# Capturing topological and geometric features for protein docking

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Joint Work with

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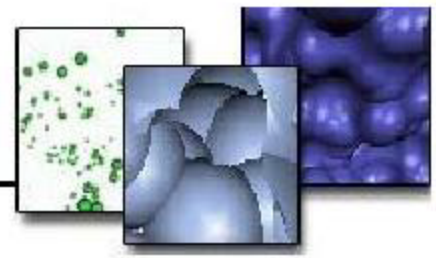
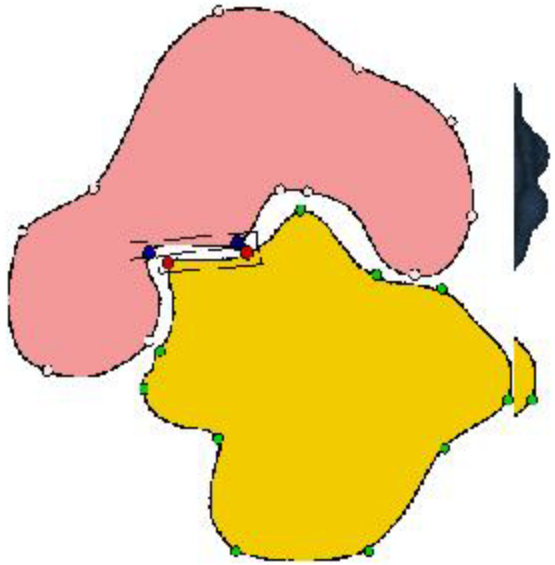
BioGeometry



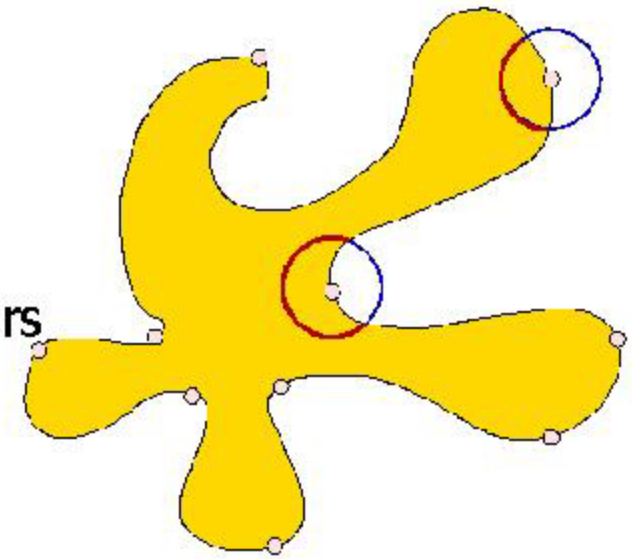
# Motivation

- Docking problem
  - Partial matching
- Extract features
  - Extract feature points
  - More global features?



# Related Work

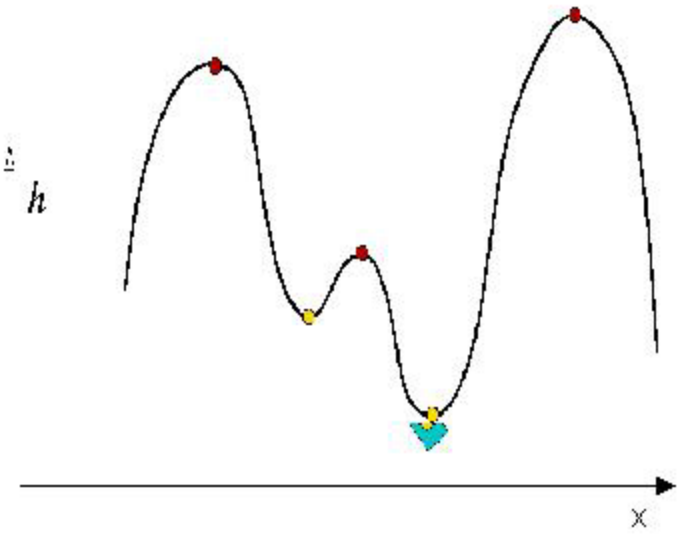
- Curvature
  - Too local
- Connolly function
  - Ratio of inside/outside perimeters
- Atomic density (Kuhn et al.)
  - FADE, PADRE



