale, simplification, VORONOI–diagram, DELAUNAY–diagram, graph analysis, similarity detection, classification (with and without supervision), filtering



# Polygonal approximation

type of clustering

- Given a set of points of a plane curve,
- construct a polygonal structure
- interpolating the sample points
- that reasonably captures the shape of the point set.

# Three approaches for polygonal approximation

- $\alpha$–shapes
- crust
- curve approximation



# Alpha–shapes

## application

The algorithm is able to detect

- the outer boundary of a set of points
- which covers more or less evenly distributed the interior of a shape.



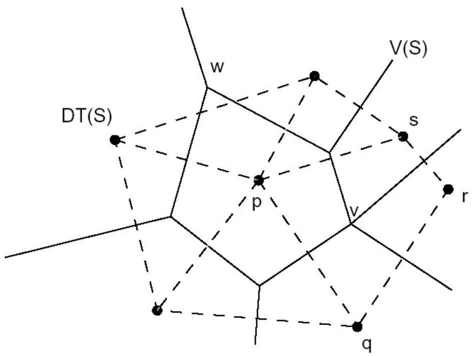
# Alpha–shapes

## algorithm

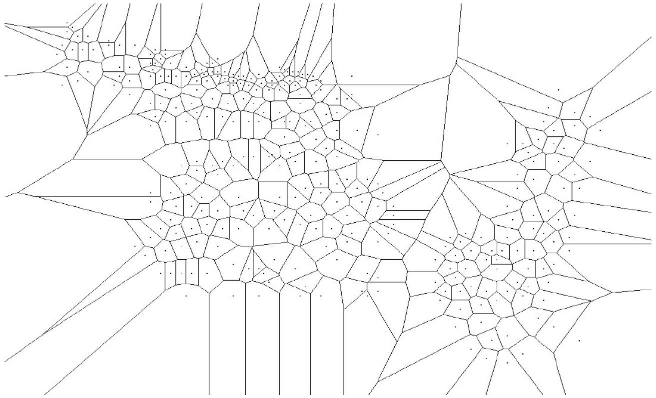
- Compute the DELAUNAY triangulation of the point set.
- Eliminate all triangles of the resulting graph which have a radius larger than $\alpha$ times the minimum radius.
- The final shape is given by the outer edges of the remaining graph.



# VORONOI–diagram

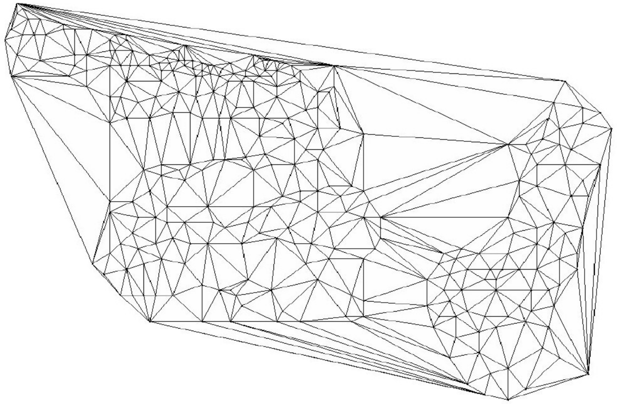


## VORONOI–diagram with more points



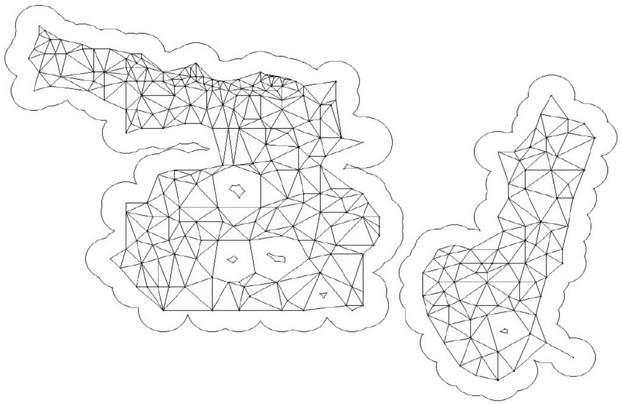


## DELAUNAY–diagram





## Alpha–shapes
Example





## Alpha–shapes
short comings

- Need of suitable alpha.
- Alpha is constant over the entire point set.
- Interior points needed.

