Optimization and search in discrete spaces

Own investigation

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Three applications

- approximate point set match in 2D and 3D
- selection of node B sites in UMTS wireless networks
- approximation of point sets with shapes

First application
psm

approximate Point Set Match in 2D and 3D

¿Dónde está Wally?

Motivation
psm

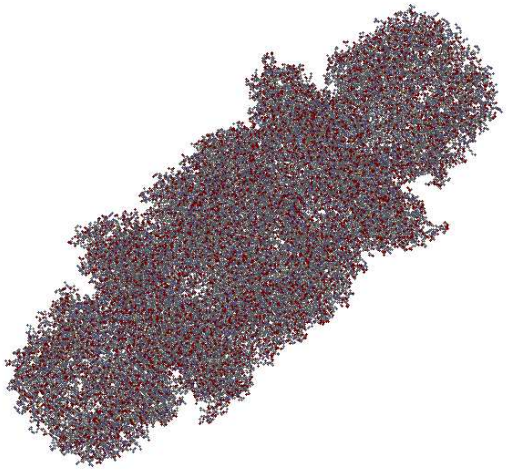
- searching of patterns
  (relatively small sets of two– or three–dimensional points),
  within search spaces
  (relatively large point sets)
- comparing point sets
- key words
  geometric pattern matching, *structure comparison*, *point set matching*, *structural alignment*, *object recognition*

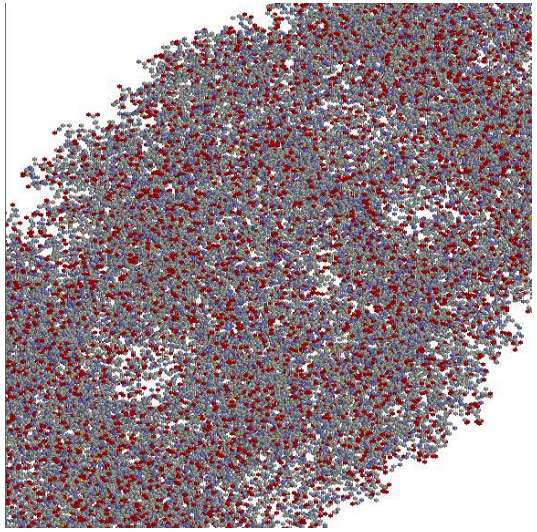
Joint work with

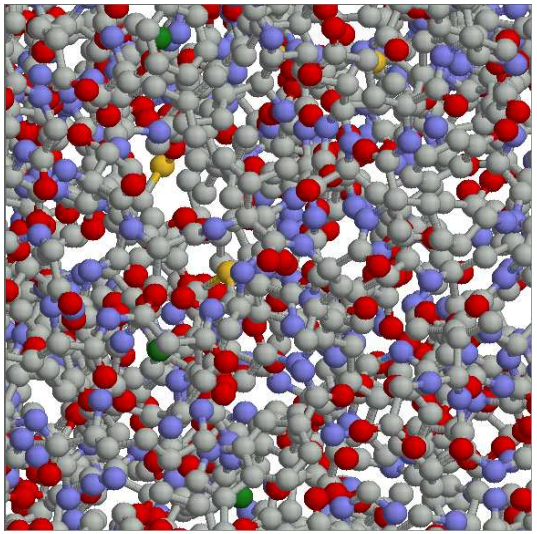
- Thorsten Pöschel
- some ideas from: Kristian Rother, Stefan Günther
- Humboldt Universität—Charité Berlin
  `http://www.charite.de/bioinf/people.html`
- Current project: `superimpose` (Raphael Bauer)
- there will be other algorithms to compare with

Search of a substructure in a protein

search space







Search of a substructure in a protein

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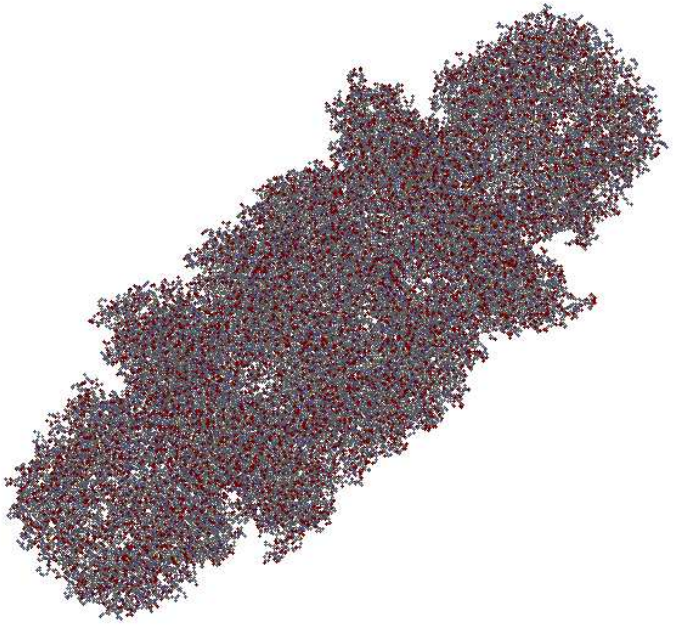
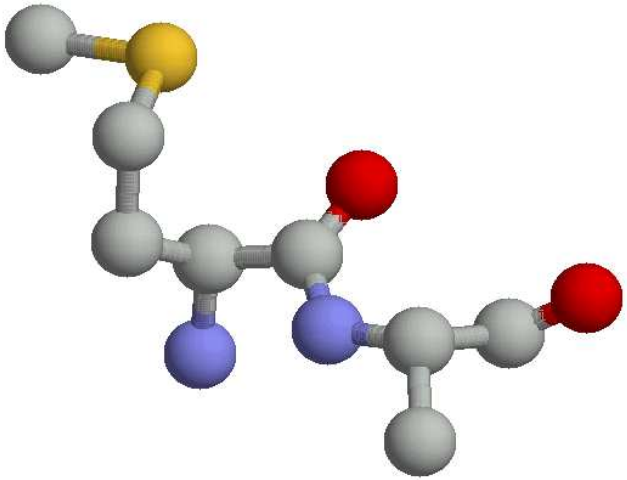




¿Dónde está Wally?

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 $\quad d = 2 \quad$ or $\quad d = 3$

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)

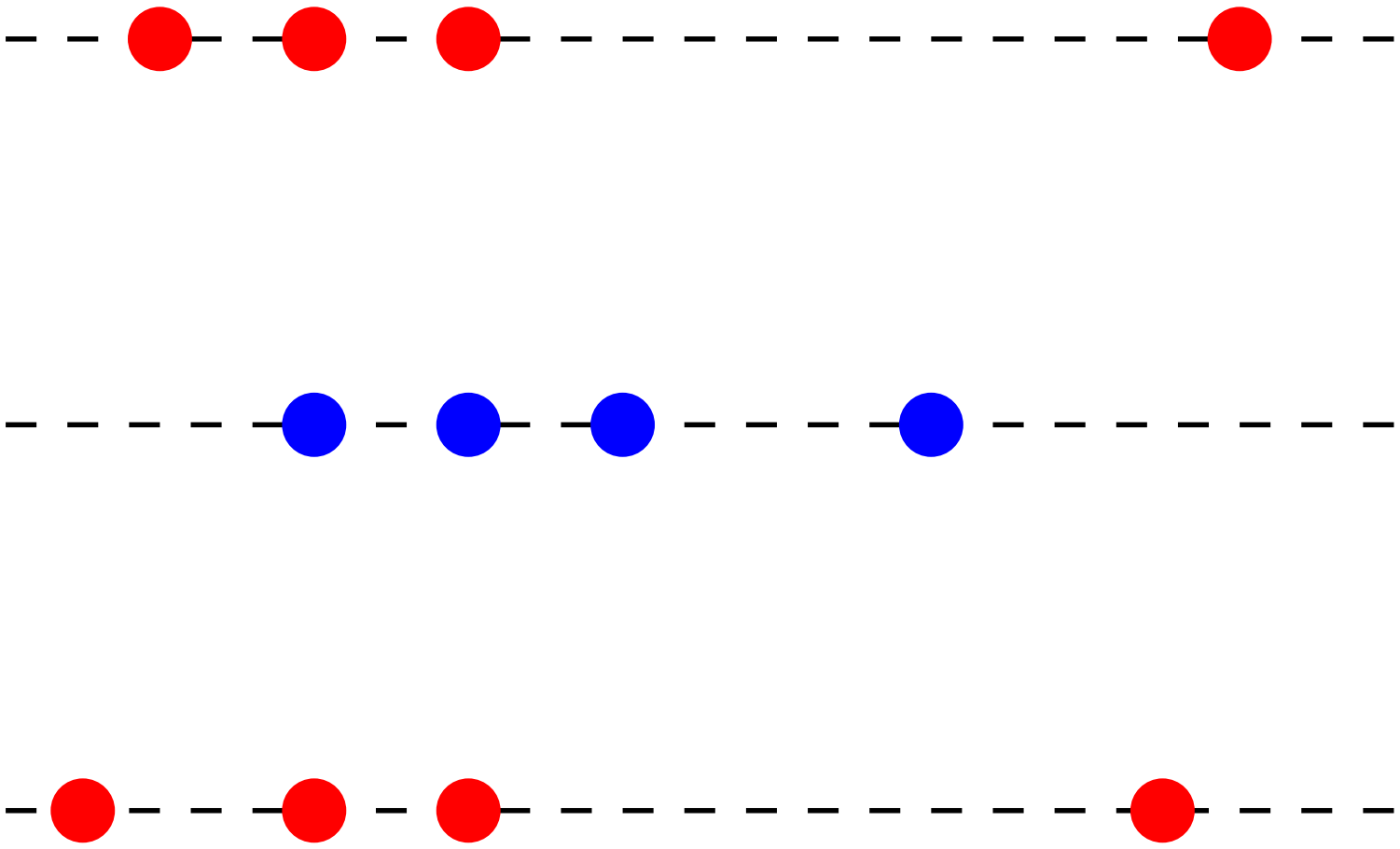
Congruent and similar transformations

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

One–dimensional example



Distance of an alignment

- let (μ, 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 $\quad d_i = 0 \quad$ 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, $\quad Q \in]0, 1]$
- 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 (μ, 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

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

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 μ (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

$$
\begin{aligned}
d &= \sqrt{\frac{1}{n}\sum_i d(p'_i, s'_i)^2} \\
&= \sqrt{\frac{1}{n}\sum_i (U \cdot p_i + t - s'_i)^2}
\end{aligned}
$$

- 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

$$\begin{aligned} t &= -U \frac{1}{n} \sum_i p_i + \frac{1}{n} \sum_i s'_i \\ &= -U \cdot p_c + s'_c \end{aligned}$$

- where p_c and s'_c are the centroids of both sets

Optimal Rotation

- with the above, d can be written as

$$
\begin{aligned}
d &= \sqrt{\frac{1}{n}\sum_i (U \cdot p_i + t - s'_i)^2} \\
&= \sqrt{\frac{1}{n}\sum_i (U \cdot (p_i - p_c) - (s'_i - s'_c))^2}
\end{aligned}
$$

- 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 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 $U = \mathbf{B} \cdot \mathbf{A}^\top$

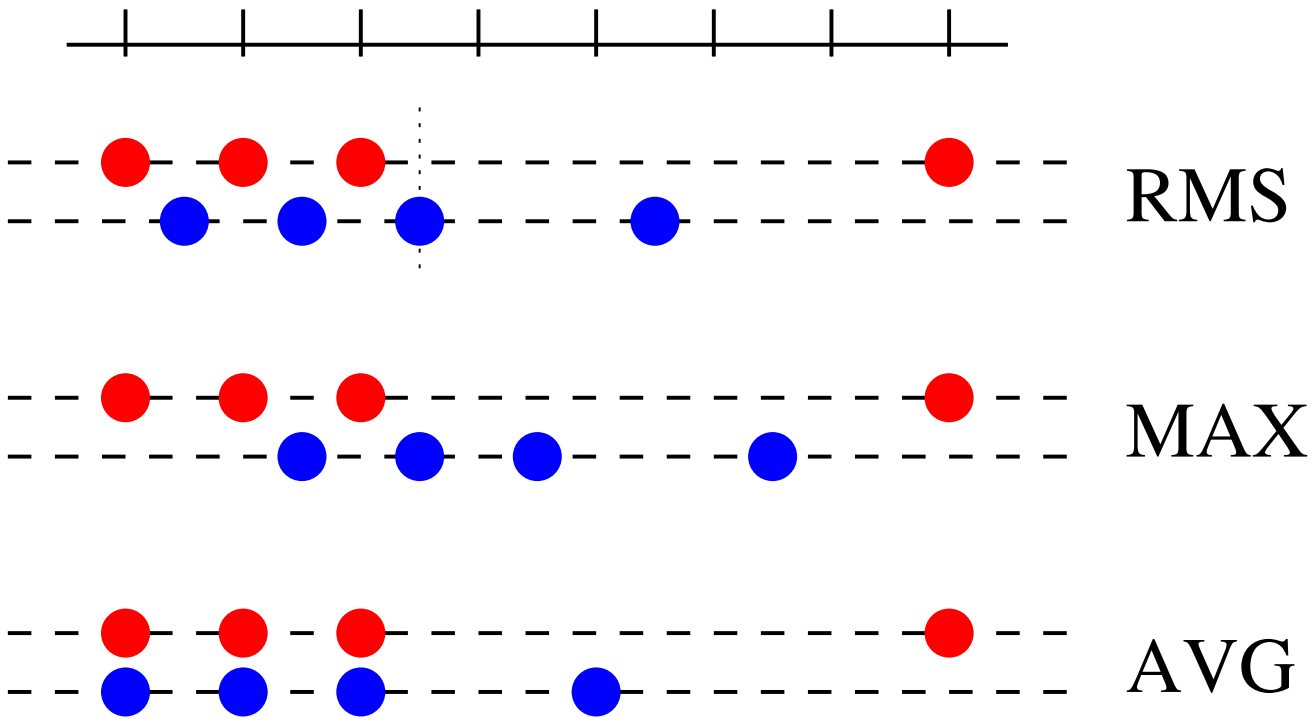
Introduction of scaling

- 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 σ: $\sigma = \dfrac{\sum_i \langle s''_i, p''_i \rangle}{\sum_i \langle p''_i, p''_i \rangle}$

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 φ the angle of rotation)
- instead of U with 9 constraint variables
  we have u and φ, 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