Our goal: more than good feature pts

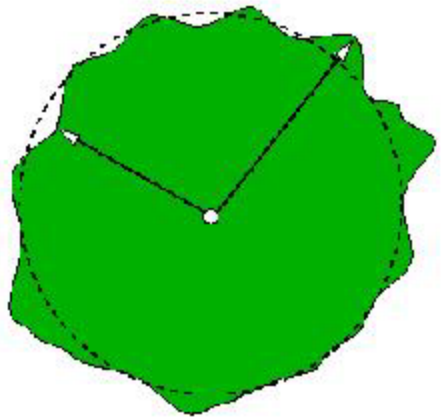
# Height Function

- Height function $h : M \rightarrow R$
- Morse function
  - No degenerate critical pts
  - No two critical pts have same function value
- Critical points
  - Capture topological features
- Pairs of critical pts
  - Persistence Alg. (ELZ01)
  - *Pairing decided by order of heights*



# General Manifold

- Height function + persistent alg.
  - Good at capturing/measuring vertical features
- All direction
  - Elevation on earth
- For general manifolds
  - No good choice for origin

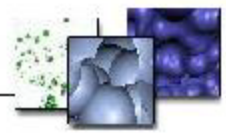


Function invariant under rigid motion

# Family of Height Functions

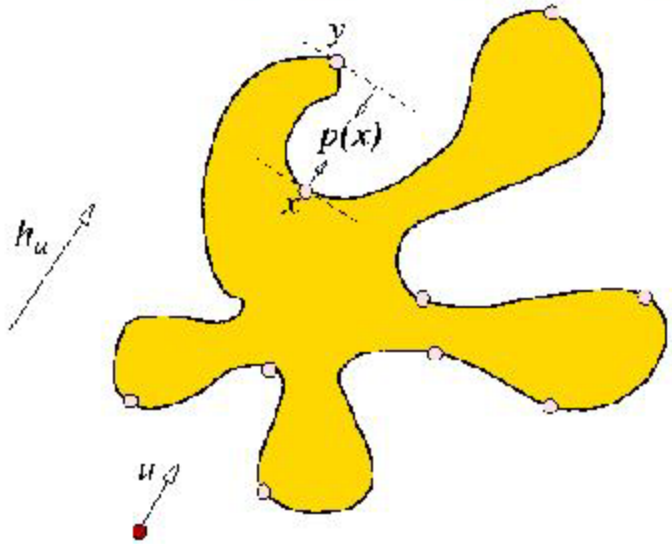
- Fix an arbitrary origin
- Given $u \in S^2$, define $h_u : M \rightarrow R$ , as
  - $h_u(x) = \langle x, u \rangle$
- $H : M \times S^2 \rightarrow R$ : a family of height functions
  - $H(x, u) = h_u(x)$





# Illustration

- Each $x \in M$ critical in normal direction
  - Pair $(x,y)$
  - Persistence $p(x) = p(y) = |h_u(x) - h_u(y)|$

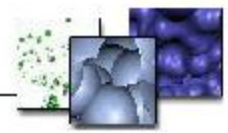


# Elevation $E$

- Define $E : M \rightarrow R$ as
  - $E(x) = p(x)$
- Interested in **max** of $E$
  - Each $x \in M$ captures feature in its normal direction
  - $E(x)$ indicates size of feature