## CRUST
### application

The algorithm is able to reconstruct

- a curve
- that is sampled sufficiently dense
- especially smooth curves, i.e., possibly many component curves without branches, endpoints, or self–intersections.



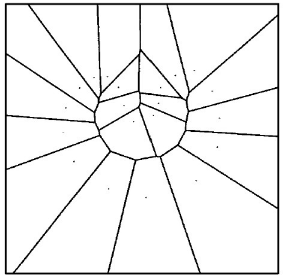
## CRUST
### algorithm

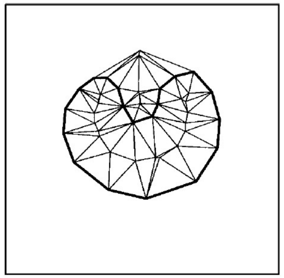
The crust

- is the set of edges
- selected from the Delaunay triangulation of the initial point set
- extended by its Voronoi points
- where both endpoints of the edges belong to the initial set.



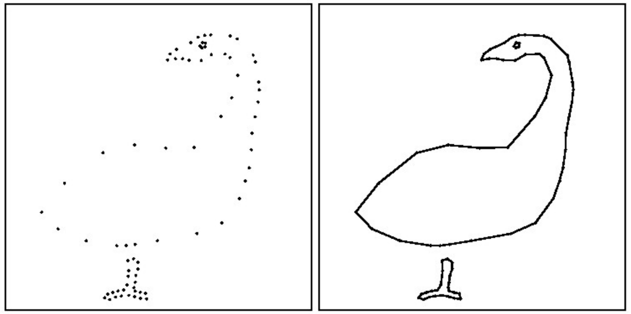
## CRUST
### Example







## CRUST
### Example



## Curve reconstruction
algorithm

- Computes the GABRIEL graph as a subgraph of the Delaunay graph
- (an edge between two input points belongs to the Gabriel graph if a disk with this edge as diameter does not contain any other input point).
- Eliminate the edges which do not fulfill the local granularity property,
- i.e., at each point only the two shortest edges are maintained.

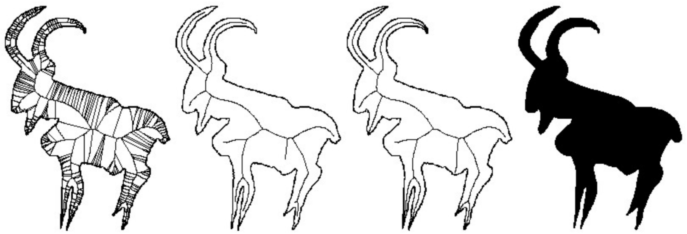


## Curve reconstruction
application

- The method works well if there exists a regular interpolant,
- that is, a polygonal closed curve such that the local granularity,
- defined as minimum distance to an input point,
- at each point of the curve is strictly smaller
- than the local thickness at that point,
- defined as the distance to the medial axis of the shape.

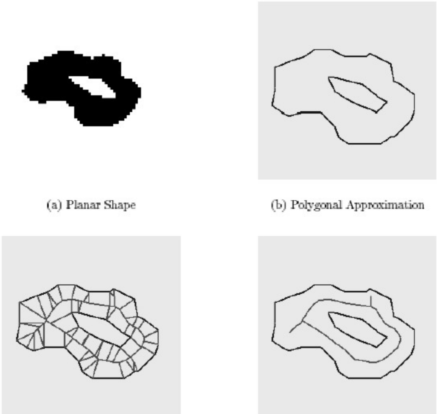


## Skeleton





## Skeleton



(a) Planar Shape (b) Polygonal Approximation

(c) Voronoi Diagram (d) Pruned Skeleton

## Simplification problem
### objective

- Given polygonal chain (or polygon) $P$ (with $n$ vertices),
- approximate $P$ by another one $Q$ whose vertices are a subset of $k$ vertices of $P$.



