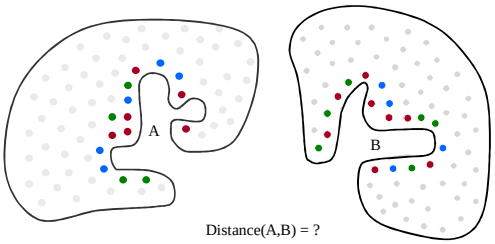
Registration of Point Sets with Rigid Transformations

Thomas Funkhouser
Princeton University
CS526, Fall 2010

Point Set Matching

Goal is to compute a similarity measure for a pair of attributed point sets

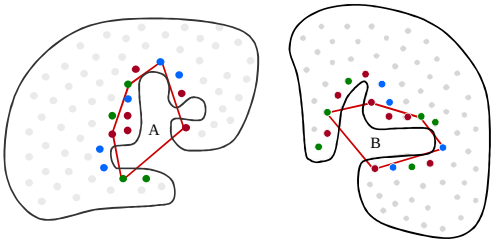


Distance(A,B) = ?

Point Set Matching

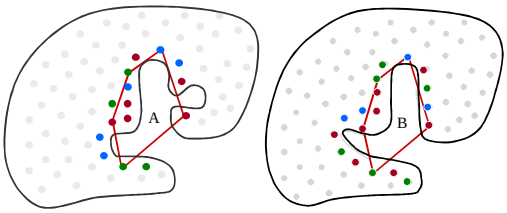
Challenge is to find corresponding points

- "Subset of points in A" may match "subset of points in B"



Point Set Matching

Calculating a superposition and distance measure is easy if correspondences are known (proposed)



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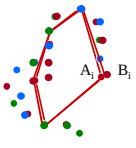
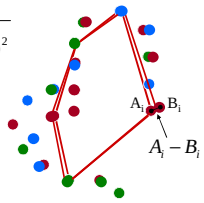


Least-squares optimal superposition of corresponding points

Point Set Matching

Calculating a superposition and distance measure is easy if correspondences are known (proposed)

$$RMSD(A,B) = \sqrt{\sum_{i=1}^{N} (A_i - B_i)^2}$$



Distance(A,B) = RMSD(A,B) + OtherTerms …

Outline

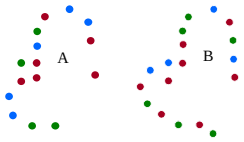
Introduction

Point set matching
- Brute force search
- RANSAC
- Geometric hashing
- Assocation graphs
- Iterative closest point

Discussion

Brute Force Search

Simple method:
- Try all possible sets of point correspondences
- Score the alignment for each one



Problem:
- O(n^m) possible sets of m correspondences among n points

Brute Force Search

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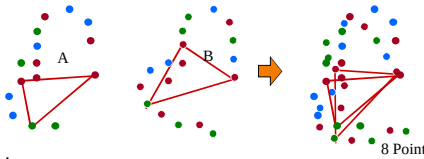

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Brute Force Search

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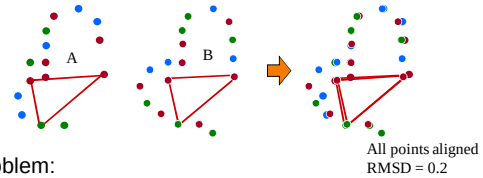

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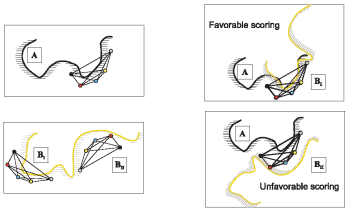
RANSAC

Randomly sample set of possible correspondences
- Randomly generate a small set of point correspondences
- Compute the aligning transformation for correspondences
  Score how well other points align after that transformation



[Schmitt02]

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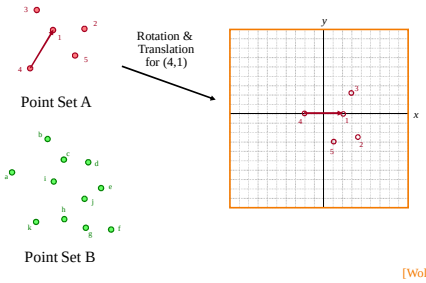
Geometric Hashing