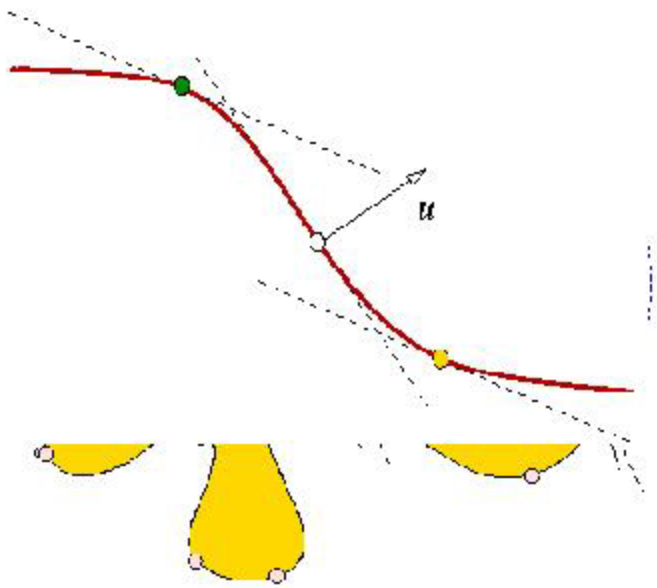
However, E not everywhere continuous





# Surgery

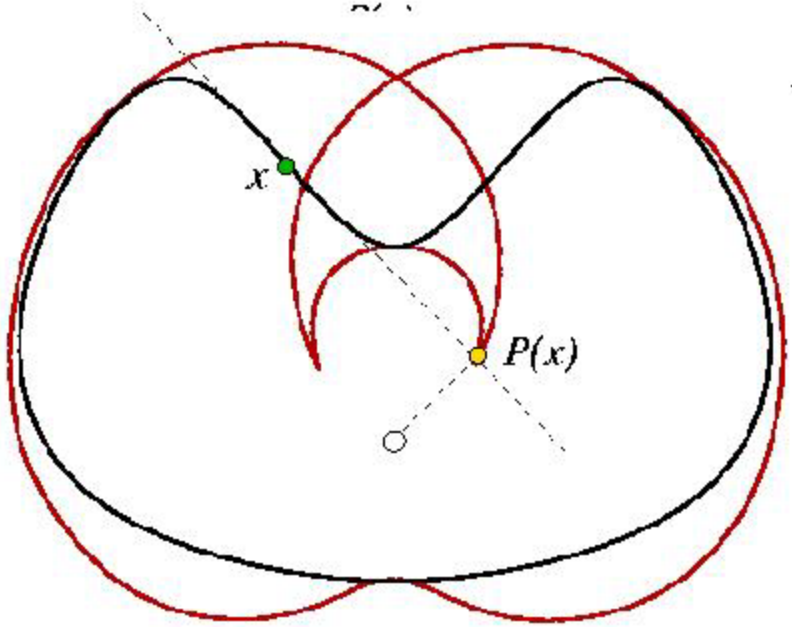
- Reason: singular tangency
  - Inflexion pt (birth-death pt)
  - Double tangency (interchange)




- Blame the manifold!
  - M' : apply surgery on M
  - Elevation function:
    - $E : M' \rightarrow R$