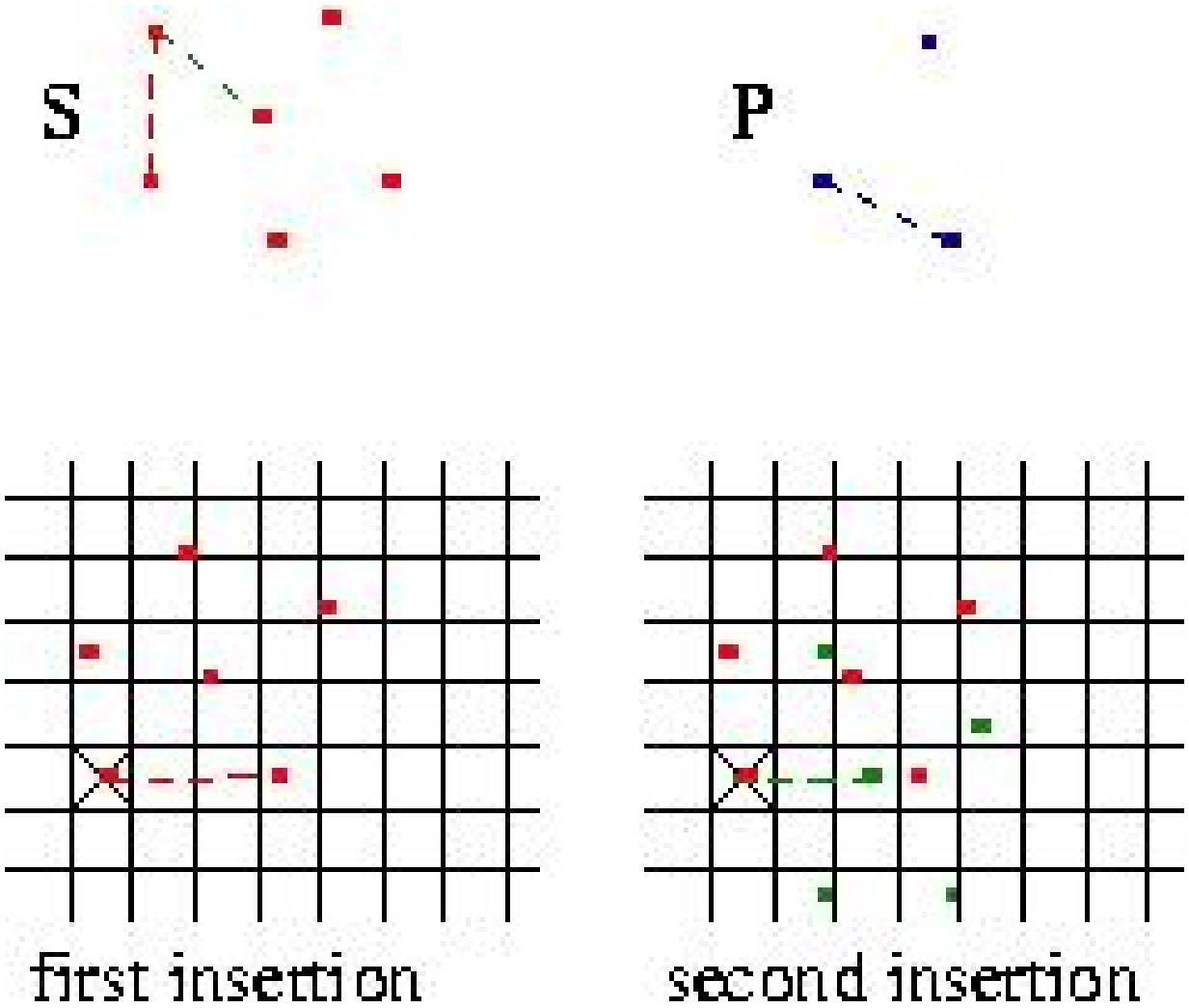
Properties of Clique Detection

- 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

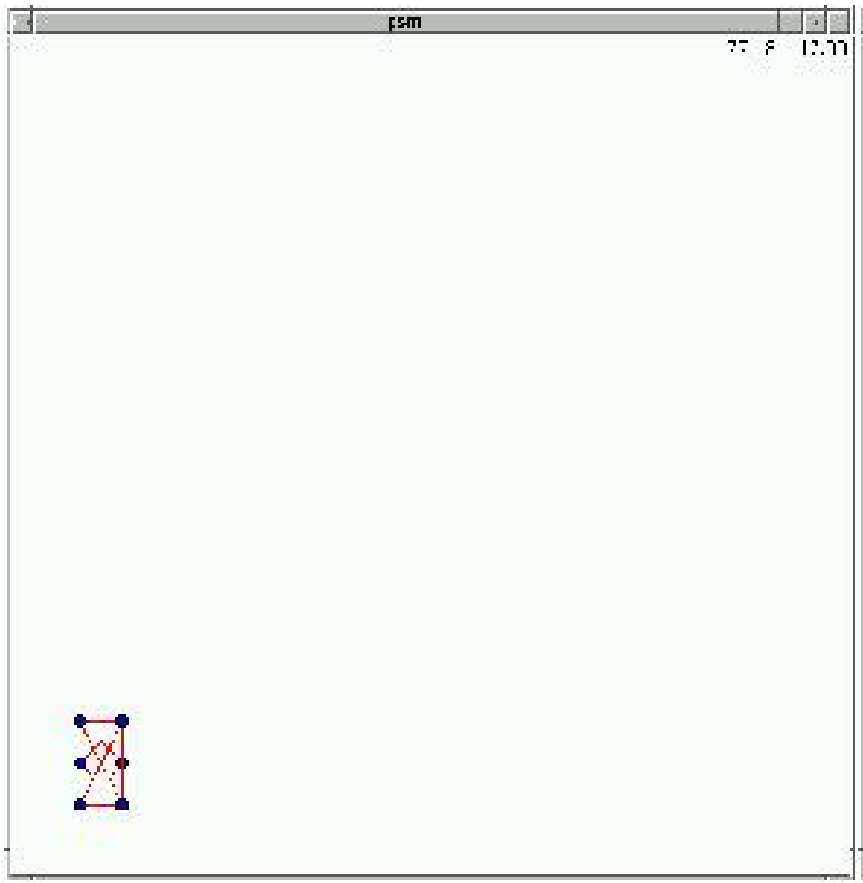
- let $d_{ij} = d(p_i, p_j)$ be the distance between two points of P
- the dictionary will contain the interval

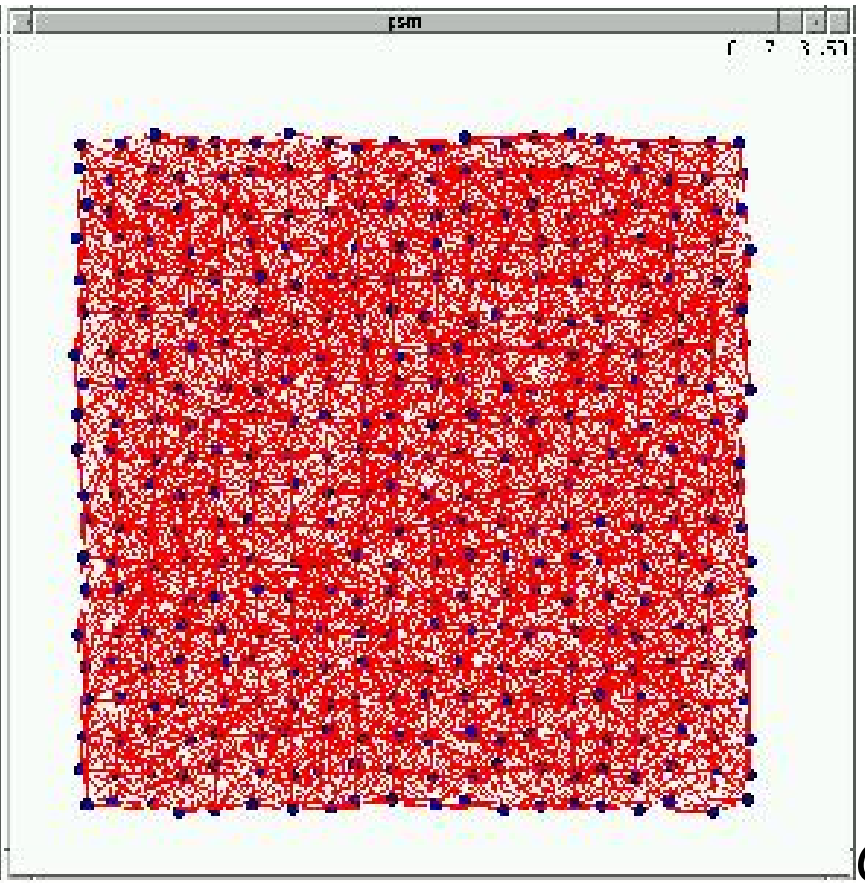
$$[\quad (1-\varepsilon)\cdot d_{ij} \quad , \quad (1+\varepsilon/(1-\varepsilon)\cdot d_{ij} \quad] \quad \in D$$

  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





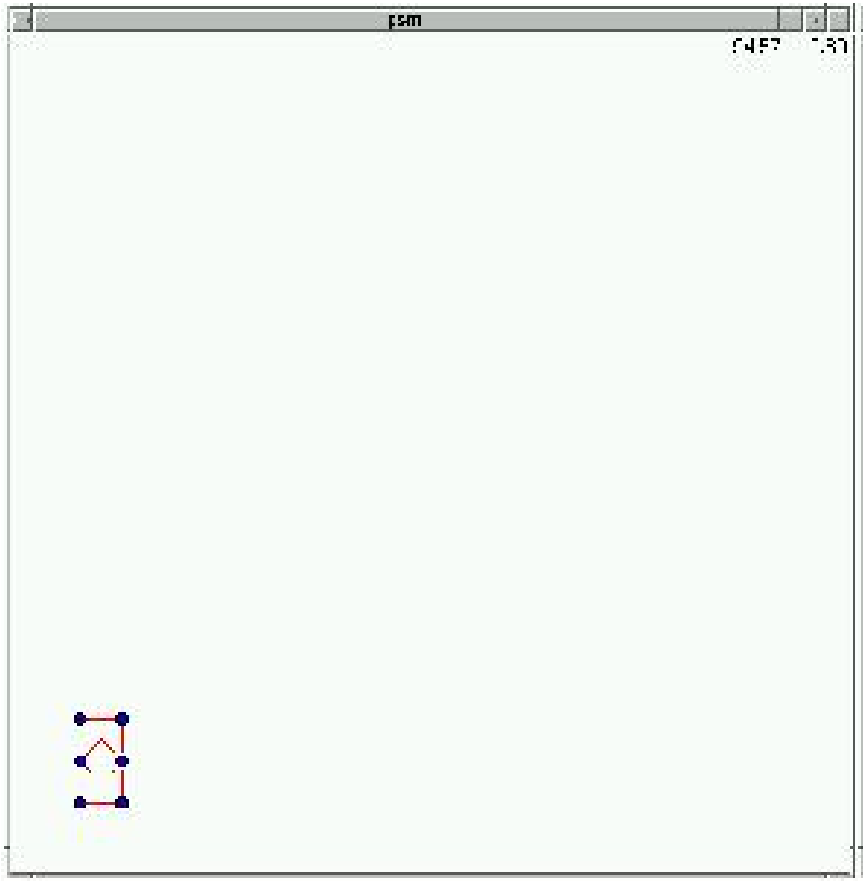
G_S

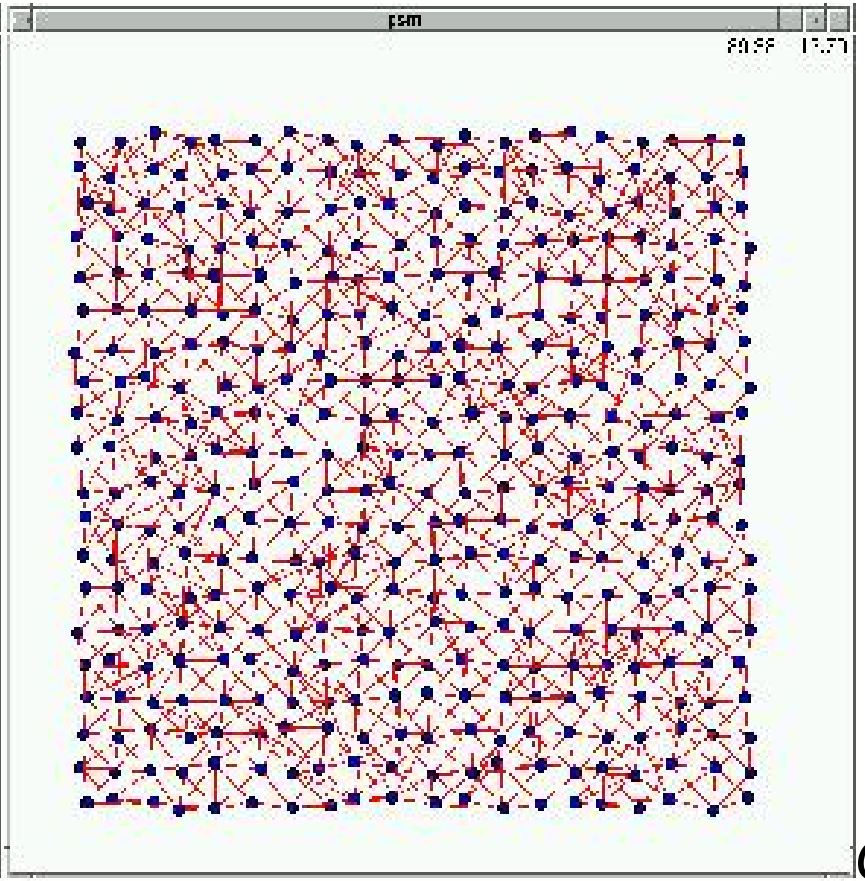
Fast construction of the graphs

- 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 $|\mathcal{P}(P)| = 2^k$ 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 si 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)

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: $|P| + 1$

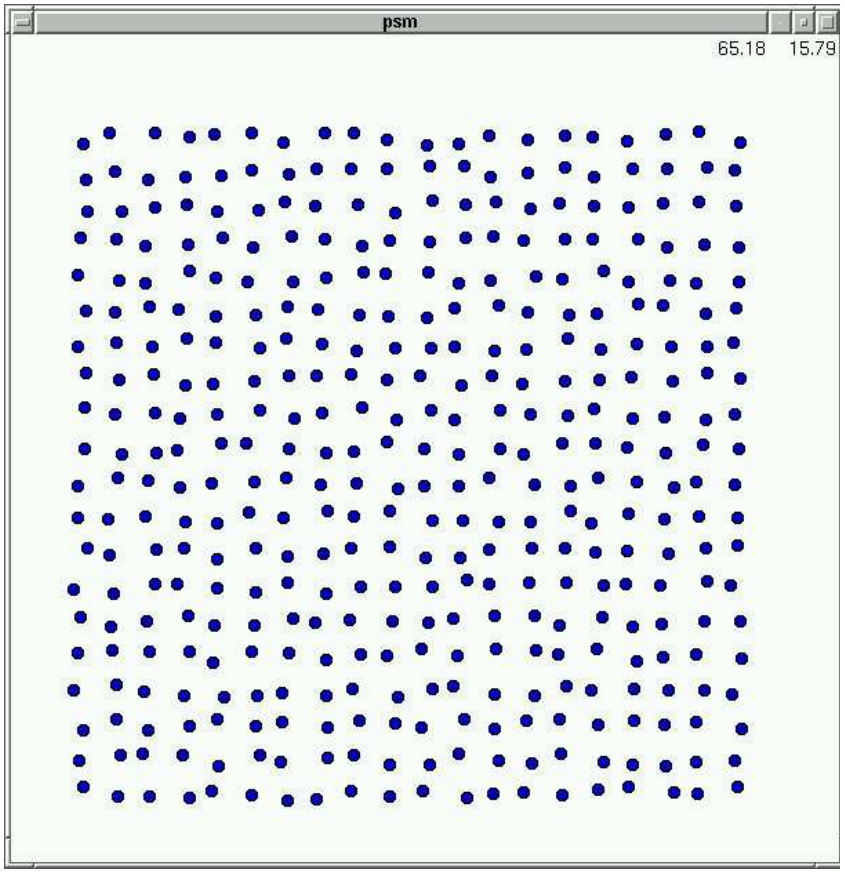
Reactive Tabu Search for `psm`

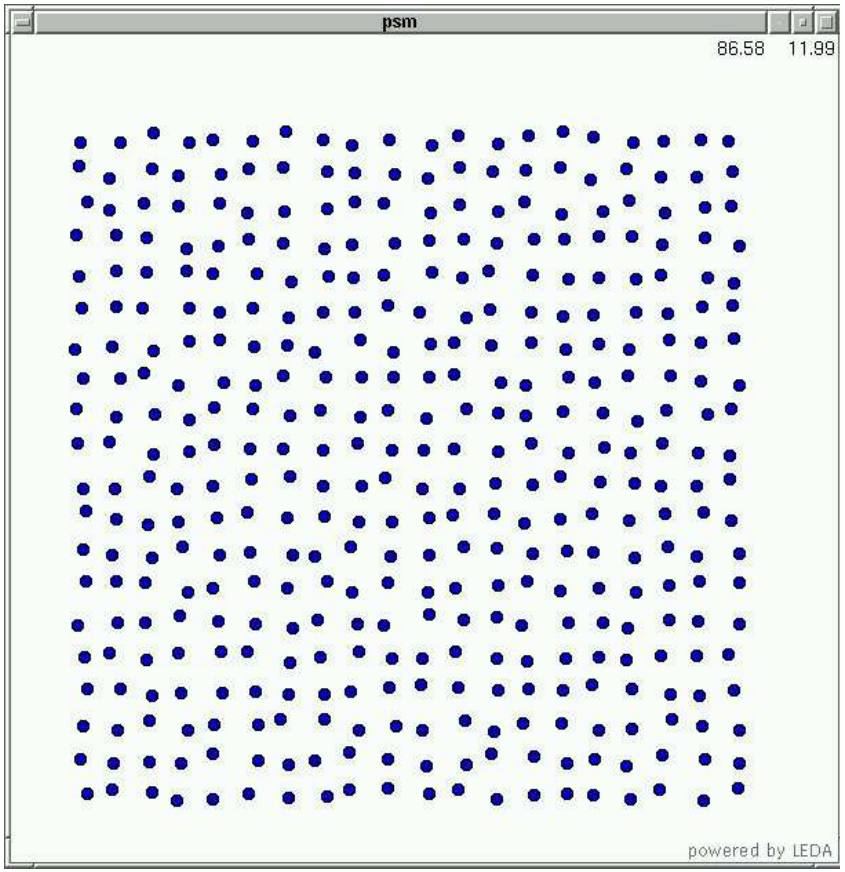
- representation of the problem:
  sets of indices of the matched points
- search for candidates to improve (*add*):
  (rigidly) connected neighbors within graph G_S
- search for candidates to reduce (*drop*):
  any point of the current solution that mantains the graph G_S connected (and rigid)

¿When do we terminate?