## Simplification problem
### two variants

- min–#–problem: minimize the number of vertices of an approximating polygonal chain (or closed polygon) with the error within a given bound;
- min–$\varepsilon$–problem: minimize the error of an approximating polygonal chain (or closed polygon) consisting of a given number of vertices.



## Simplification problem
### solutions

- Both problems can be solved in optimal time $O(n^2)$.
- There exist near–optimal algorithms for solving the min–#–problem for the Euclidean distance which for practical problems outperform the optimal algorithms.
- There exists a genetic algorithm to cope with the min–#–problem which found near optimal solutions in the presented experiments.



## Approximation problem
### objective

- Given polygonal chain (or polygon) $P$ (with $n$ vertices),
- approximate $P$ by another one $Q$ whose $k$ vertices can be placed arbitrarily in the plane.
- min–#–problem: minimize the number of vertices with the error within a given bound;
- min–$\varepsilon$–problem: minimize the error consisting of a given number of vertices.

## Approximation problem
### solutions

- There exists an algorithm that approximates the point set with a set of individual lines.
- Joining the lines is problematic in certain cases.
- There exists an algorithm that approximates with a linked chain whenever the input polyline is monotonic (runtime $O(n^k)$).
- There exists an approximation version of this algorithm which runs much faster (no implemention known).



## shaprox
### shape description

A shape $\mathscr{S}$ is defined by a number of points and certain parameters:

- line: a point $L \in \mathbb{R}^2$ and an angle $\varphi \in \mathbb{R}$;
- circumference: a center point $C \in \mathbb{R}^2$ and a radius $\rho \in \mathbb{R}$;
- set of circumferences: set of pairs of center points and corresponding radii, i.e., $(\mathscr{C}, \mathscr{R}) \subset \mathbb{R}^2 \times \mathbb{R}$;
- polyline or polygon: an ordered set of corner points $\mathscr{Q} = \{Q_1, Q_2, \ldots, Q_k\}, Q_j \in \mathbb{R}^2, j = 1, \ldots, k$, where the only difference between the two shapes is that for a polygon the last and first corner are connected;
- rounded box: a line segment defined by two points $Q_1, Q_2 \in \mathbb{R}^2$, an aspect ratio $\alpha \in \mathbb{R}$, and a corner radius $\rho \in \mathbb{R}$.



## shaprox
### distance functions: point—shape I

- line
$$\delta_{L_2}(P_i, \mathscr{S}) = \left|\mathrm{Det}(P_i - L, (\cos\varphi, \sin\varphi)^T)\right|$$
- circumference
$$\delta_{L_2}(P_i, \mathscr{S}) = |\|P_i - C\| - \rho|$$
- set of circumferences
$$\delta_{L_2}(P_i, \mathscr{S}) = \min_{(C_j, \rho_j) \in (\mathscr{C}, \mathscr{R})} |\|P_i - C_j\| - \rho_j|$$



## shaprox
### distance functions: point—shape II

- polyline or polygon, first we need the distance for a segment $\overline{QQ_j} = Q_{j+1} - Q_j$:
$$\delta_{L_2}(P_i, \overline{QQ_j}) = \begin{cases} \|P_i - Q_j\| & \text{if } (P_i - Q_j)^T \overline{QQ_j} < 0 \\ \|P_i - Q_{j+1}\| & \text{if } (P_i - Q_{j+1})^T \overline{QQ_j} > 0 \\ \left|\frac{\mathrm{Det}(\overline{QQ_j}, P_i - Q_j)}{\|\overline{QQ_j}\|}\right| & \text{otherwise} \end{cases}$$
and obtain for a polyline or polygon
$$\delta_{L_2}(P_i, \mathscr{S}) = \min_{Q_j \in \mathscr{Q}} \delta_{L_2}(P_i, \overline{QQ_j})$$
where for a polyline the index $j$ runs from $1, \ldots, k-1$ and for a polygon from $1, \ldots, k$ with $Q_{k+1} = Q_1$.