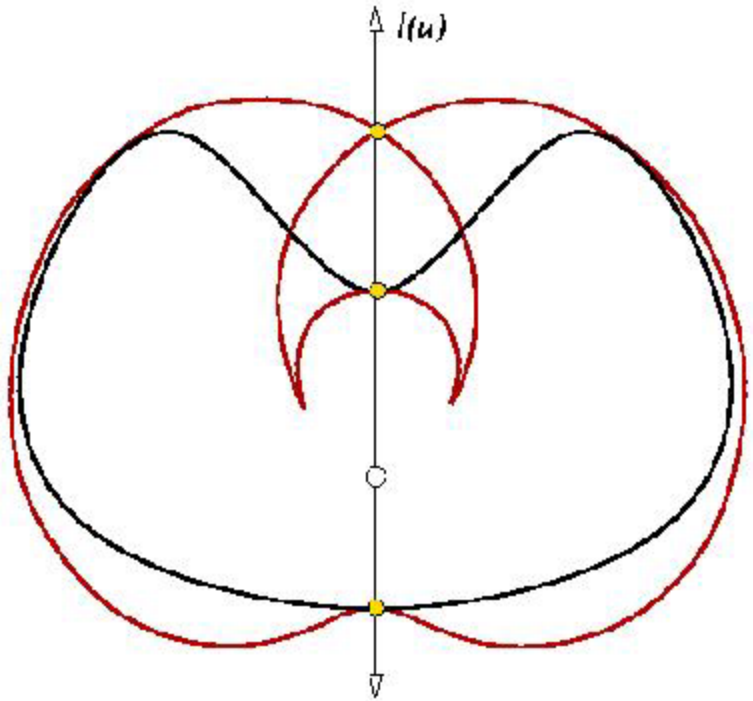
# Pedal Surface

- Goal: help understand E
- Definition for $P : M \rightarrow R^3$
- Singularities
  - Inflexion pt $\Leftrightarrow$ cusp
  - Double tangency $\Leftrightarrow$ xing



# Relation

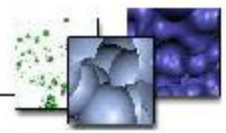
- Critical pts for $h_u \Leftrightarrow P \cap l(u)$
  - $P = P(M)$
- Singularities of $P$ along $l(u)$



# Dictionary of Singularities

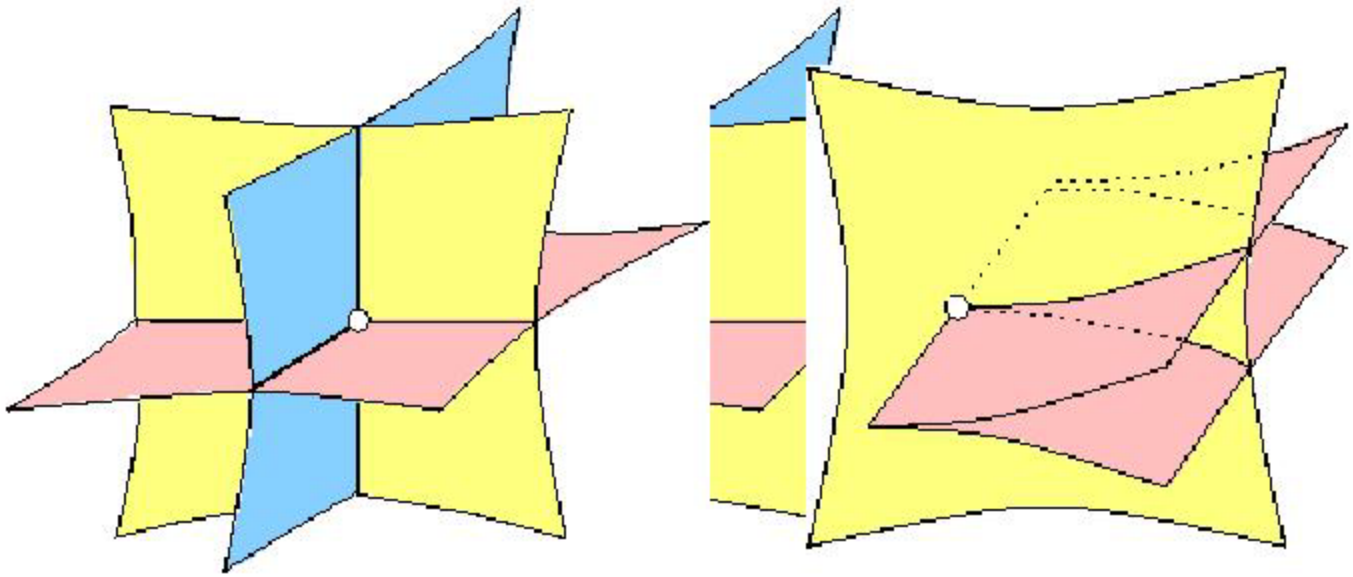
| M | Height | P |
|---|---|---|
| inflexion pt<br>double tangency | birth-death pt<br>interchange | cusp<br>xing |
| Jacobi pt<br>triple tangency | 2 birth-death pts<br>3 interchanges<br>bd-pt + interchange | dovetail pt<br>triple pt<br>cusp intersection |
| | 2 birth-death pts<br>2 interchanges<br>bd-pt + interchange | cusp-cusp crossing<br>xing-xing crossing<br>cusp-xing crossing |