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

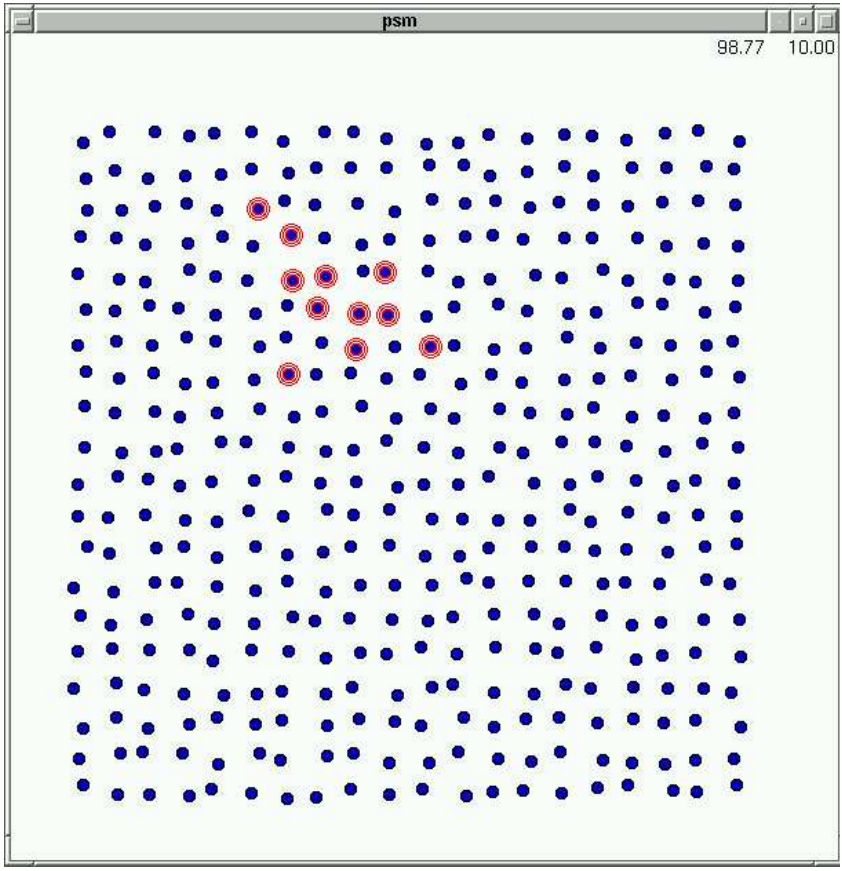
Search for the largest common pattern

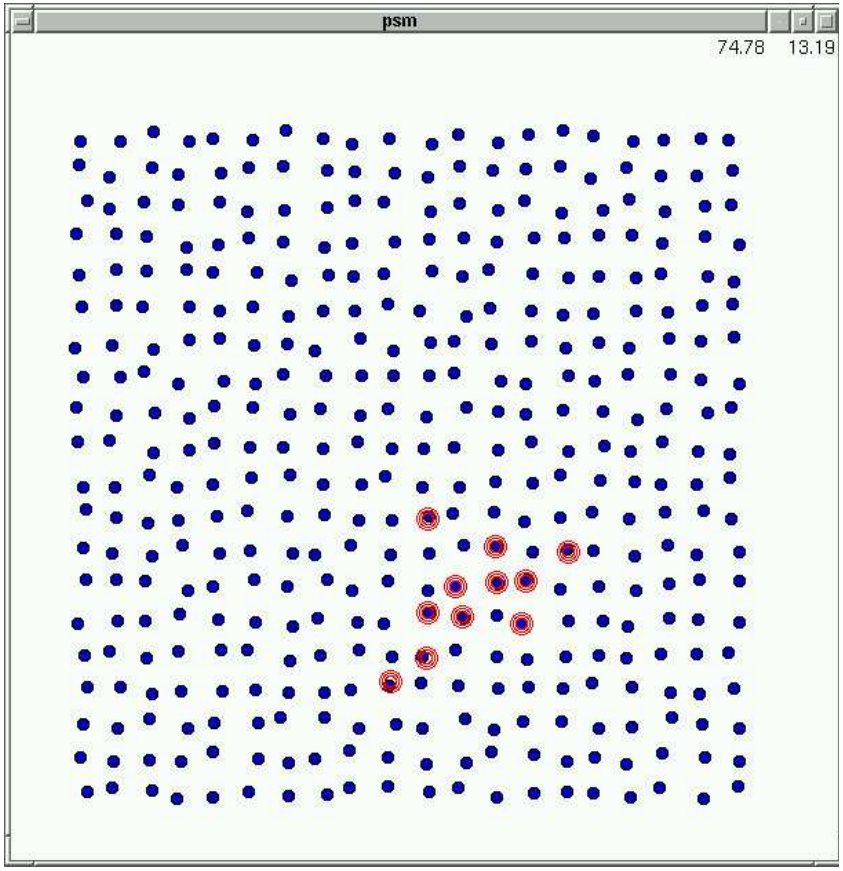




P S

Search for the largest common pattern

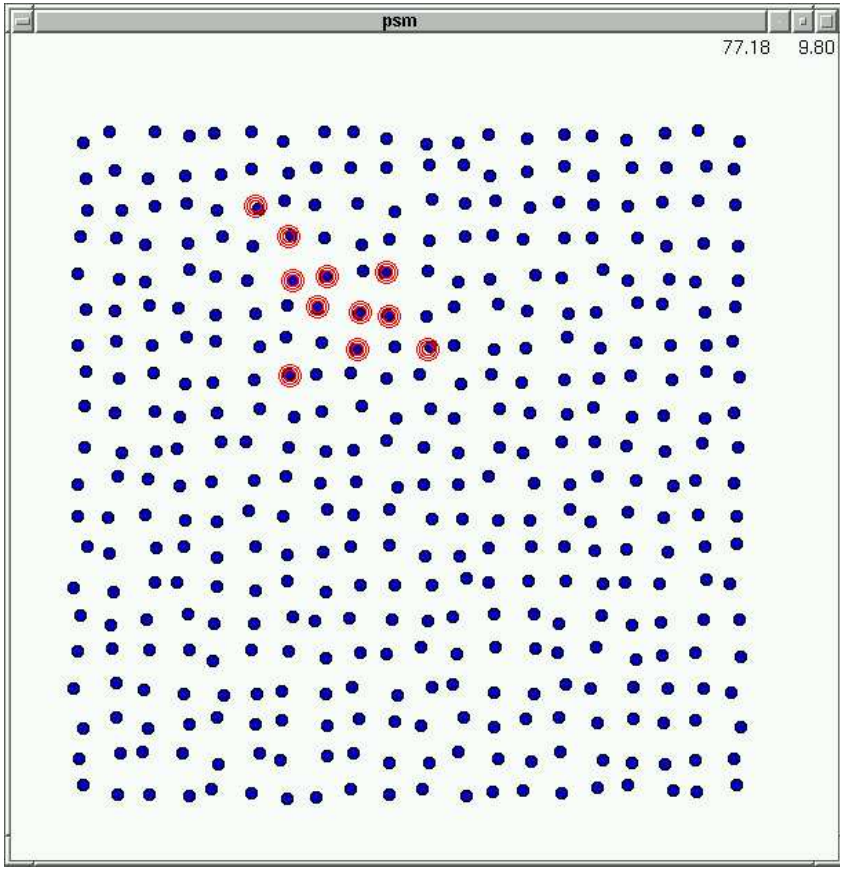


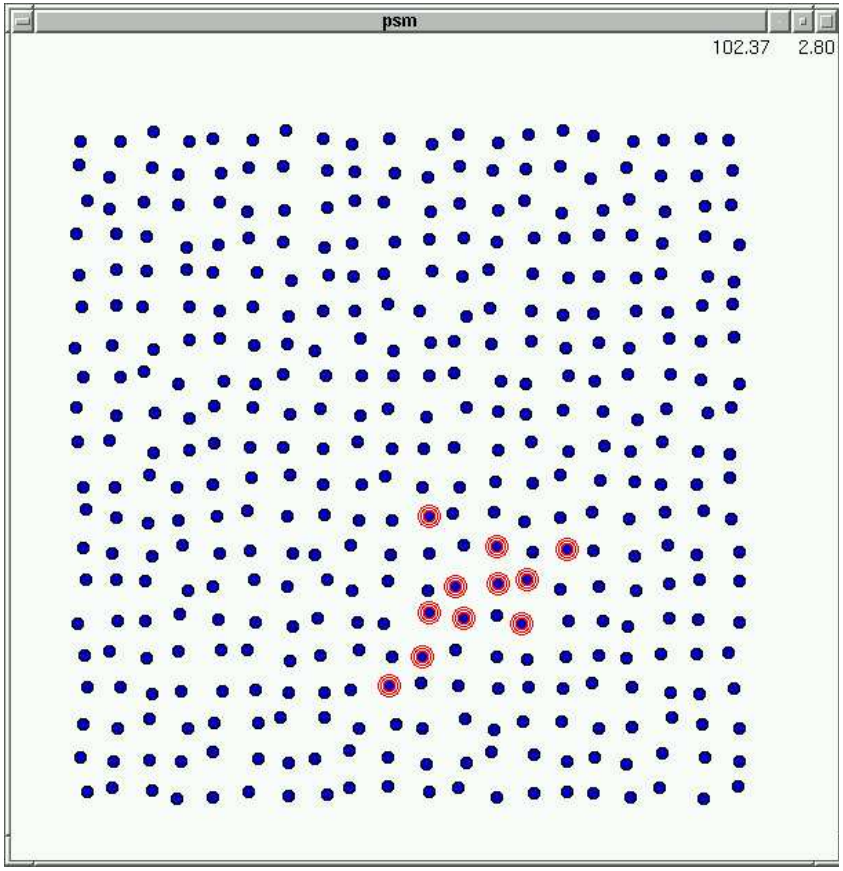


p/P

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

Software

old version

- almost 13.000 specific lines of C++
- uses the libraries:
  - Leda (*library of efficient data structures and algorithms*)
  - gsl (*Gnu scientific library*)
  - GAlib (genetic algorithms, MIT)
  - Gtkmm (graphical user interface)
  - own libraries

Software

newer version

- almost 11.000 specific lines of C++
- uses the libraries:
  - mtl (*matrix template library*)
  - Gtkmm (graphical user interface)
  - own libraries

psm

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)
- improve the user interface
- more applications

`optimUMTS`

Optimization of wireless UMTS networks

Joint work with

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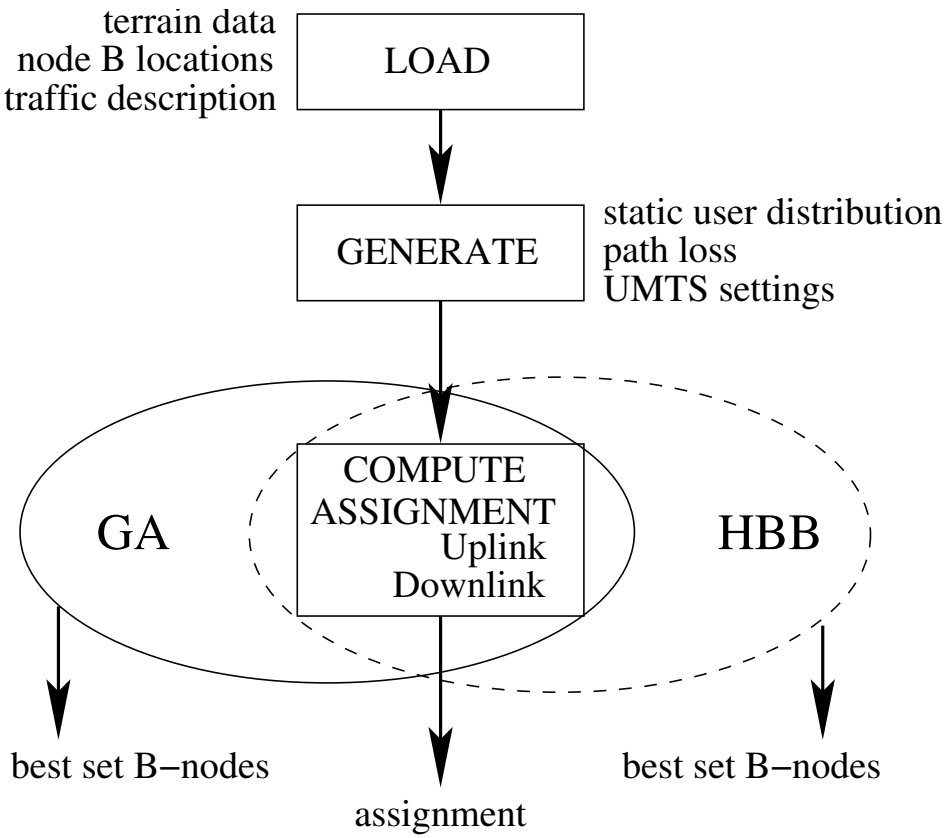
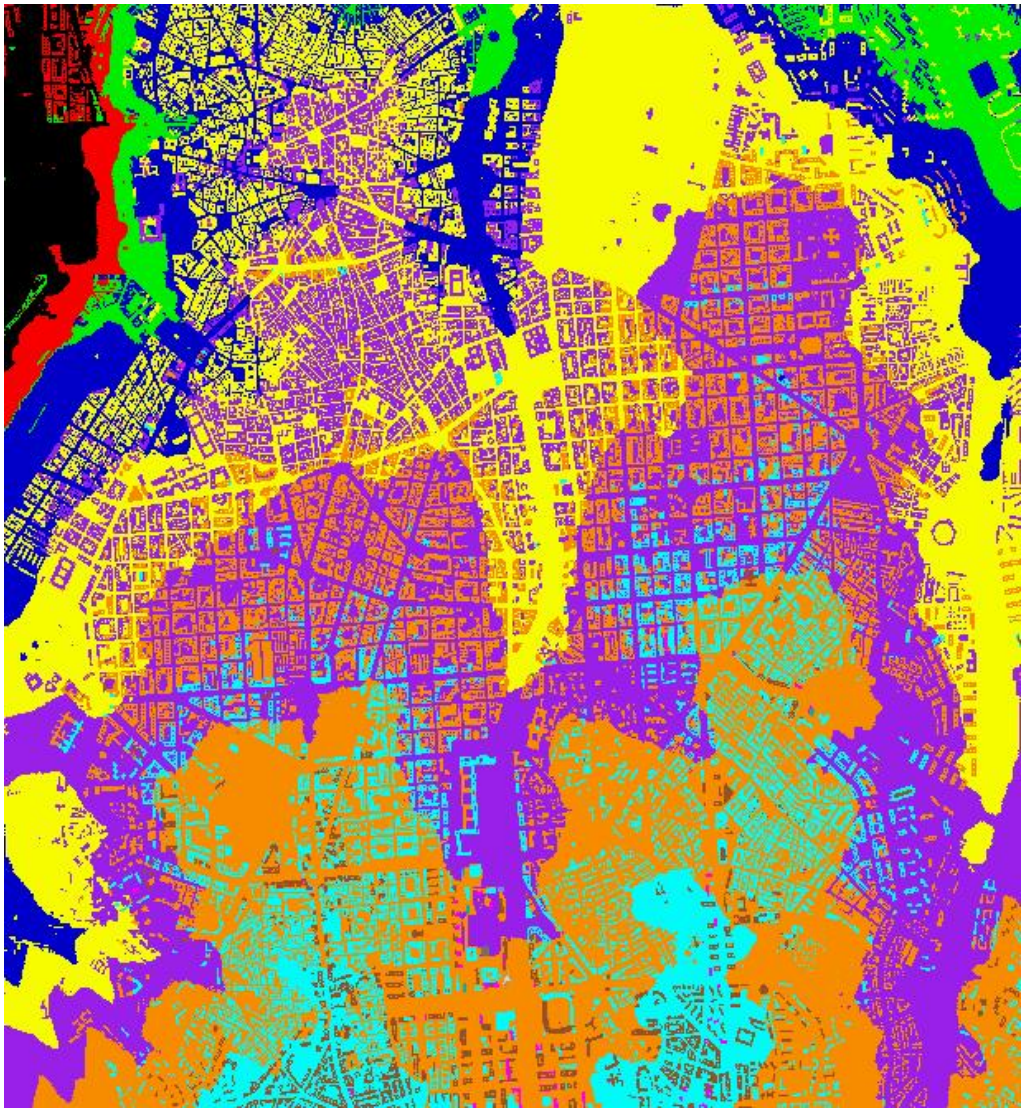
Objectives

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

Principal algorithm



Cartography of Madrid



Calculation of attenuation matrix α

- simple logarithmic decay

$$
\begin{aligned}
L(m,k) &= 10^{0.1\cdot(32.2+35.1\cdot\log(d(m,k)))} \\
\alpha(m,k) &= \frac{G_{\text{eff}}(m)\cdot G_{\text{eff}}(k)}{L(m,k)}
\end{aligned}
$$

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

Coverage around a node B

Traffic distribution

- 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

- uplink SIR γ_{UL}:

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

- downlink SIR γ_{DL}:

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

Calculation of noise

- 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)

- 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

$$\exists k \text{ with } P(k) > P_{\max}(k) \implies \text{no assignment}$$

$$i > I_{\max} \implies \text{no assignment}$$

$$\max_k \left\{ \frac{P_i(k)}{P_{i-1}(k)}, \frac{P_{i-1}(k)}{P_i(k)} \right\} \leq \Delta \implies \text{assignment possible}$$

Calculation of assignment

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

Validation of assignment

- uplink:

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

preliminaries

- downlink:

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

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

$$
\begin{aligned}
H(m,n) &= \delta_{m,n} - \sum_{k \in \mathcal{A}^{-1}(m)} \frac{\alpha(n,k) \cdot \beta(n,k,m) \cdot \tilde{\gamma}(m,k)}{\alpha(m,k)} \\
\nu(m) &= P_{\mathrm{plt}}(m) + \sum_{k \in \mathcal{A}^{-1}(m)} \frac{\tilde{\gamma}(m,k) \cdot N(k)}{\alpha(m,k)} \\
H \cdot T &= \nu
\end{aligned}
$$

Validation of power restrictions

- validation of maximum power of transmitter m:

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

Validation of power restrictions

- 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

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 branch&bound

Termination with heuristic backtracking

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

Heuristics

- 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.