- rounded box

$$\delta_{L_2}(P_i,\mathscr{S}) = \left| \min_{j=1,\ldots,4} \delta_{L_2}(P_i,\overline{QQ_j}) \pm \rho \right|$$

where $Q_3 = Q_2 + \alpha\, Q_{12}^{\top}$ and $Q_4 = Q_1 + \alpha\, Q_{12}^{\top}$ being $Q_{12}^{\top}$ the left turned perpendicular vector to $Q_2 - Q_1$ of same length. $+\rho$ is taken when the point $P_i$ lies inside the rectangular box through $Q_1,\ldots,Q_4$, and $-\rho$ when $P_i$ lies outside.





- vertical distance to a line:

$$\delta_V(P_i,\mathscr{S}) = \left| P_i^2 - L^2 - (P_i^1 - L^1)\cdot \sin\varphi / \cos\varphi \right|$$

- length of the segments could have an influence as a weight

$$\delta_{wL_2}(P_i,\overline{QQ_j}) = \left| \mathrm{Det}(\overline{QQ_j}, P_i - Q_j) \right|$$





- RMS

$$\delta_{\mathrm{RMS},L_2}(\mathscr{P},\mathscr{S}) = \sqrt{\frac{1}{I}\sum_{P_i\in\mathscr{P}} \delta_{L_2}(P_i,\mathscr{S})^2}$$

- AVG

$$\delta_{\mathrm{AVG},L_2}(\mathscr{P},\mathscr{S}) = \frac{1}{I}\sum_{P_i\in\mathscr{P}} \delta_{L_2}(P_i,\mathscr{S})$$

- MAX

$$\delta_{\mathrm{MAX},L_2}(\mathscr{P},\mathscr{S}) = \max_{P_i\in\mathscr{P}} \delta_{L_2}(P_i,\mathscr{S})$$

- or $\delta_{\mathrm{RMS},V}(\mathscr{P},\mathscr{S})$ or $\delta_{\mathrm{AVG},L_1}(\mathscr{P},\mathscr{S})$, etc



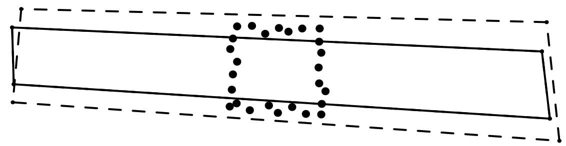


- Algorithm of RODRÍGUEZ/GARCÍA–PALOMARES
- derivative–free minimization method
- proved convergence for either locally strictly differentiable or non–smooth locally convex functions.

- Til now concentrated on the minimization of a single function.
- However, in our optimization problem, it can happen that there is no change in the value of the distance function although the shape is modified.











- Minimize perimeter as well.





- Formulate a convex combination of all objectives,
- i.e., optimize the single–objective function

$$f(x) = \beta_1 f_1(x) + \beta_2 f_2(x) + \cdots + \beta_l f_l(x)$$

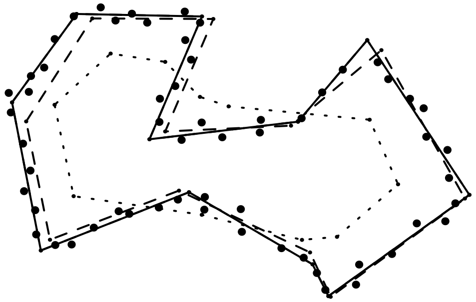
- where the $\beta_j > 0$, for $j = 1, \ldots, l$, are strictly positive weights,
- $f_j(\cdot) : \mathbb{R}^n \longrightarrow \mathbb{R}$ are the individual objective functions.

## shaprox
### Subsidiary objective: short coming of possible solution

- Explores the Pareto front defined by the weights $\beta_j$,
- it might be difficult to find weights such that the encountered minimum is sufficiently close to the minimum considering only the principal objective $f_1(\cdot)$.