# Examples

Examples of *triple pt* and *cusp + intersection*



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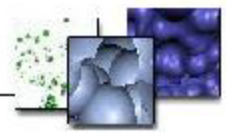
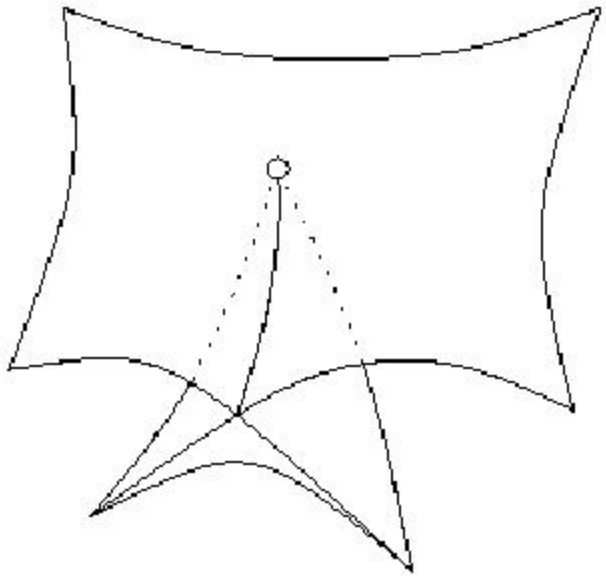


# Another Example

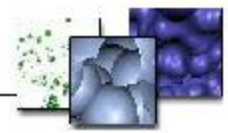


dovetail

# Max of E

An inflexion pt x **cannot** be a maximum





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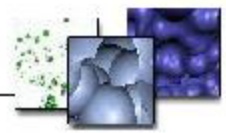
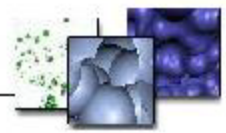