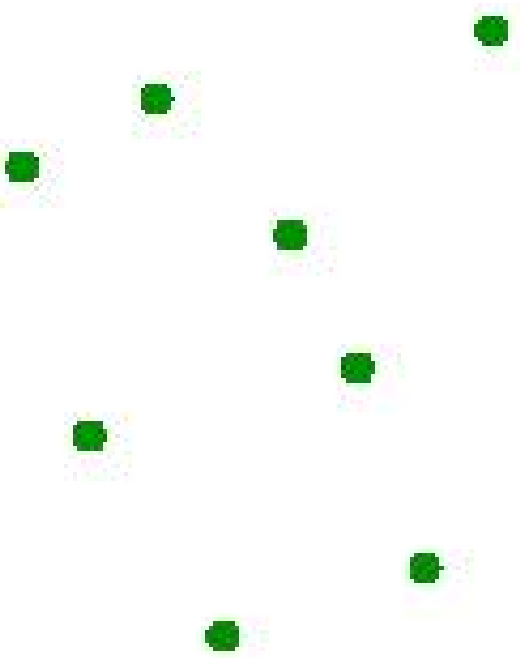
Optimization with genetic algorithm (GA)

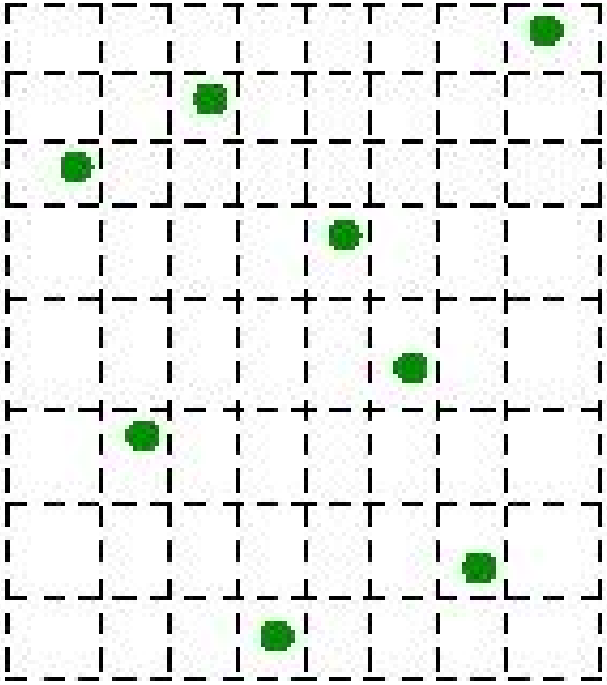
- steady-state incremental evolution
  (in each iteration two new decendents are generated)
- selection: roulette wheel
- mutation: flip
- crossover: two–point–cyclic
- quality: number of nodes B plus power as tiebreak

Genom generation I

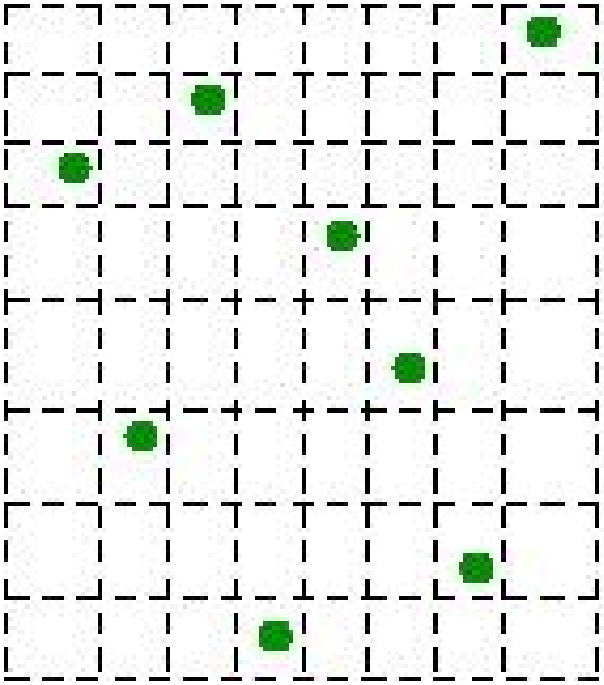
- matrix representation of nodes B
- exploiting locality properties
- using allele: usable, unusable, used, fixed

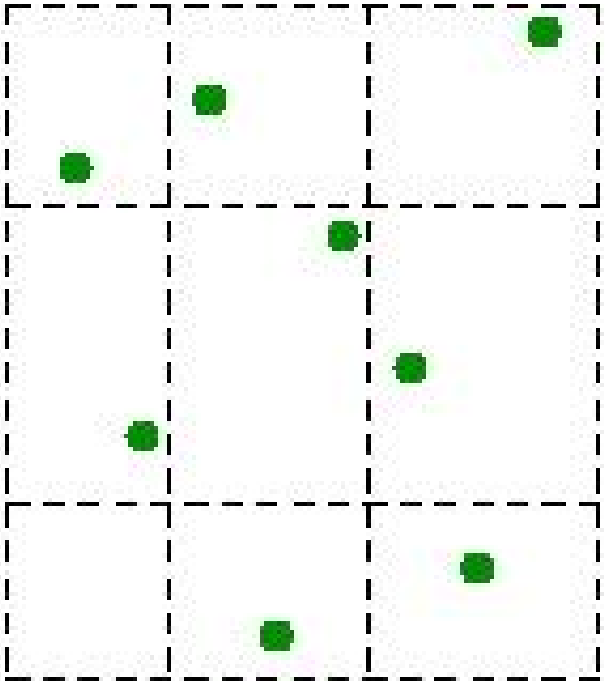
Genom generation II



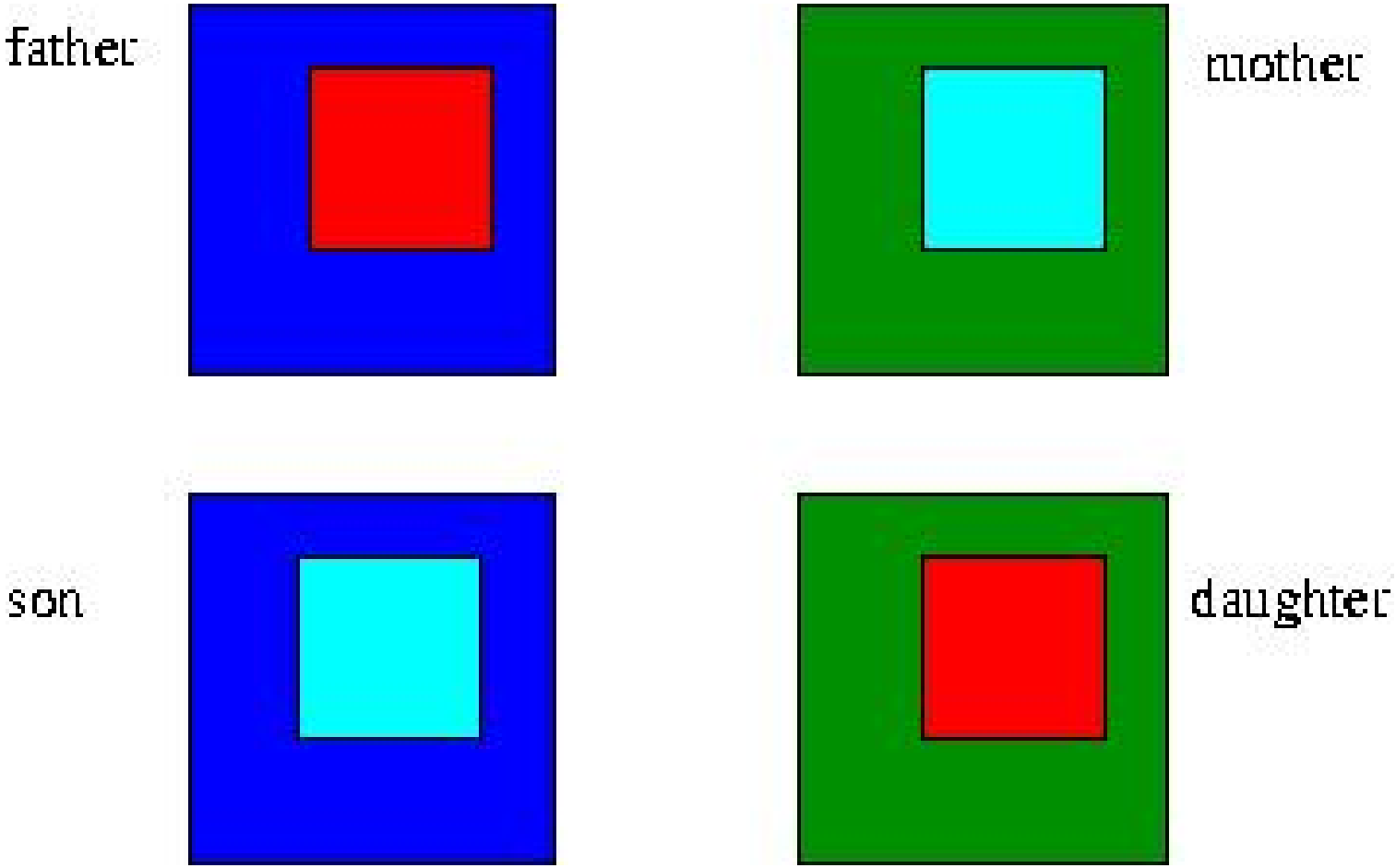


Genom generation III

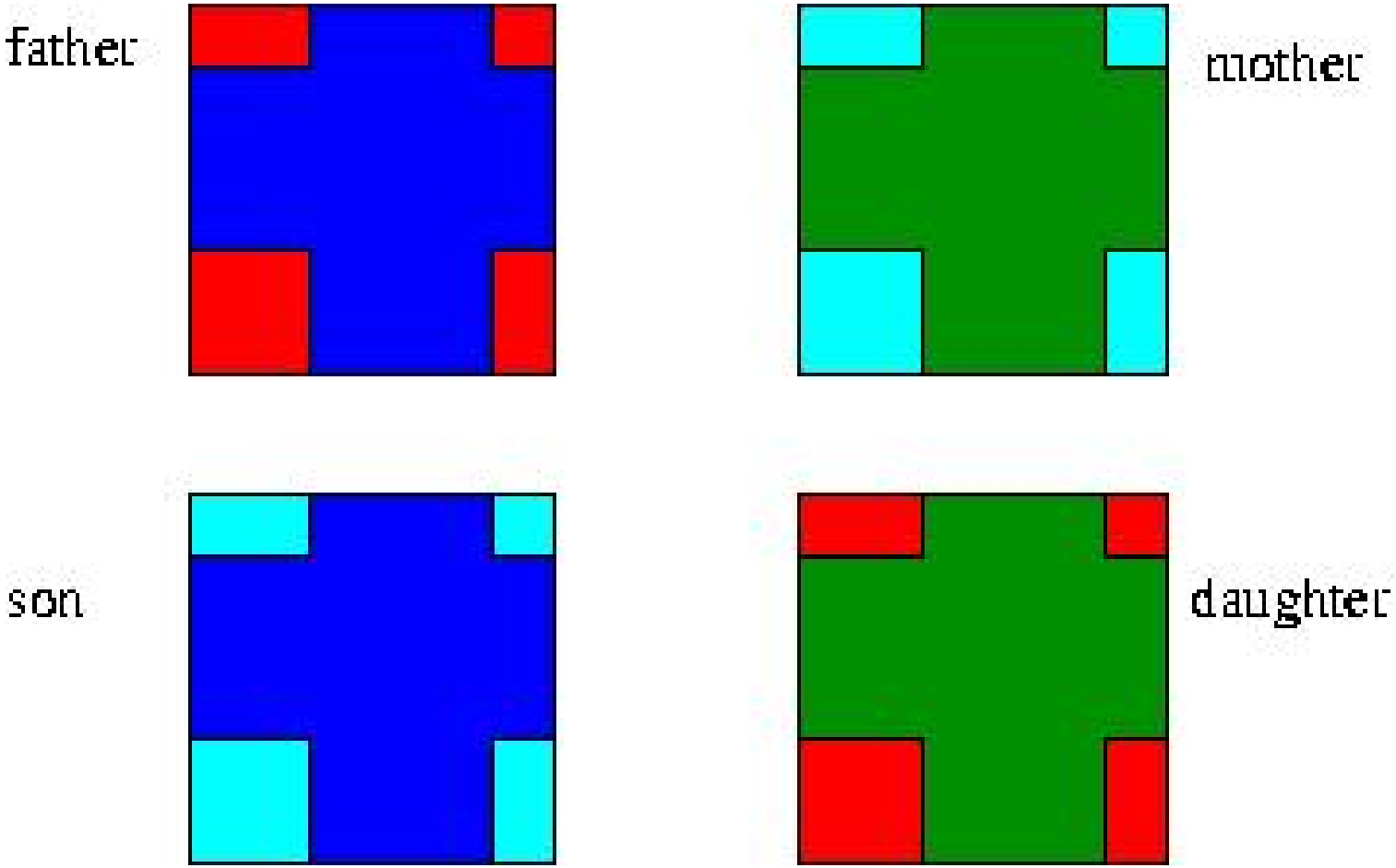




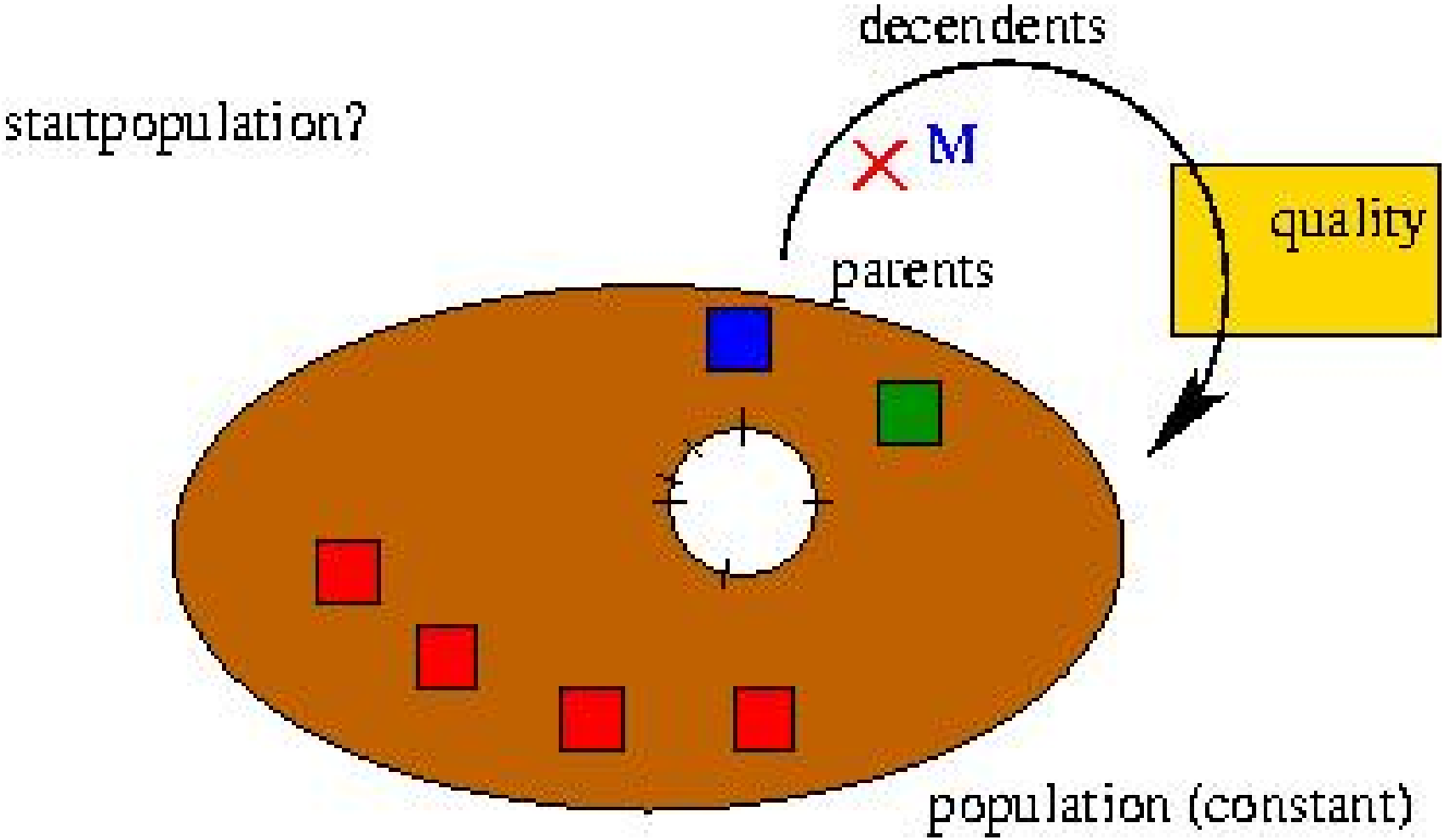
Crossover I



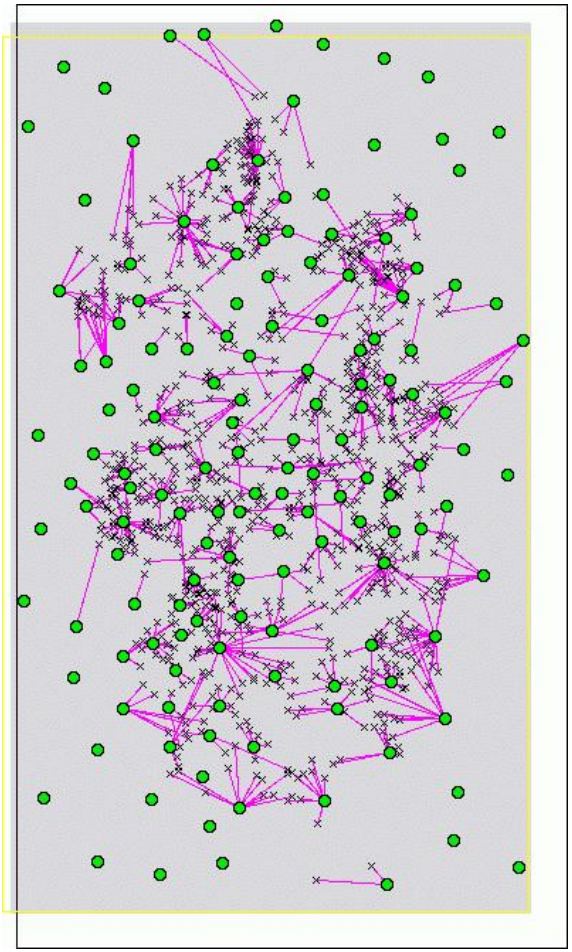
Crossover II

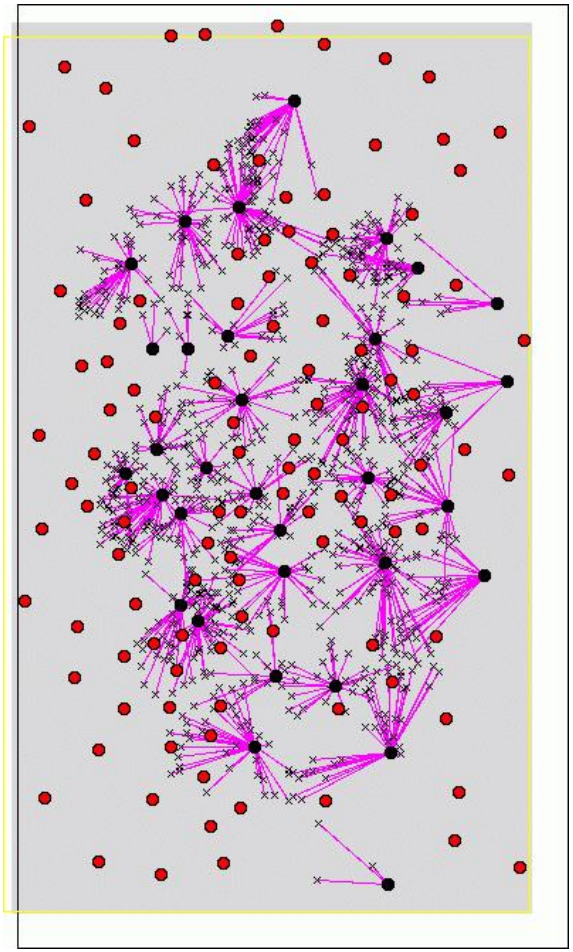


Evolution

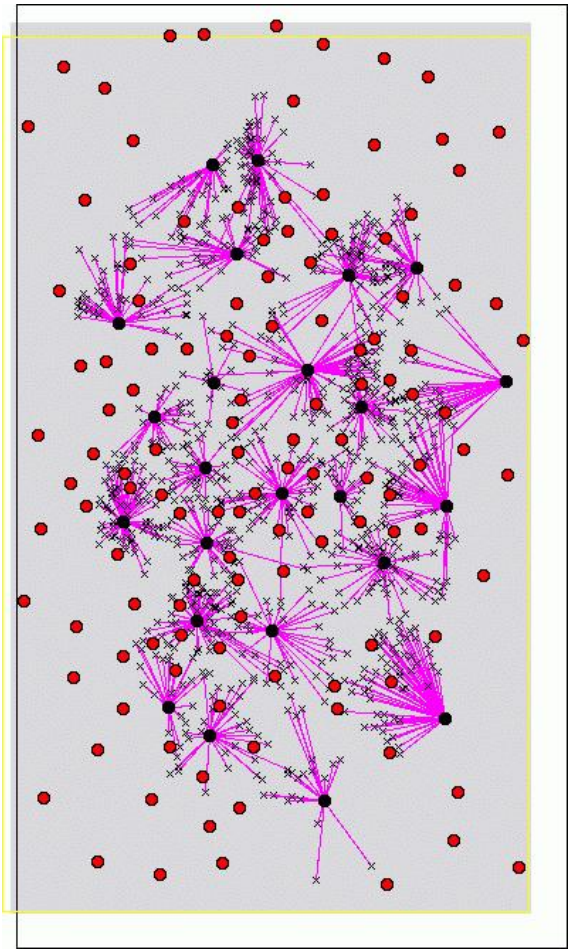

decendents
startpopulation?
M
quality
parents
population (constant)