## shaprox
### Example: convex combination as objective function





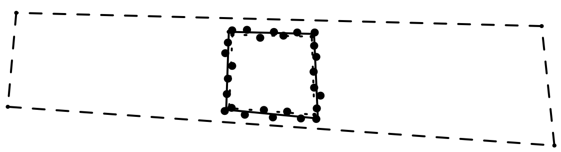
## shaprox
### Subsidiary objective: better solution

- modify the comparison $f(z) \leq f(x) - \tau^2$ (in the local search algorithm)
- with the following iteratively defined comparison function for $l$ objectives:

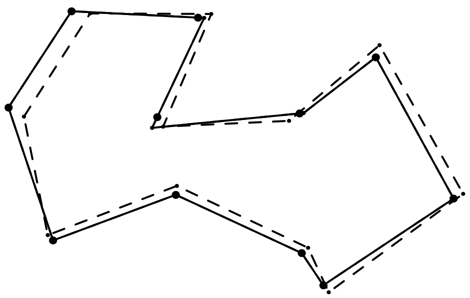
$$[f_1(z), \ldots, f_l(z)] \leq_{\tau^2} [f_1(x), \ldots, f_l(x)] \iff$$
$$\forall j = 1, \ldots, l : f_j(z) \leq f_j(x) - \tau^2 \text{ or}$$
$$(j < l \text{ and } f_j(z) \leq f_j(x) \text{ and } f_{j+1}(z) \leq f_{j+1}(x) - \tau^2)$$