Discretize transformations and scoring

[Wolfson97]

Geometric Hashing

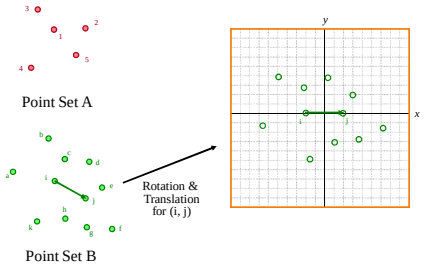
Discretize transformations and scoring



[Wolfson97]

Geometric Hashing

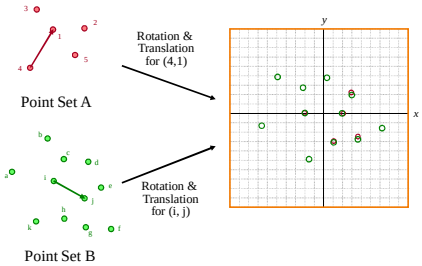
Discretize transformations and scoring



[Wolfson97]

Geometric Hashing

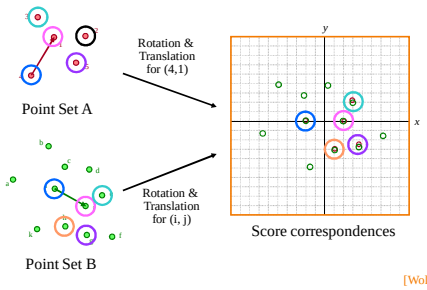
Discretize transformations and scoring



[Wolfson97]

Geometric Hashing

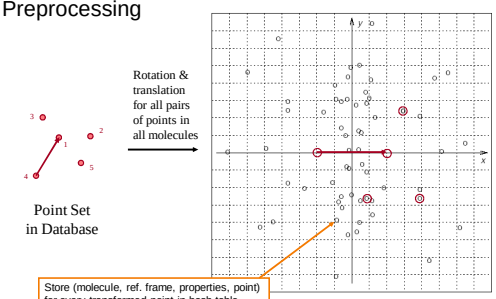
Discretize transformations and scoring



[Wolfson97]

Geometric Hashing

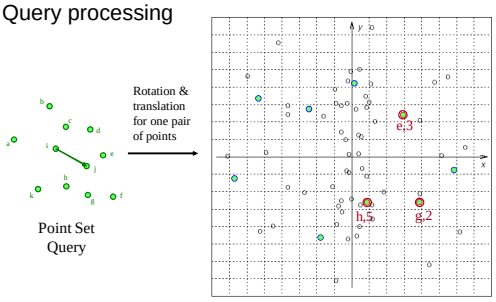
Preprocessing



[Wolfson97]

Geometric Hashing

Query processing



[Wolfson97]

Geometric Hashing

Preprocessing
- For each triple of points
  - Compute reference frame
  - For each point
    - Transform point into reference frame
    - Hash (molecule, ref. frame, properties, point)

Query processing
- Choose any triple of points
- Compute reference frame
- For each point
  - Transform point into reference frame
  - For each entry in hash bin for transformed point
    - Check point properties
    - Vote for (molecule, ref. frame)

Geometric Hashing

Preprocessing complexity
- $O(n^4)$ for n points per binding site
  - $O(n^3)$ possible triples * O(n) transformations per triple

Query complexity
- O(m) * binsize for m points in query binding site
  - 1 triple * O(m) transformations per triple * binsize hash processing per transformation

[Wolfson97]

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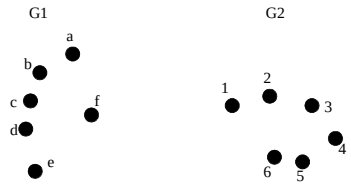
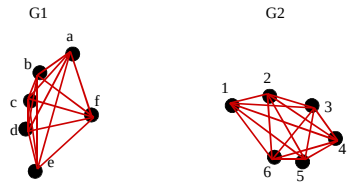
Association Graphs



[Schmitt02, Brown82]