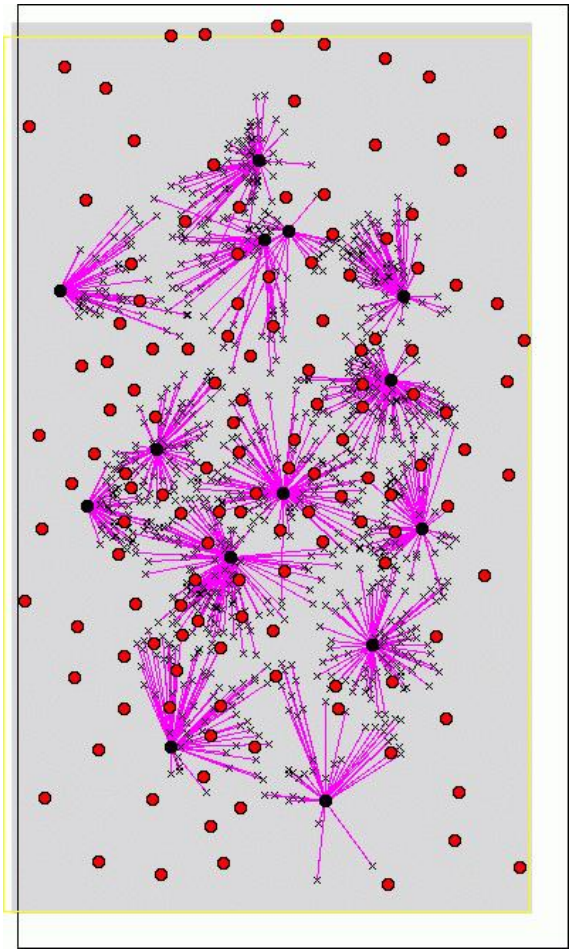
Assignment and heuristic branch result





GA results with and without downlink





Software

- almost 22.000 specific lines of C++
- uses the libreries:
  - Leda (*library of efficient data structures and algorithms*)
  - GAlib (genetic algorithms, MIT)
  - own libraries

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

Approximation of point sets with shapes

Informal problem description

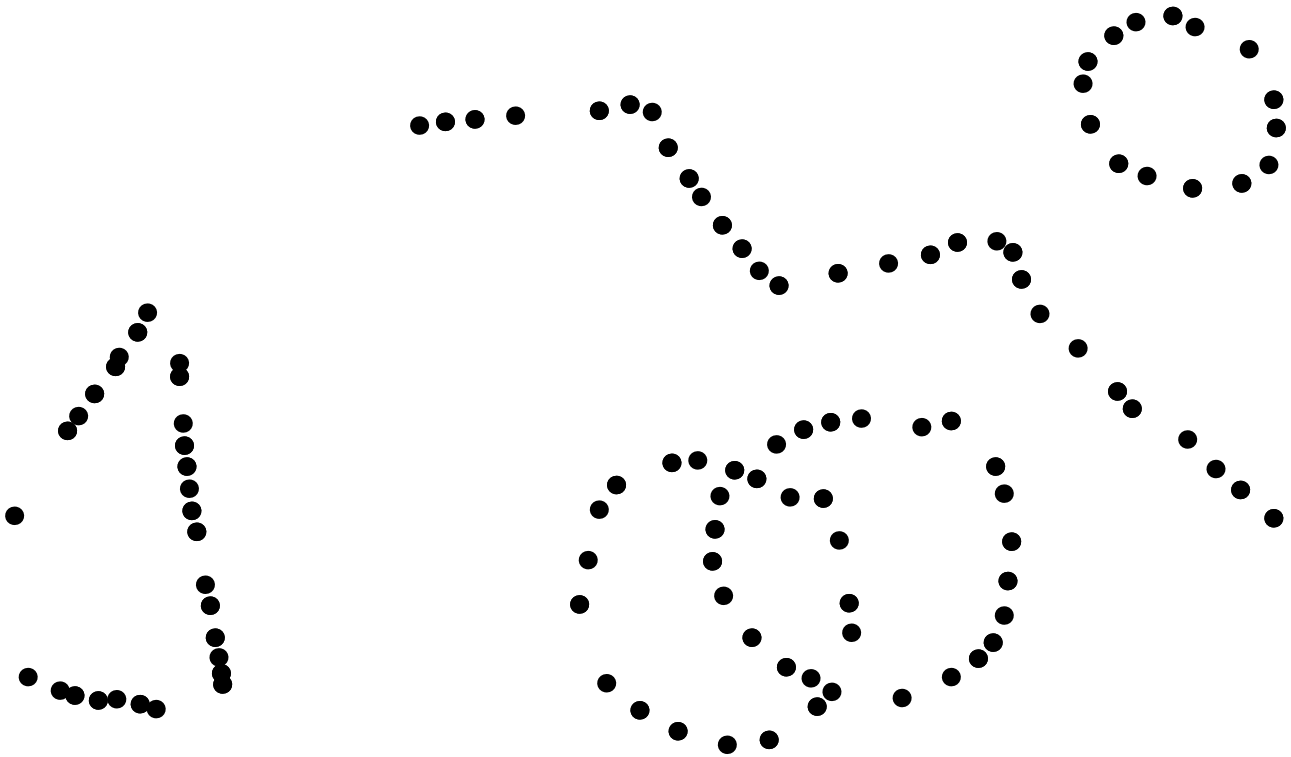
- given a set of points in the plane
- construct a geometric figure interpolating the sample points
- that reasonably capture the shape of the point set

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.

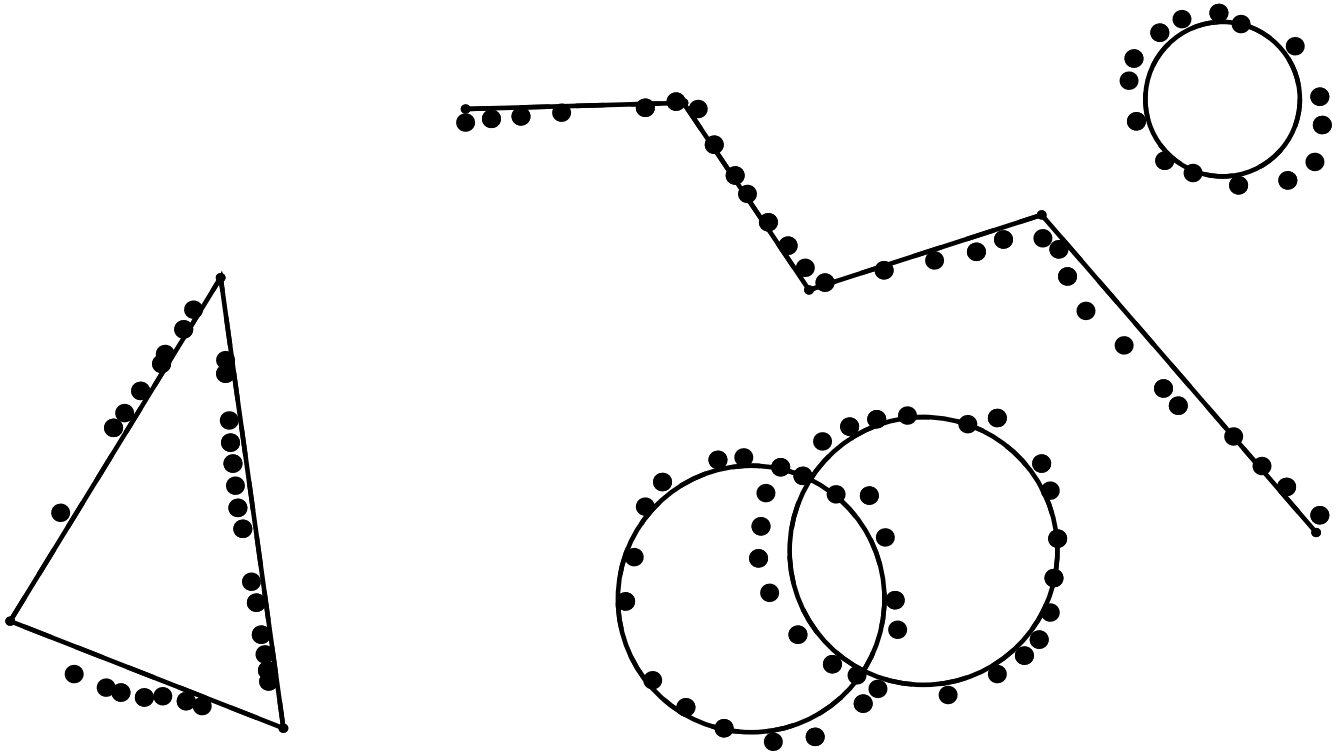
Example

point set



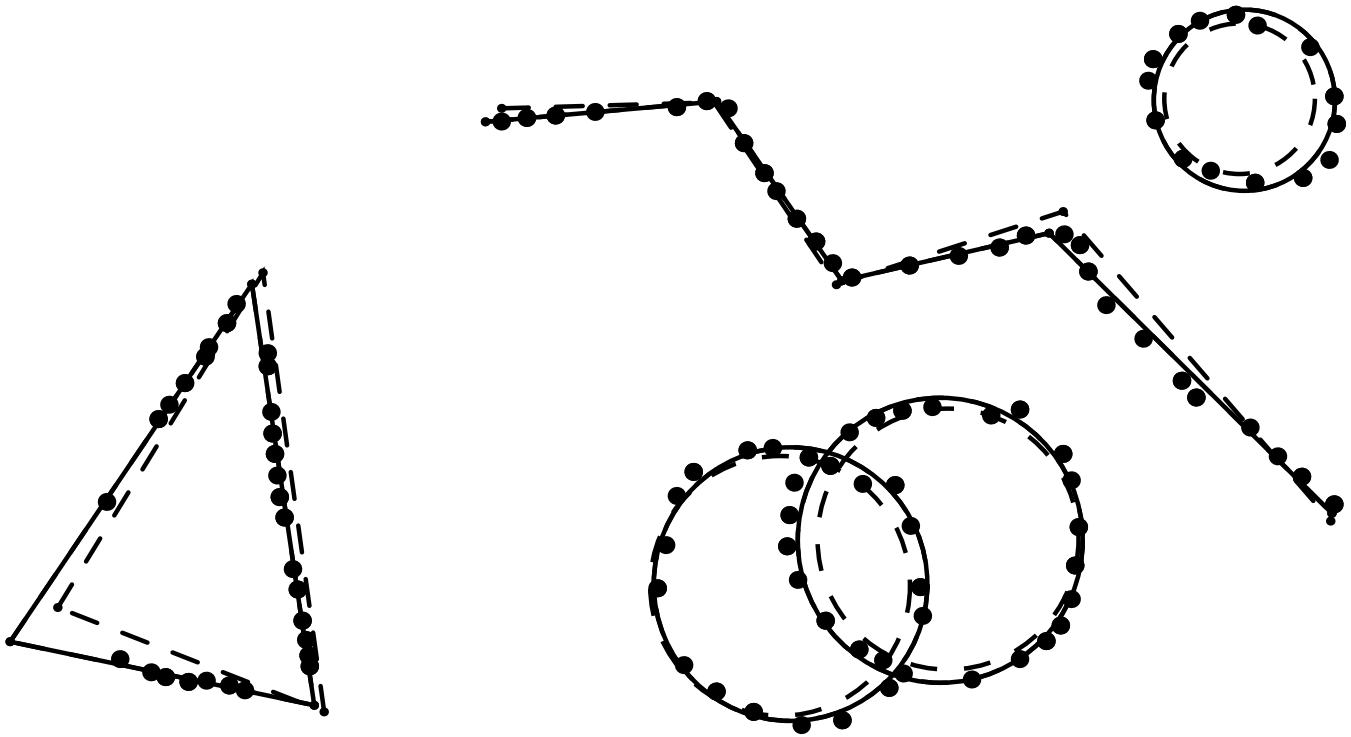
Example

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, clasification (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

- α–shapes
- crust
- curve approximation

Alpha–shapes

application

The algorithm is able to detect

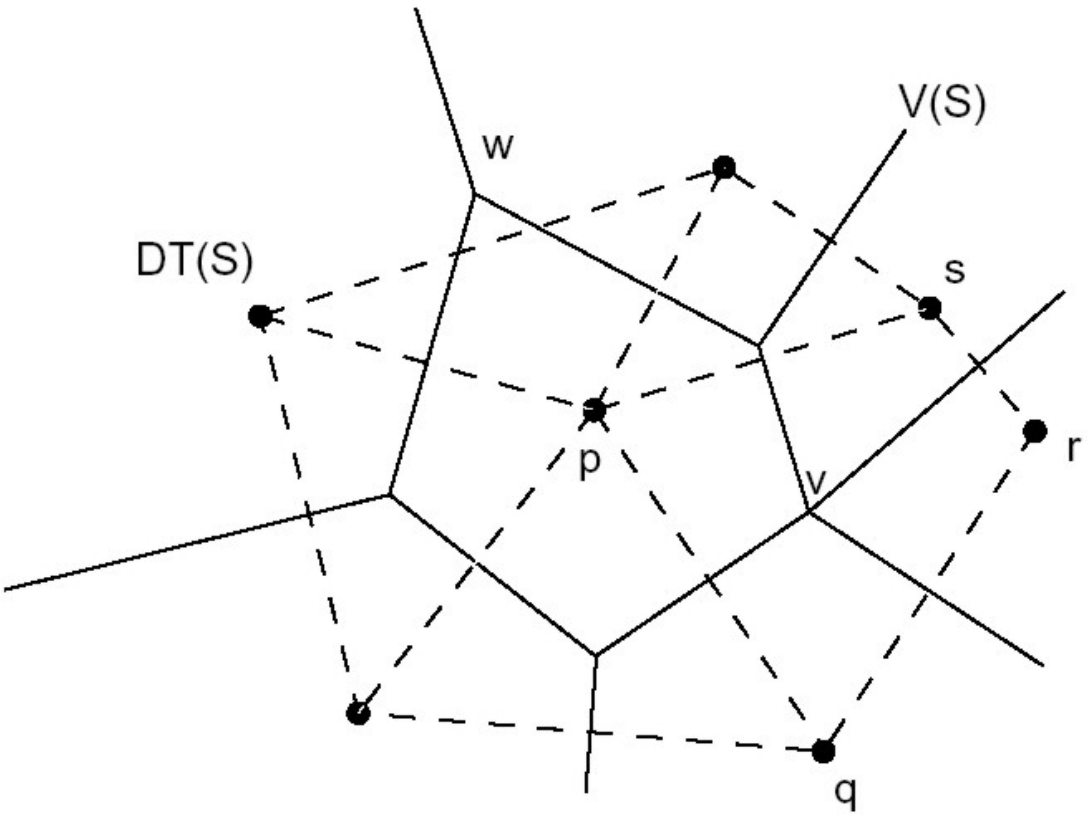
- the outer boundary of a set of points
- which covers more or less evenly distributed the interior of a shape.