## shaprox
### Example

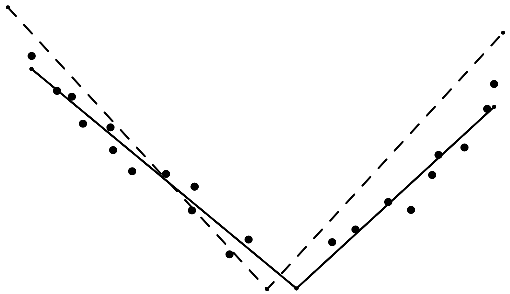


## NP–Completeness and non–convexity of the objective function



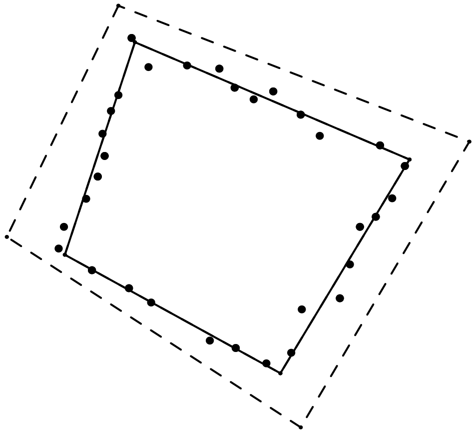


## shaprox
Examples: wedge



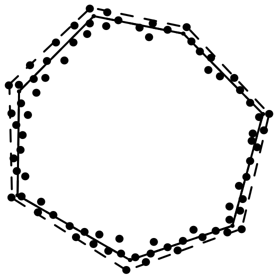


## shaprox
Examples: simple polygon

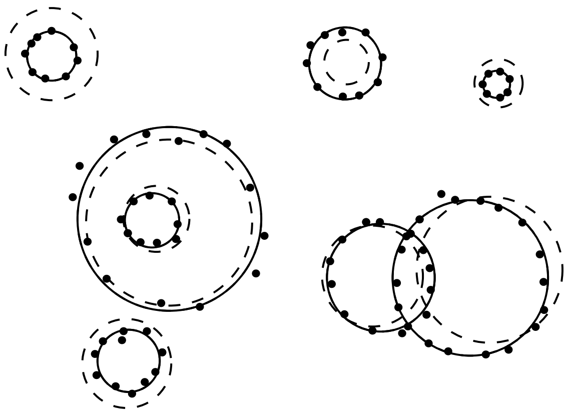




## shaprox
Examples: convex hull

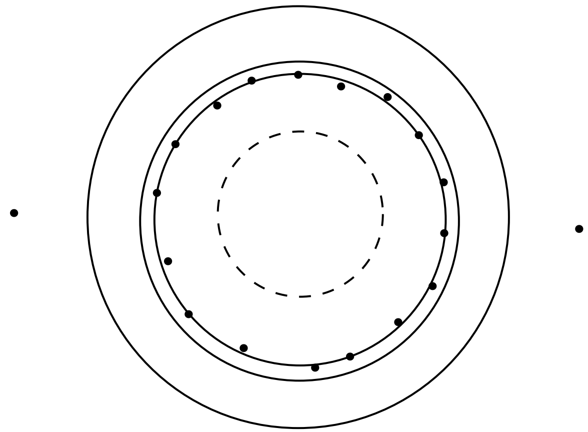


## shaprox
Examples: circumferences



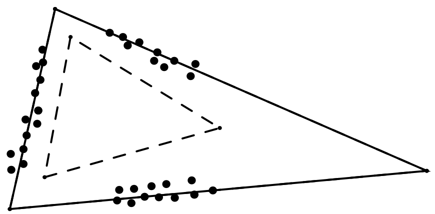


## shaprox
Examples: influence of metrics



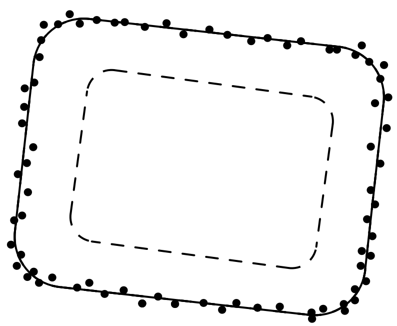


## shaprox
Examples: completing shapes

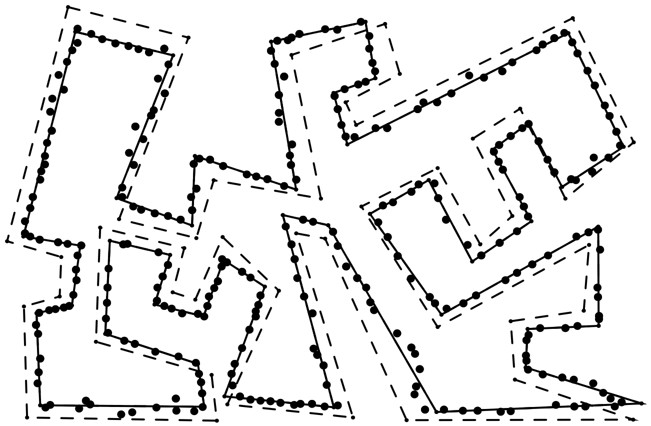




## shaprox
Examples: rounded rectangle



## shaprox
### Examples: complex polygon





## Evolutive methods
### based on natural fenomena

- simulated anealing
- cristalizaton of materials
- evolution (mutation, recombination, selection)
- competitive/colaborative systems
- social interactions



## Evolutive methods
### with meta heuristics

- (reactive) tabú search (since 1986)
- random search (since 196X)
- simulated anealing (since 196X)

- genetic algorithms (since 1975)
- genetic programming
- (neural networks)
- ant colony optimization (since 1992)
- particle swarm optimization (since 1995)
- guided local search (since 1997)
- iterated local search (since 1999)
- variable neighborhood search (since 1999)



## Evolutive methods
### paradigms

- work with populations of individuals
  (only one individual and a memory...)
- there are modification processes
  (mutation, modification, reproduction)
- *performance* of the individuals in the environment based on a *fitness* which usually is the objective function (but not necessarily)
- decisions are drawn probabilistically

# Evolutive methods
## genetic algorithms

- one distinguishes genotype (codification) and fenotype
- there exists a bijection between genotype and fenotype
- modifications (mutation and crossover) is done over the genotypes
- the fitness is evaluated over the fenotypes
- mutation (which one?), recombination (types?), selection (types?)



# Evolutive methods
## evolutive programming

- there exists only the fenotype (with its codification)
- modification (mutation) is realized over the fenotypes of copies
- the fitness is evaluated over the fenotypes
- mutation (types?), selection (types?)