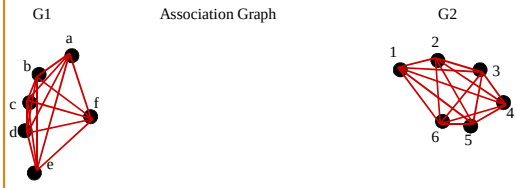
Association Graphs



Represent both points sets as complete graphs (G1 and G2).
(edges connect all pairs of vertices within each point set)

[Schmitt02, Brown82]

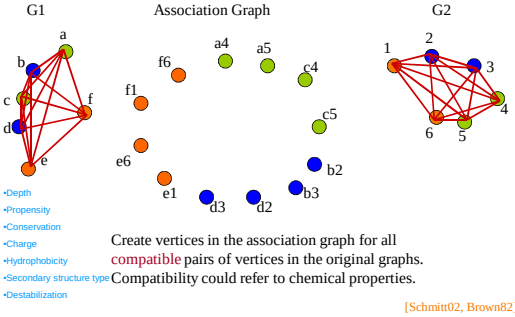
Association Graphs



Create vertices in the association graph for all compatible pairs of vertices in the original graphs.
This can lead to a large number of vertices.

[Schmitt02, Brown82]

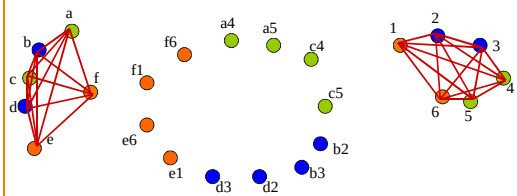
Association Graphs



Create vertices in the association graph for all compatible pairs of vertices in the original graphs.
Compatibility could refer to chemical properties.

[Schmitt02, Brown82]

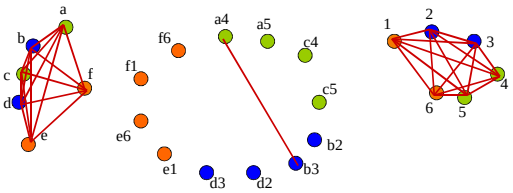
Association Graphs



Create edges between (uv) and (wx) if the edges between (u) and (w) as well as between (v) and (x) match.

[Schmitt02, Brown82]

Association Graphs



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For this example, edge length is the only consideration

[Schmitt02, Brown82]

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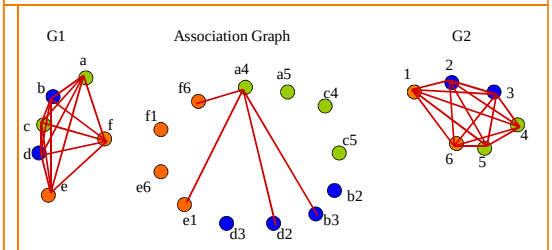

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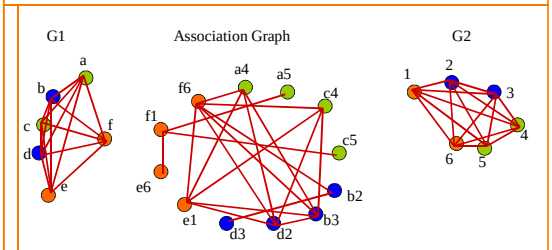

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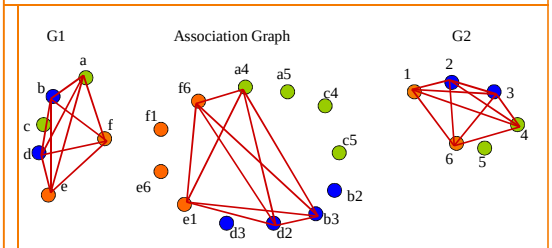


Finding correspondences: The the largest set of corresponding nodes in the same configuration is the maximal clique in the association graph

[Schmitt02, Brown82]

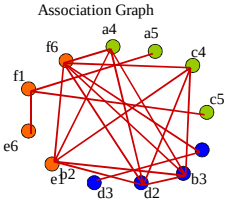
Association Graphs

Computational complexity:

- $O(2^n)$ for n points
- NP-complete
- Branch and bound algorithms

```
Find the Maximal Clique{
    return Cliques(empty, all nodes)
}

Cliques(X, Y){
    if (no node in Y-X is connected to all of X){
        return X;
    }else{
        y = node in Y connected to all of X;
        return Largest(Cliques(X union y, Y},
                       Cliques{X, Y-y});
    }
}
```