Alpha–shapes

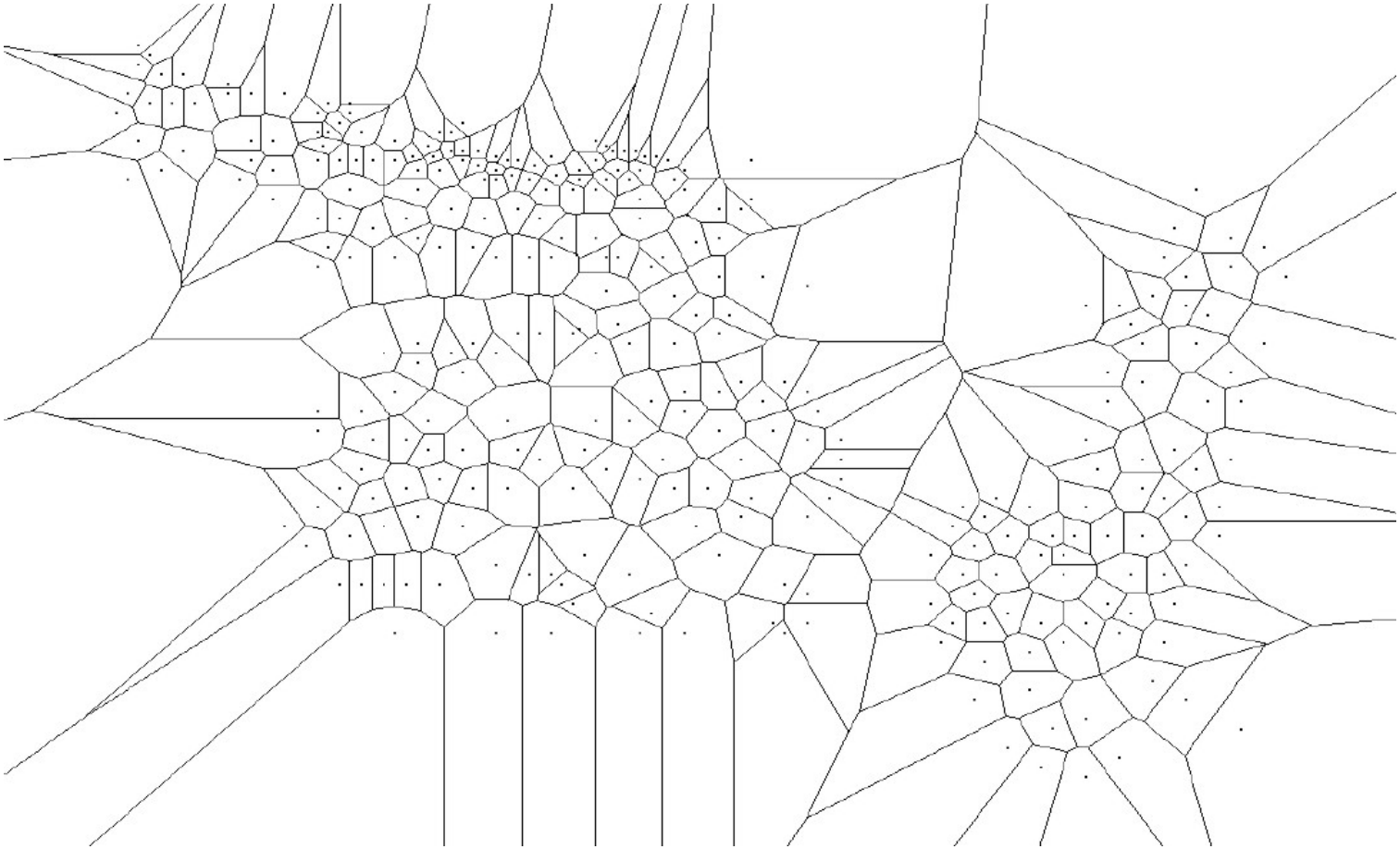
algorithm

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

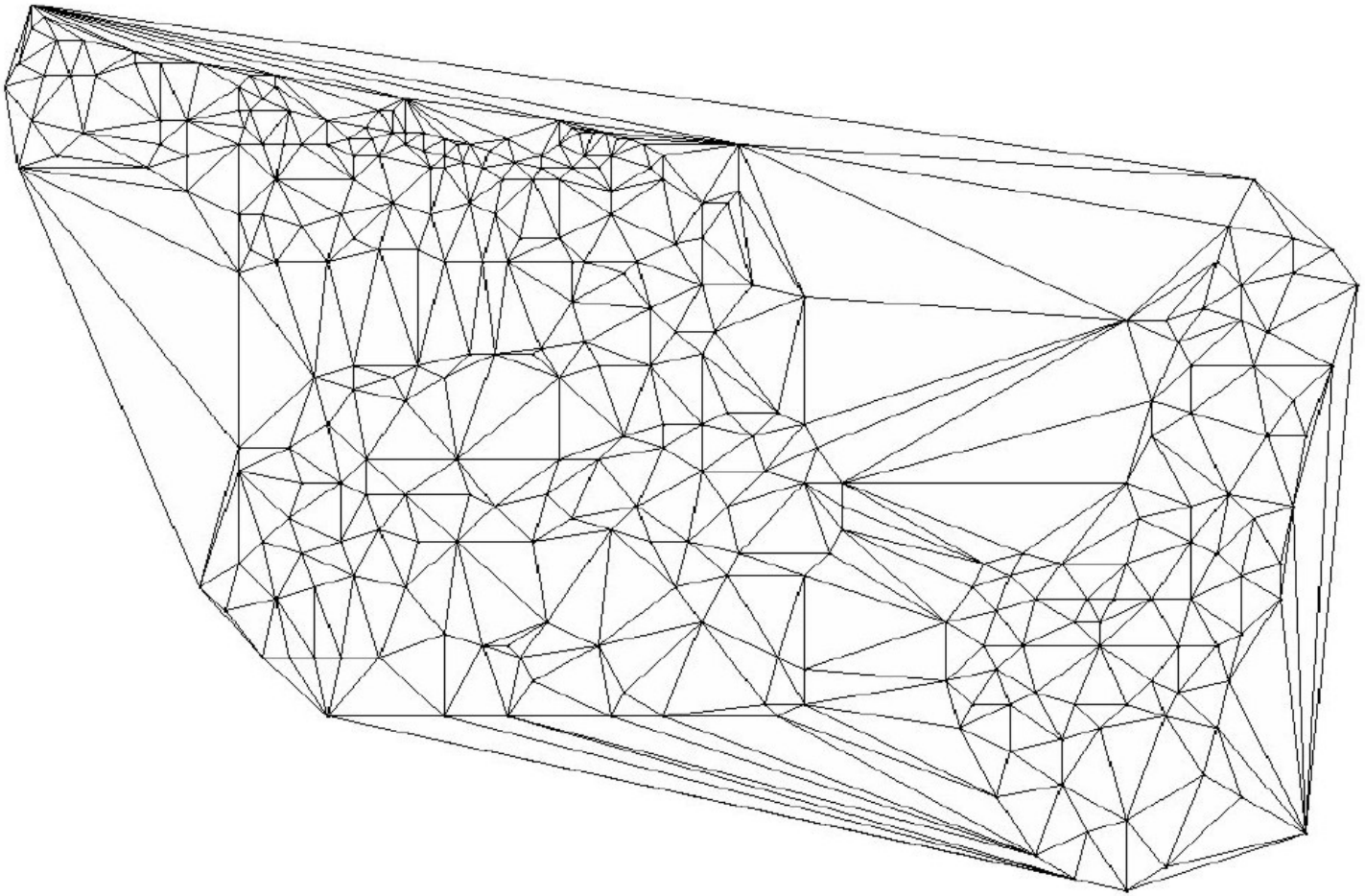
VORONOI–diagram



VORONOI–diagram with more points

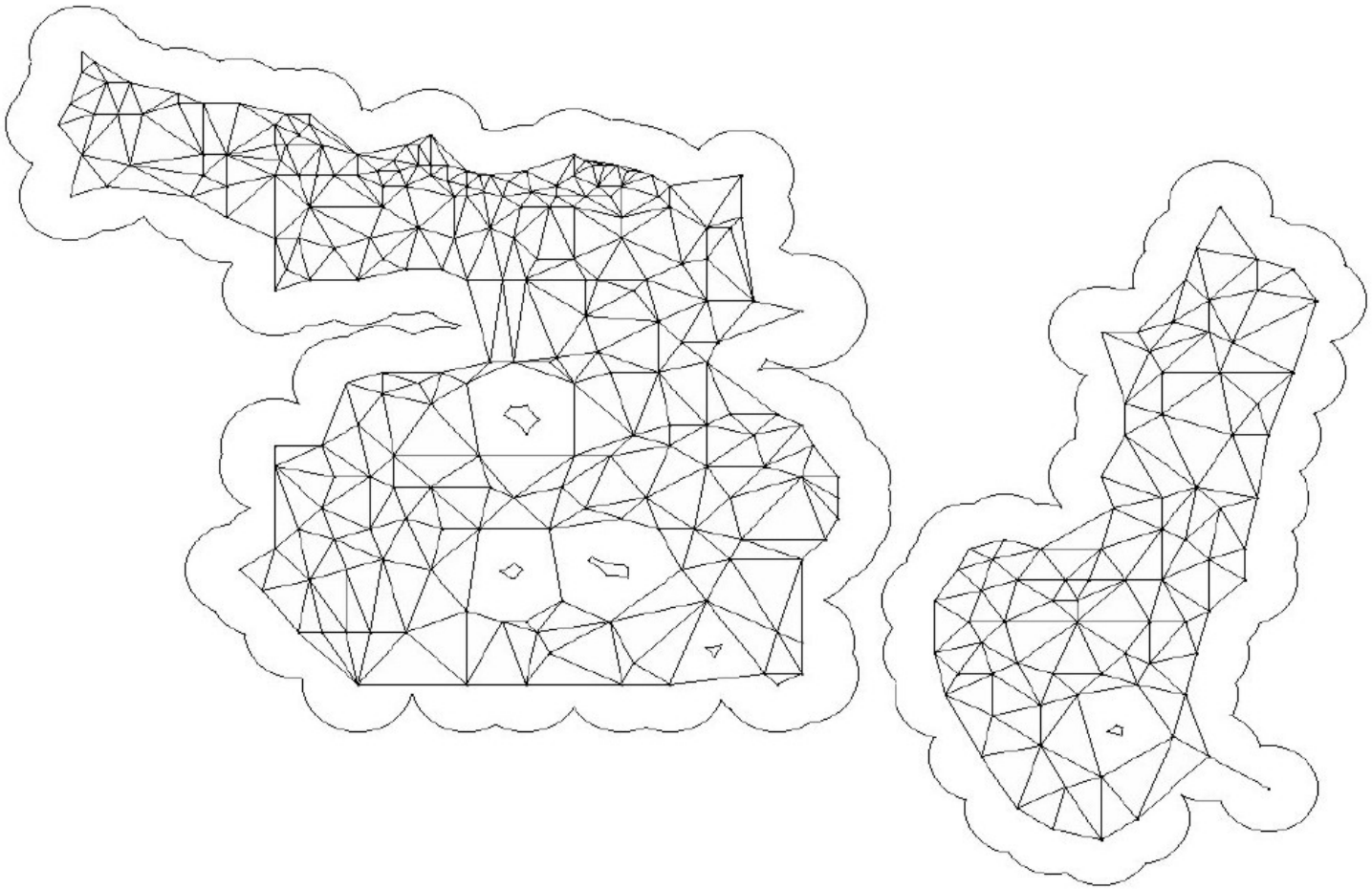


DELAUNAY–diagram



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

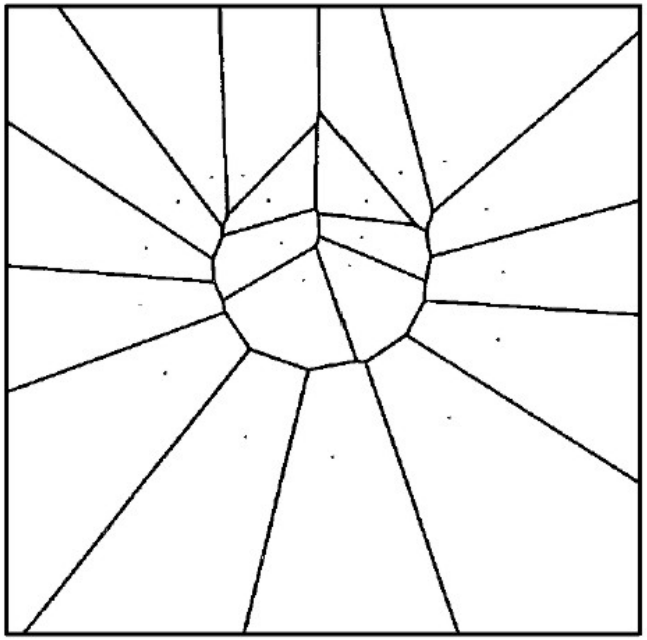
algorithm

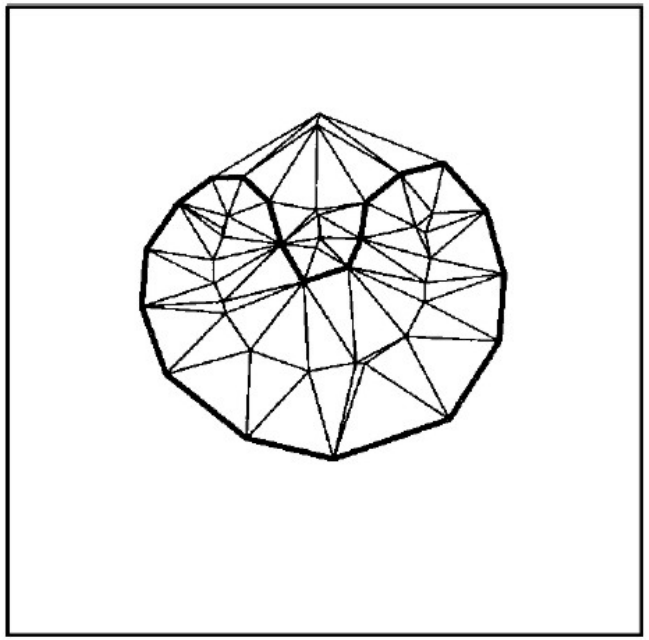
The crust

- 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

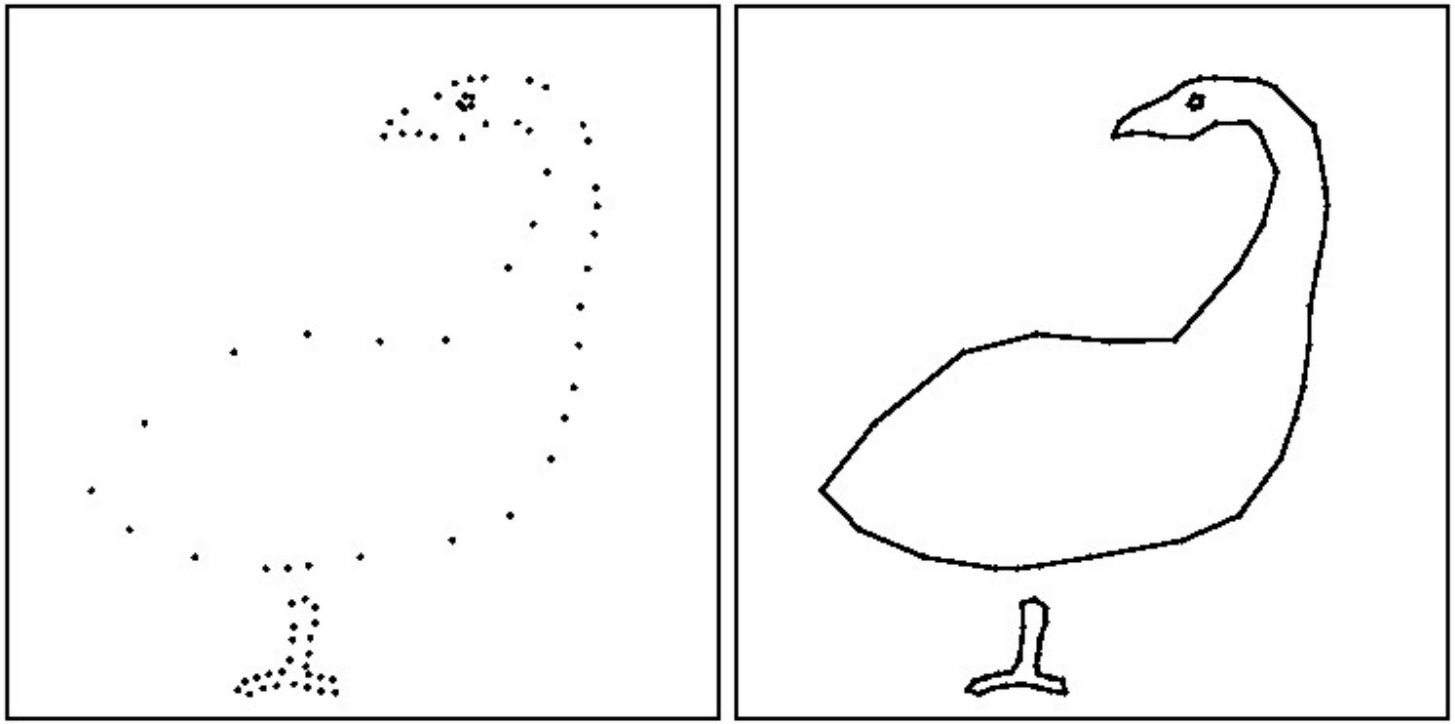
Example





CRUST

Example



Curve reconstruction

algorithm

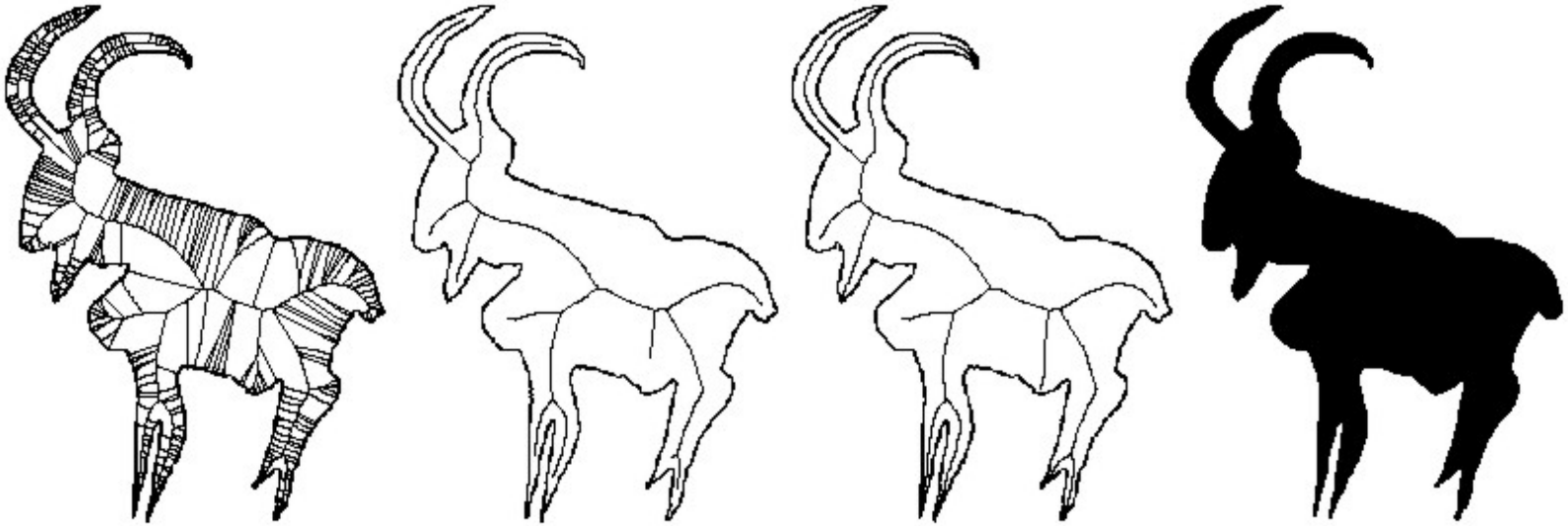
- Computes the GABRIEL graph as a subgraph of the Delaunay graph
- (an edge between two input points belongs to the Gabriel graph if a disk with this edge as diameter does not contain any other input point).
- Eliminate the edges which do not fulfill the local granularity property,
- i.e., at each point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