# Evolutive methods
## evolutive strategies

- an amplification of evolutive programming
- each individual maintains parameters that guide the mutations
- these parameters are modified in the same way as the proper fenotypes
- mutation (types?), selection (types?)



# Evolutive methods
## genetic programming

- the codification of the fenotype is a program
- the programs are modified with adecuate operations
- mutation (types?), selection (types?)

recent example (André Falcão, Residue fragment programs for enzyme classification, Proceedings BKDB2005, pp.24–28, 2005).

## Evolutive methods
### differential evolution

- the codification of the fenotype is a vector of characteristics
- the vector of an individual is modified with the differences to other vectors (individuals)
- modifications (types?), selection (types?)



## Evolutive methods
### swarm intelligence

- the individuals of the population interact in a social way
- the decisions of each individual depend on the own wishes and the information available from the others
- ant colonies
- particle swarms



## Evolutive methods
### ant colonies

- the individuals leave information (feromonas) in the search space
- the decisions are based on individual information and on the feromonas encountered
- the information (feromonas) is volatile
- the feromonas or statistical behavior of the individuals define the solution



## Particle swarm optimization
### characteristics

- simple to describe
- simple to implement
- few parameters to adjust
- usually small population are used
- the number of objective function evaluations is usually small
- usually is very fast

premature convergence occurs whenever all individuals are located in a small area of the search space

## Particle swarm optimization

some details

- each individual communicates with its neighborhood (usually, the neighborhoods overlap)
- and maintains local information (best solutions viewn til now, search direction, etc.)
- in most cases, the neighborhood is fixed
- the local information is modified with the help of the information gathered in the neighborhood (or just from the best neighbor)
- local changes are confined to avoid *explosions* (dramatic changes)
- the method is able to solve discrete problems



## Particle swarm optimization

velocity actualization

$$v_i = \xi(v_i + U[0,\varphi_1](p_i - x_i) + U[0,\varphi_2](p_g - x_i))$$
$$x_i = x_i + v_i$$

con

- $x_i$ vector of current positions
- $v_i$ vector of current directions
- $p_i$ best local position vector
- $p_g$ best position vector of group (neighborhood)
- $\varphi_1 = 2{,}05$
- $\varphi_2 = 2{,}05$
- $\xi = 0{,}729$



## Particle swarm optimization

versions

binary version: the variables are interpreted as binary values according to a distribution of threshold

discret version: the variables are interpreted as integer values (for instance with simple rounding)

dynamic version: the search space is reinitialized, the local variables are reset, for instance: $p_i = x_i$ or re-evaluate $p_i$ and decide between $p_i$ ans $x_i$.



## Particle swarm optimization

convergence

- the individuals should exhibit certain diversity
- one needs a similarity measure
- diversity can be forced dynamically adapting the parameters
- one might use lack of diversity as stopping condition

## multi–objective optimization

### Pareto

- there is more than one independent objective function
- Pareto optimal (global): every other component for all other solutions is worse (or equal) (other names are: efficient points, dominant points, non-interior points)
- Pareto optimal (local): every other component for all other solutions in a local neighborhood is worse (or equal)
- the Pareto frontier describes the trade-off between the different objectives



## Multi–objective

### techniques for a solution

- convex combination of the objectives (to obtain the Pareto frontier one has to explore the coefficient space)
- homotopic techniques, i.e., compute the entire Pareto frontier (works in most cases just for two objectives)
- goal programming, i.e., fix values for all objectives and minimize the distance of all objectives to the predefined goals (according to some convenient distance metric)
- priority optimization, i.e., fix thresholds for all but one objective beforehand and optimize above the threshold according the most important one
- priorization (multi-level) programming, i.e., optimize according to a predefined ordering of the objectives.



## Multi–objective optimization

### with evolutionary methods

- evolutionary methods can approximate the Pareto frontier in parallel (with the help of the diversity among the individuals)
- for instance particle swarm systems varying the weights of a convex combination periodically during the iterations