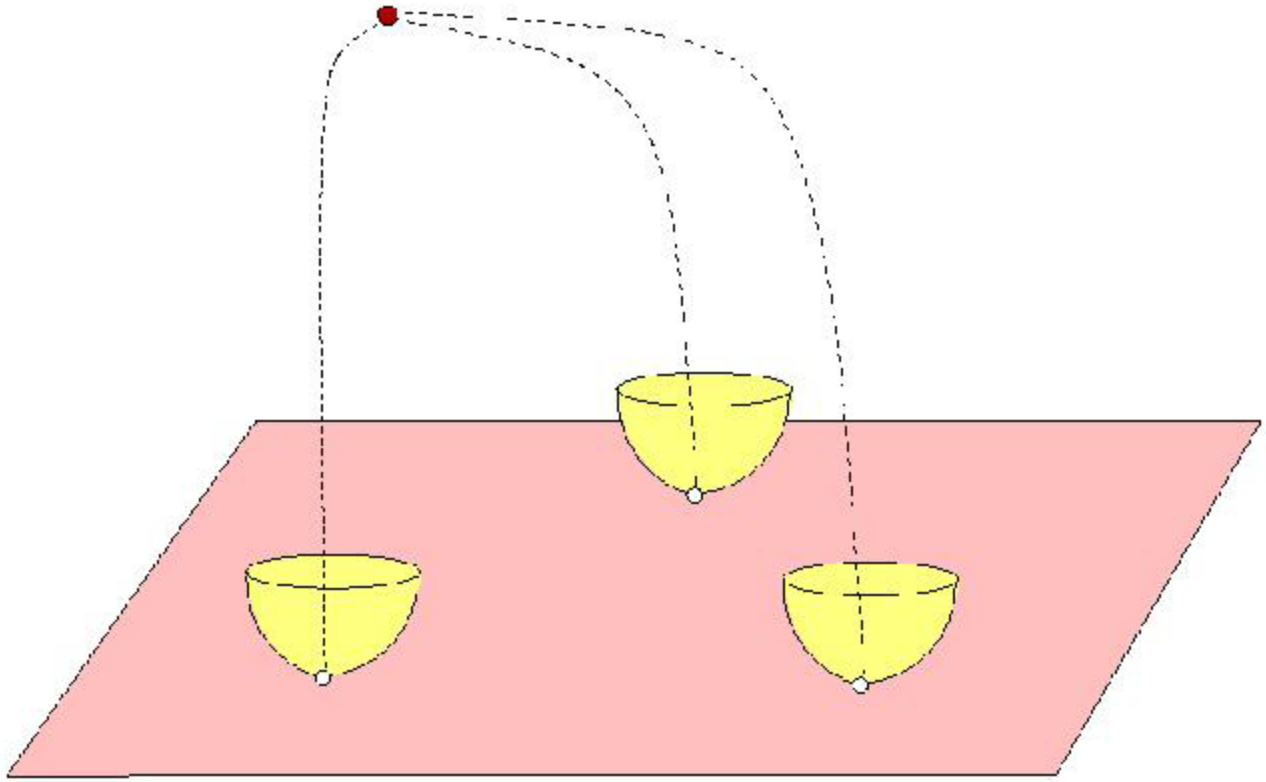
# Classification of Max for E

- Four types of max x
- No singularity involved:
  - 1-legged : x regular, paired w/ regular pt
- Singularity involved:
  - 2-legged : x regular, paired w/ double pt
  - 3-legged : x regular, paired w/ triple pt
  - 4-legged : x double pt, paired w/ double pt

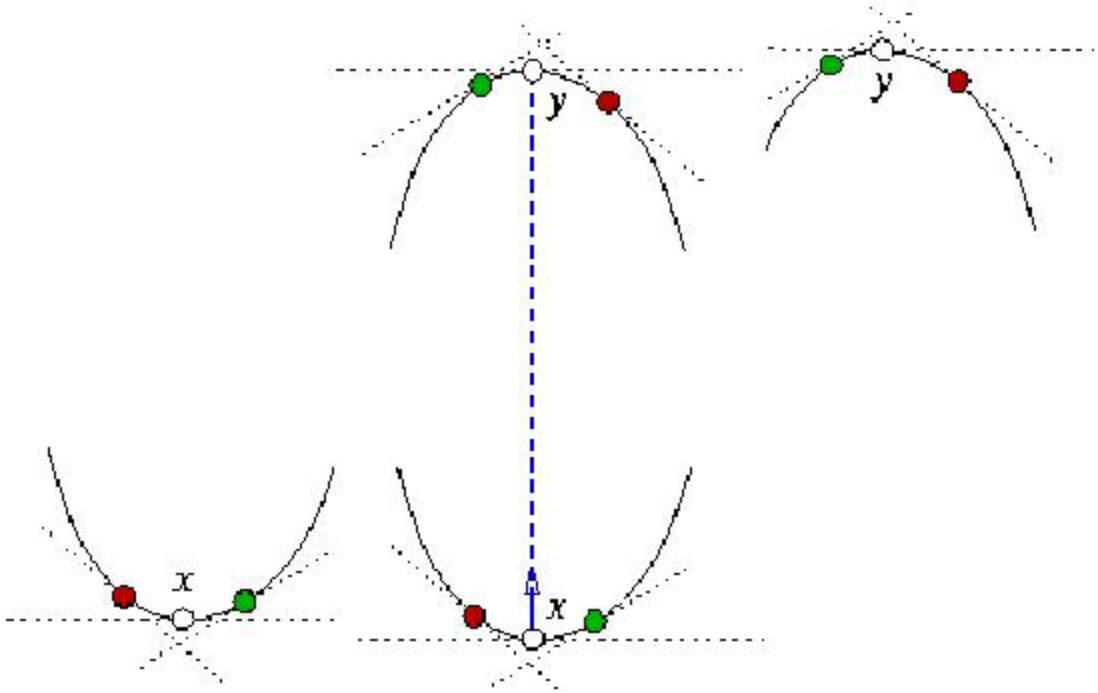




# 3-Legged Max



# Characterization of Max



# Conclusion

- Elevation function
- Relation w/ pedal function
- Classification of max of Elevation function

- Compute max for PL-case

- More efficient alg. to compute max
- Matching (docking)