Curve reconstruction

application

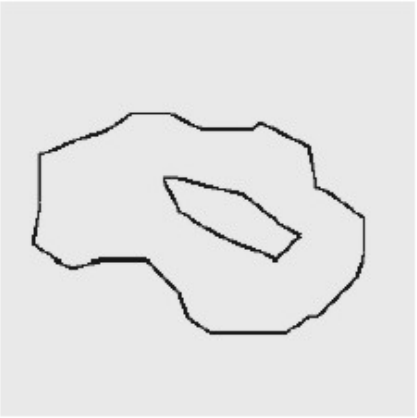
- The method works well if there exists a regular interpolant,
- that is, a polygonal closed curve such that the local granularity,
- defined as minimum distance to an input point,
- at each point of the curve is strictly smaller
- than the local thickness at that point,
- defined as the distance to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

Skeleton

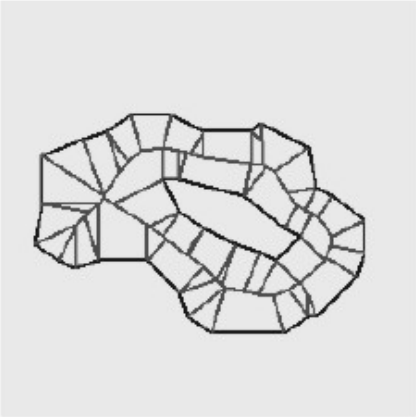


Skeleton

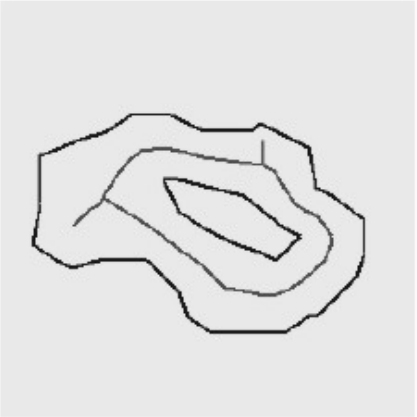
(a) Planar Shape



(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–ϵ 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 exist a genetic algorithm to cope with the min–# problem which found near optimal solutions in the presented experiments.

A shape $\mathcal{S}$ 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 $\varrho \in \mathbb{R}$;
- set of circumferences: set of pairs of center points and corresponding radii, i.e., $(\mathcal{C}, \mathcal{R}) \subset \mathbb{R}^2 \times \mathbb{R}$;
- polyline or polygon: an ordered set of corner points $\mathcal{Q} = \{Q_1, Q_2, \ldots, Q_k\}, Q_j \in \mathbb{R}^2, j = 1, \ldots, k$, 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 $\varrho \in \mathbb{R}$.

- line

$$\delta_{L_2}(P_i, \mathcal{S}) = \left|\mathrm{Det}(P_i - L, (\cos\varphi, \sin\varphi)^T)\right|$$

- circumference

$$\delta_{L_2}(P_i, \mathcal{S}) = |\|P_i - C\| - \varrho|$$

- set of circumferences

$$\delta_{L_2}(P_i, \mathcal{S}) = \min_{(C_j, \varrho_j) \in (\mathcal{C}, \mathcal{R})} \left|\|P_i - C_j\| - \varrho_j\right|$$

- 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

$$\delta_{L_2}(P_i, \mathcal{S}) = \min_{Q_j \in \mathcal{Q}} \delta_{L_2}(P_i, \overline{QQ_j})$$

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

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

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. $+\varrho$ is taken when the point P_i lies inside the rectangular box through $Q_1, \ldots, Q_4$, and $-\varrho$ when P_i lies outside.

- vertical distance to a line:

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

- 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

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

- AVG

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

- MAX

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

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

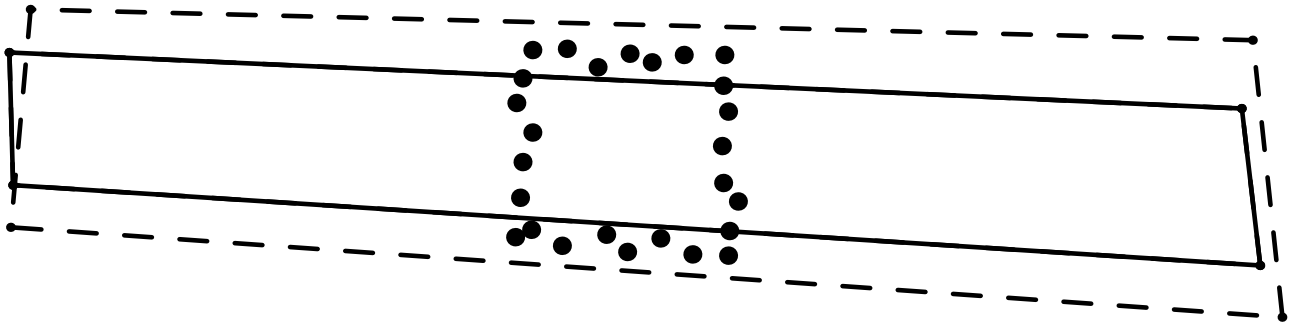
shaprox

algorithm for local search

- 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.

Example: Subsidiary objective



- 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.

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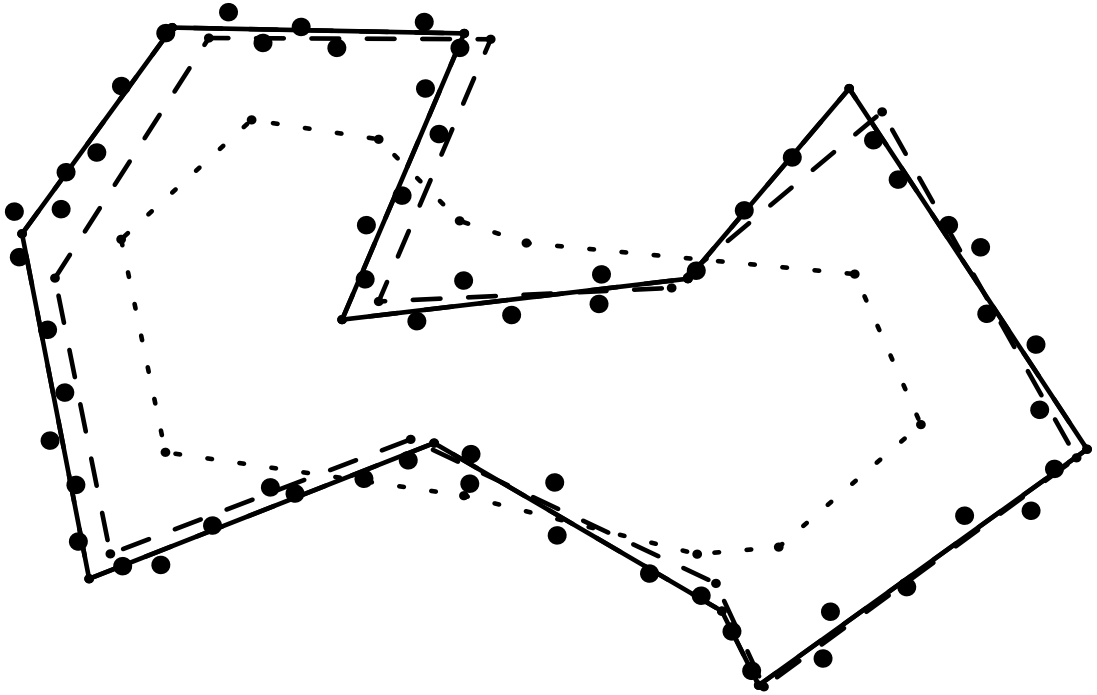
Subsidiary objective: short coming of possible solution

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

Example: convex combination as objective function



- 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:

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

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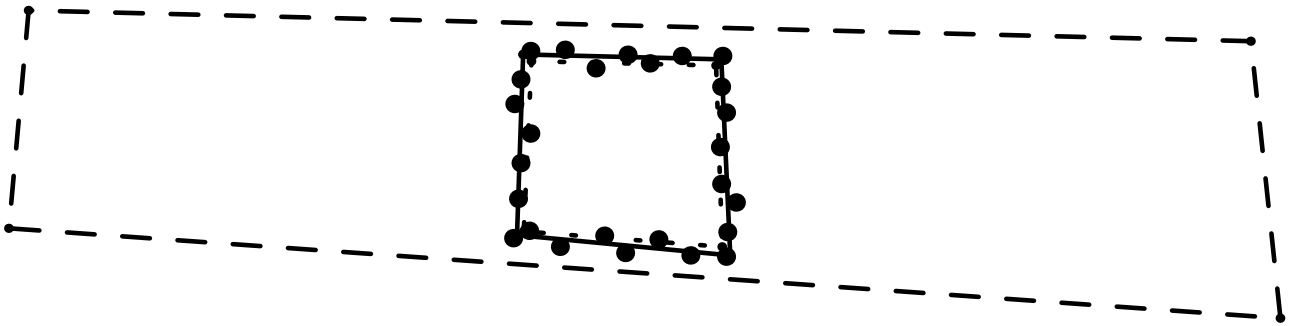
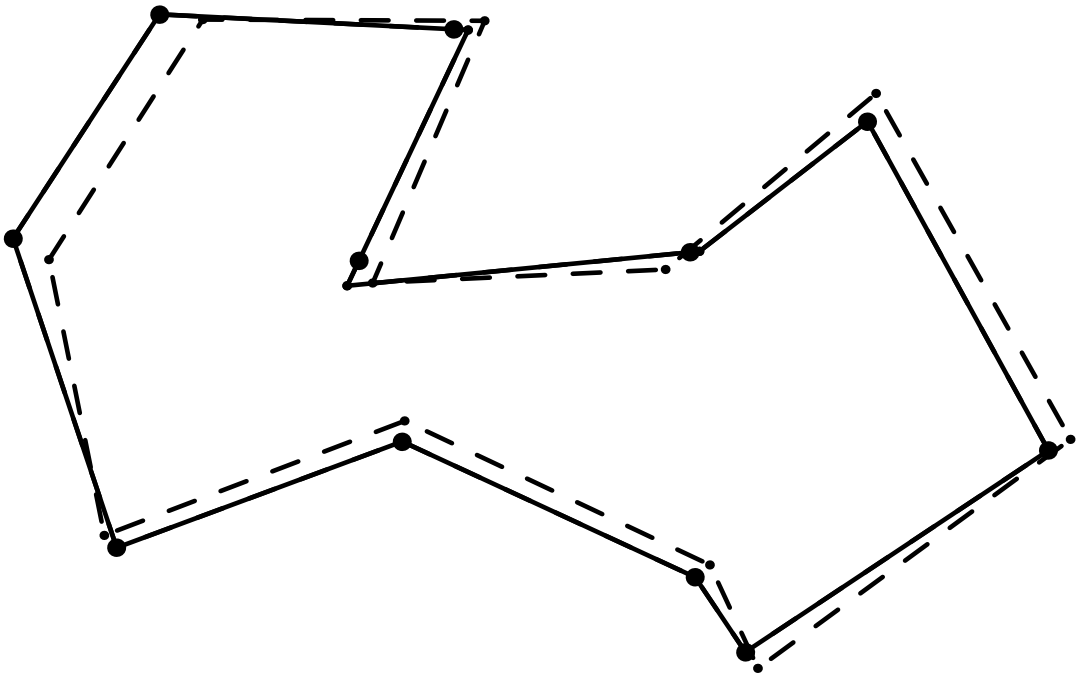
Example



NP–Completeness and non–convexity of the objective function



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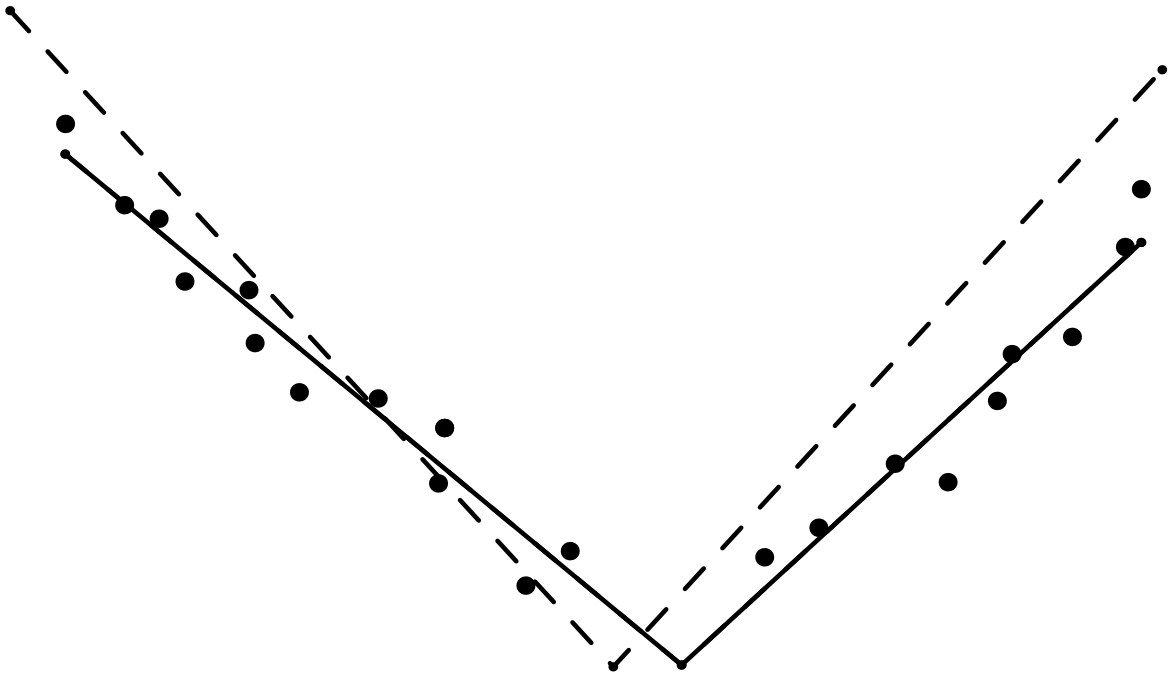
Examples: wedge



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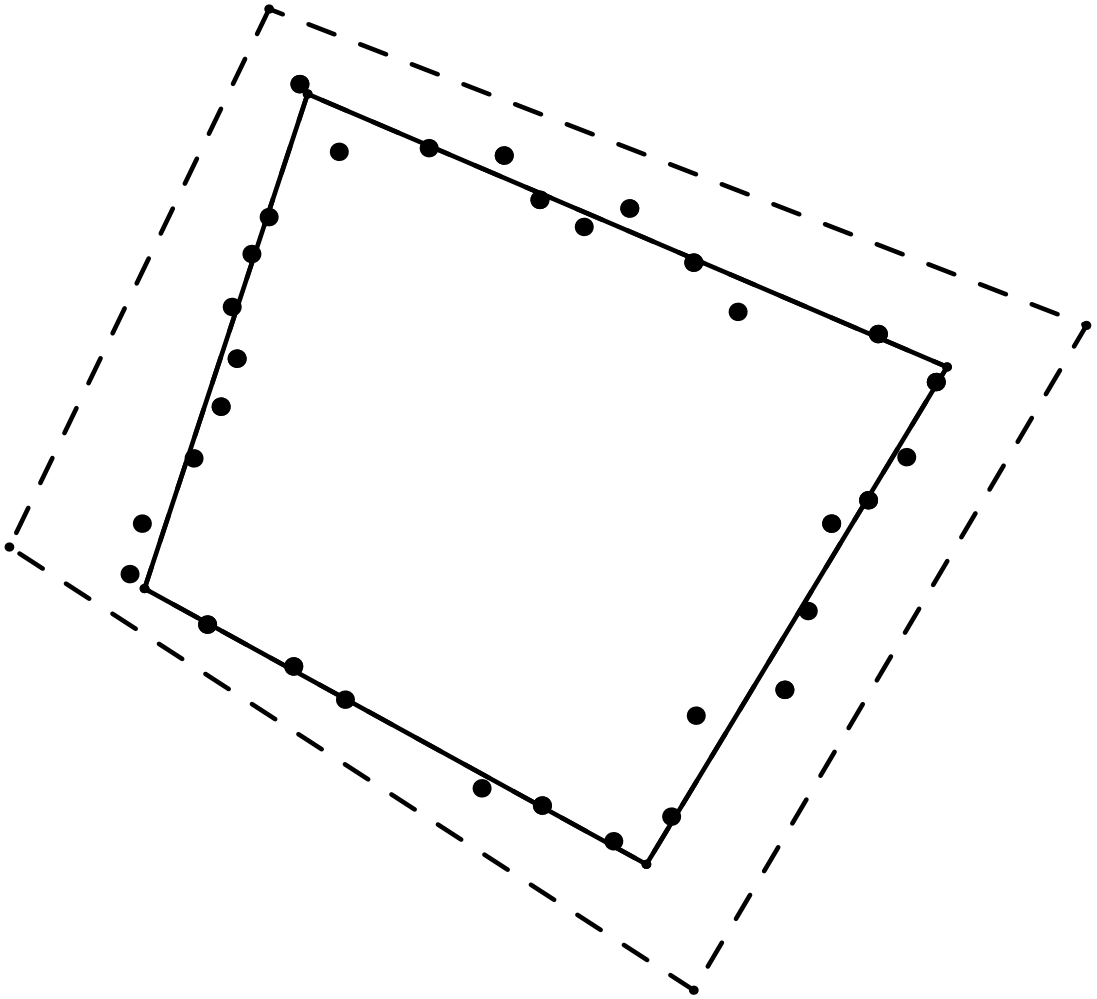
Examples: simple polygon