[Schmitt02, Brown82]

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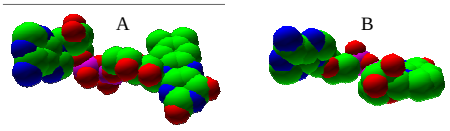
Iterative Closest Points

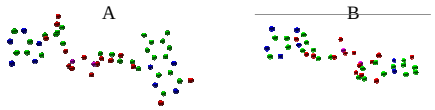
Given two point sets



[Besl92]

Iterative Closest Points

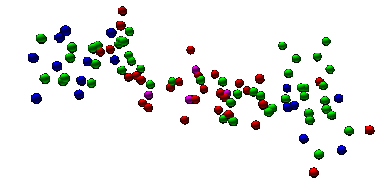
Given two point sets



[Besl92]

Iterative Closest Points

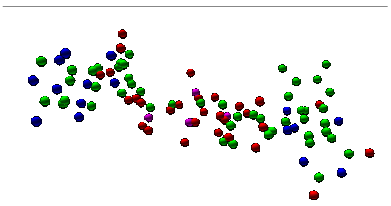
Given two point sets and an initial guess for the transformation that aligns them



[Besl92]

Iterative Closest Points

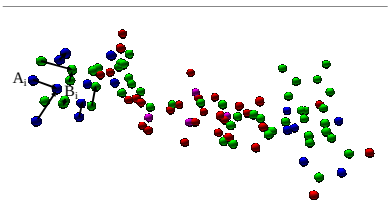
Assume closest points correspond



[Besl92]

Iterative Closest Points

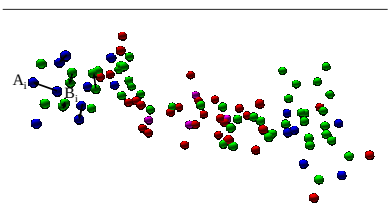
Assume closest points correspond: A→B



[Besl92]

Iterative Closest Points

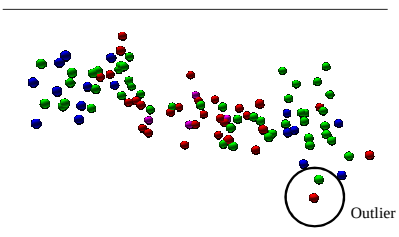
Assume closest points correspond: A→B and B→A



[Besl92]

Iterative Closest Points

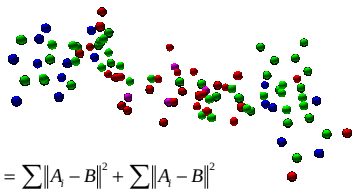
Rejecting outliers



[Besl92]

Iterative Closest Points

Find the transformation that optimally aligns proposed correspondences (superposition)



$$d(A,B) = \sum_{A_i \in A} \|A_i - B\|^2 + \sum_{B_i \in B} \|A_i - B\|^2$$

[Besl92]

Iterative Closest Points

Iterate until convergence

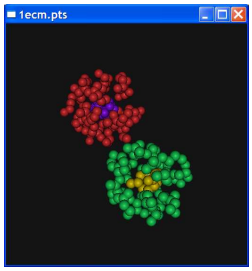
1. Select source points (from one or both molecules)
2. Match to points in the other molecule
3. Weight the correspondences
4. Reject outlier point pairs
5. Compute an error metric for the current transform
6. Minimize the error metric w.r.t. transformation

Computational complexity

- O(k * nlogn) for n points per binding site and k iterations
  - k iterations * O(n) points * O(logn) to find closest point

Slide courtesy of Szymon Rusinkiewicz

Iterative Closest Points



Demo courtesy of Szymon Rusinkiewicz

Summary

Brute force
- Accurate, slow

RANSAC
- Approximate

Geometric hashing
- Fast query, after slow preprocessing
- Distance threshold implicit in hash bucket sizes

Association graphs
- Expensive for large point sets
- Distance threshold for “associations”

Iterative closest points
- Fast, in practice
- Requires good initial guess