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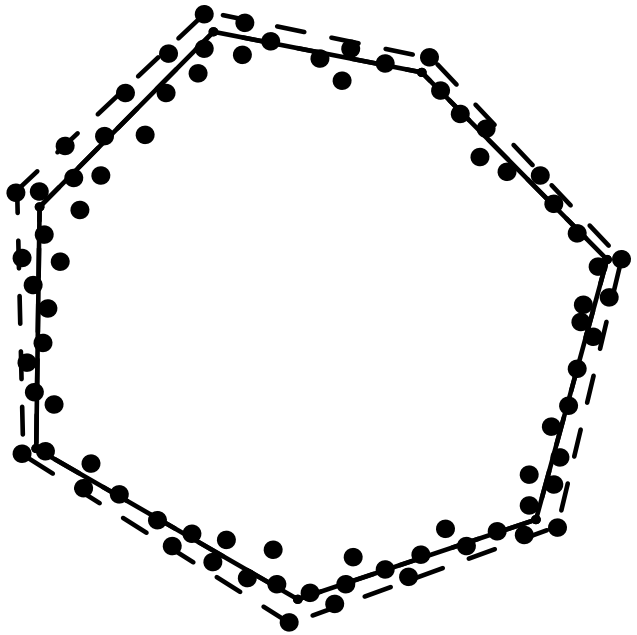
Examples: convex hull



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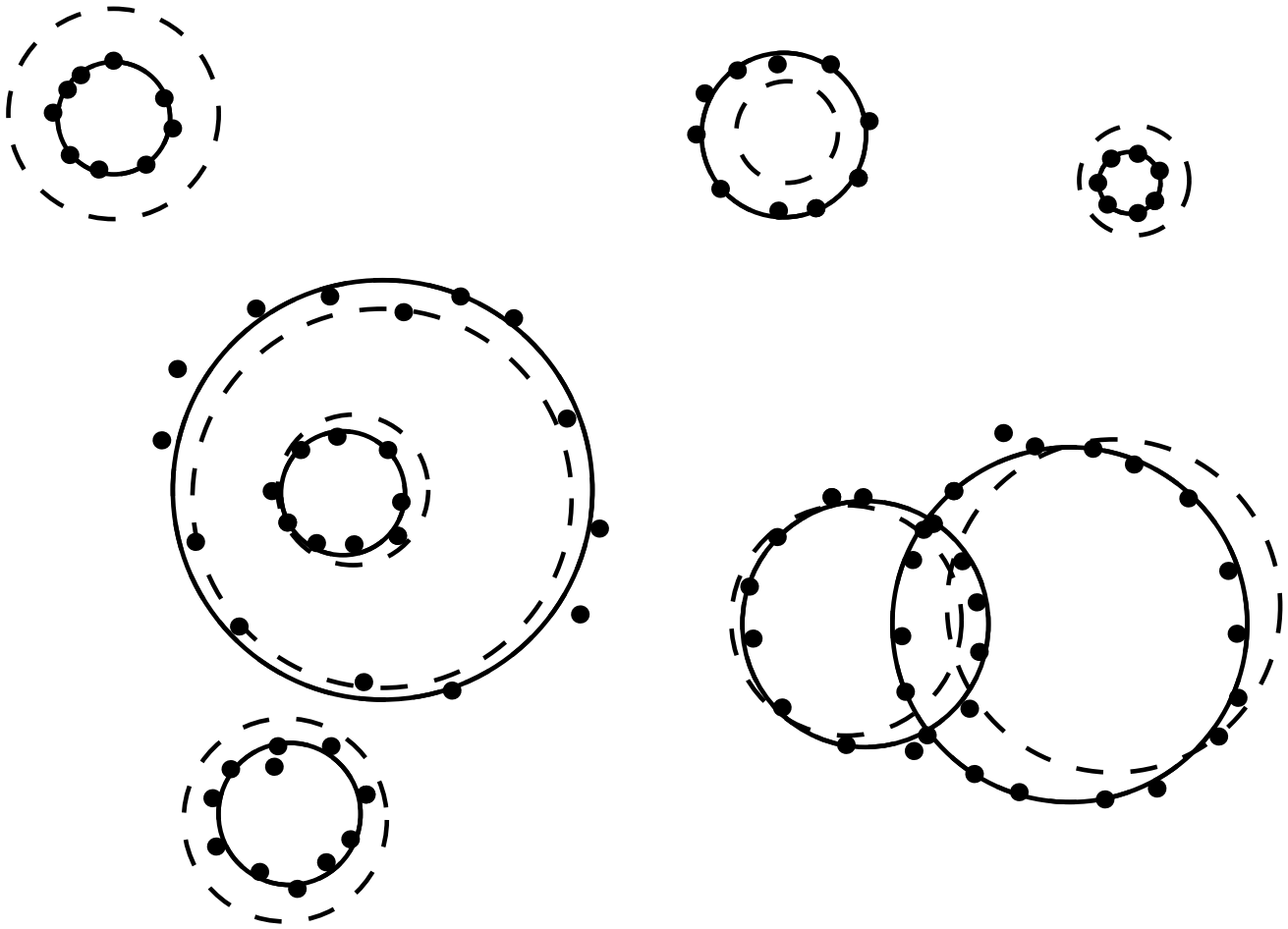
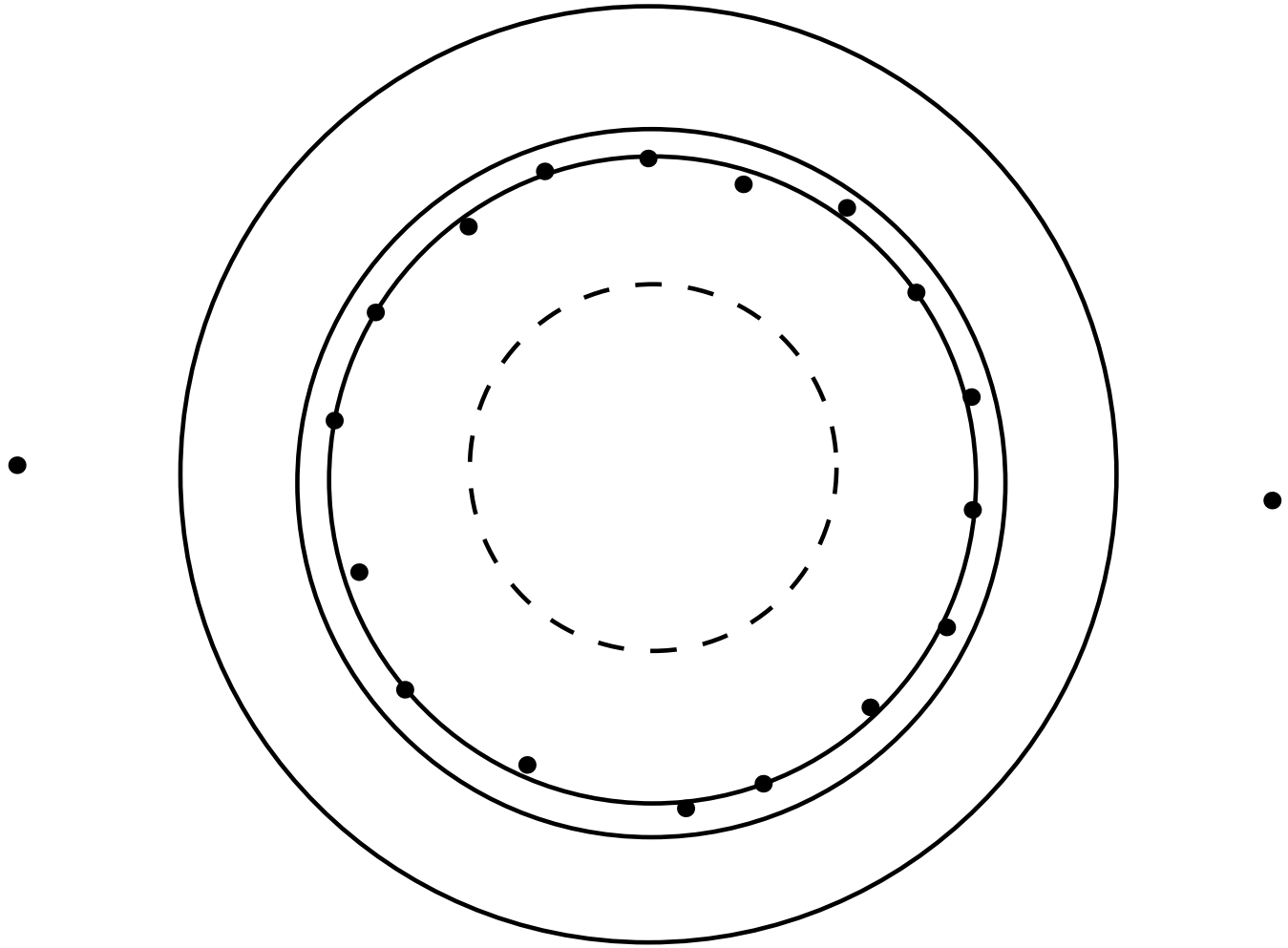
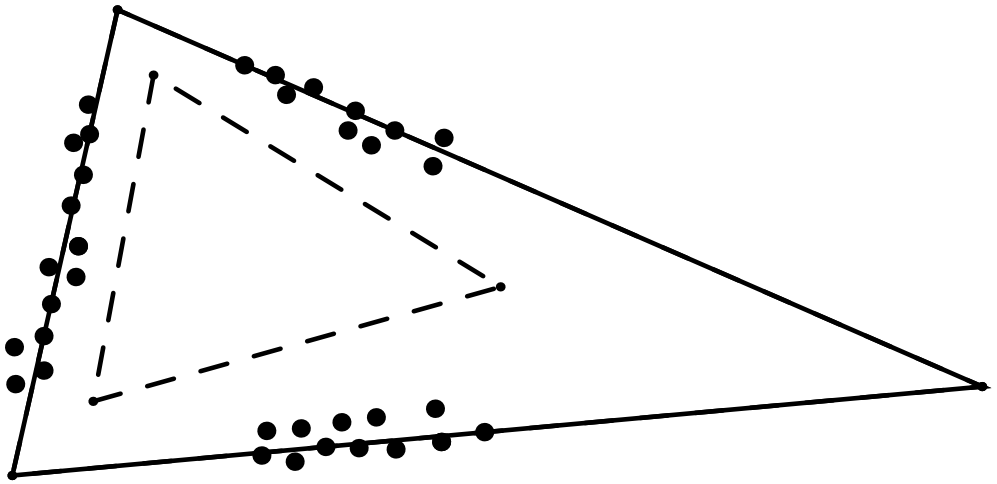
Examples: circumferences

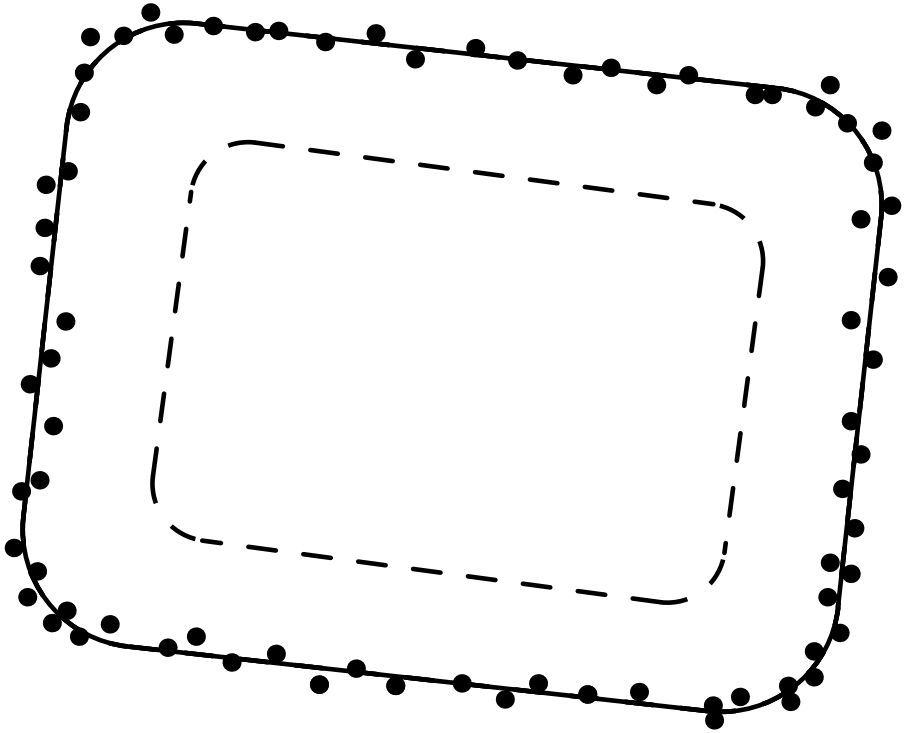


Examples: influence of metrics





Examples: rounded rectangle



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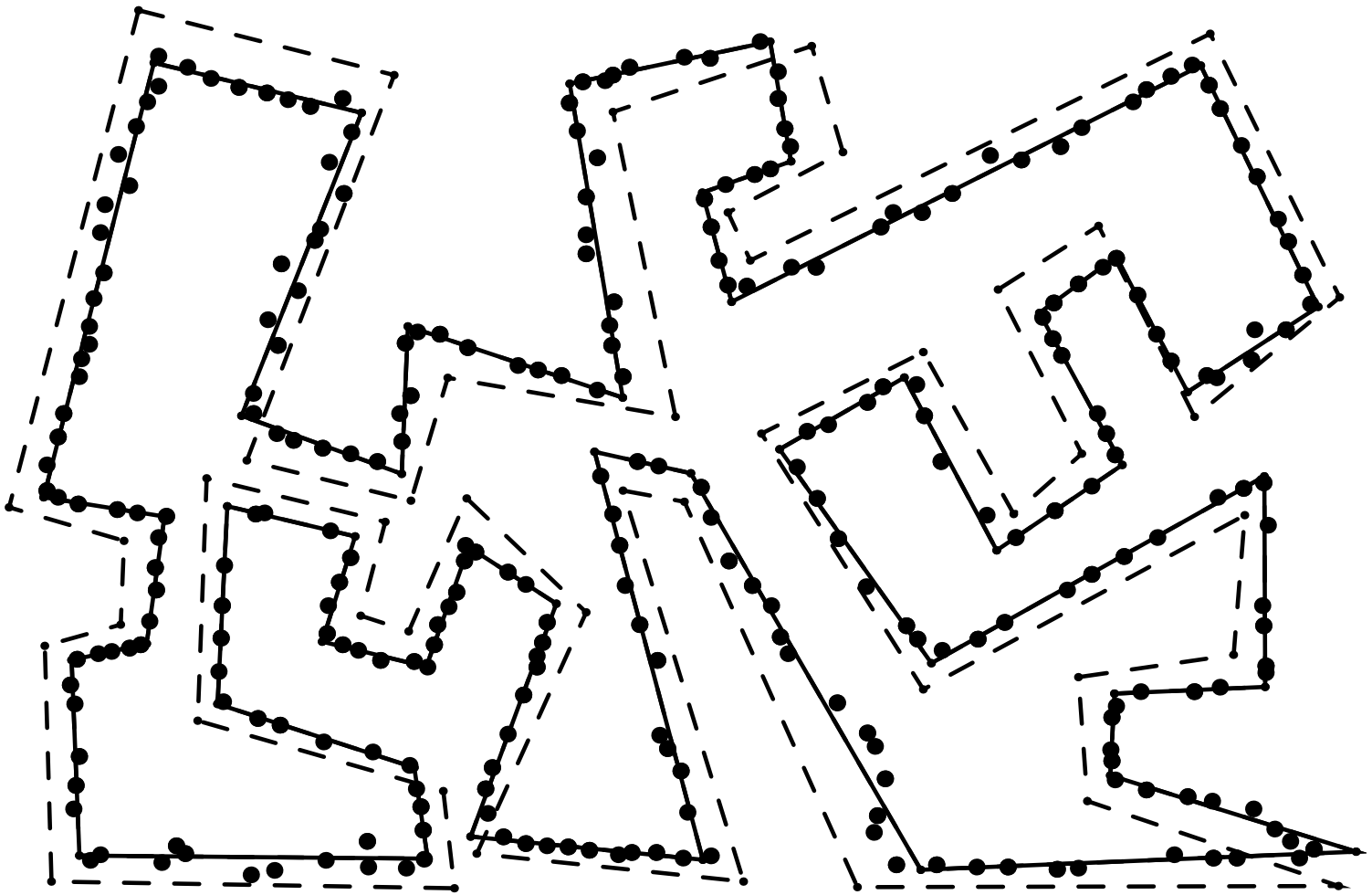
Examples: complex polygon



Software

- more than 7.000 specific lines of C++
- uses the libraries:
  - ImageMagick
  - Gtkmm (graphical user interface)
  - own libraries

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¿Questions?

¡Many thanks!