Alpha Shapes Extended
Singapore 2017

Herbert Edelsbrunner
IST Austria
I BioGeometry

II Wrap

III Persistence

IV Expectation
FROM PROTEINS TO SIMPLICIAL COMPLEXES

HEMOGLOBIN

OXYGEN TRANSPORT
From Proteins to Simplicial Complexes

Hemoglobin protein = \( \cup \) balls in \( \mathbb{R}^3 \)

Oxygen Transport

Voronoi \downarrow + nerve

\( \alpha \)-complex
FROM PROTEINS TO SIMPLICIAL COMPLEXES
From Proteins to Simplicial Complexes
From Proteins to Simplicial Complexes

Voronoi domains $V(x)$
From Proteins to Simplicial Complexes

Delaunay complex of $X$ for radius $r$ is $D_r(x) = \{ P \subseteq X \mid \bigcap_{x \in P} [B_r(x) \cap V(x)] \neq \emptyset \}$. 
From Proteins to Simplicial Complexes

DeLaunay complex of $X$ for radius $r$ is $D_r(X) = \{ p \in X | \bigcap_{x \in p} [B_r(x) \cap V(x)] \neq \emptyset \}$. 
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FROM PROTEINS TO SIMPLICIAL COMPLEXES
Inclusion - Exclusion

**Theorem:**

$$\text{Vol}(UB) = \sum_{Q \in \mathcal{Q}(x)} (-1)^{\dim Q} \text{Vol}(\cap Q).$$
**Inclusion - Exclusion**

**Theorem:**

\[
\text{Vol}(UB) = \sum_{Q \in \mathbb{D}(X)} (-1)^{\dim Q} \text{Vol}(\cap Q).
\]
Inclusion-Exclusion

**Theorem:**

\[ \text{Vol}(UB) = \sum_{Q \in \mathcal{Q}(X)} (-1)^{\dim Q} \text{Vol}(\cap Q). \]
Inclusion-Exclusion

Theorem:

\[ \text{Vol}(UB) = \sum_{Q \in D(x)} (-1)^{\dim Q} \text{Vol}(\cap Q). \]
**Inclusion-Exclusion**

**Theorem:**

\[
\text{Vol}(UB) = \sum_{Q \in D(x)} (-1)^{\dim Q} \text{Vol}(\cap Q).
\]

[E. 1995]
Inclusion - Exclusion

Theorem:

\[ \text{Vol}(UB) = \sum_{Q \in \Omega(x)} (-1)^{\dim Q} \text{Vol}(\cap Q). \]

[Ref. 1995]

Extends to voids, pockets, area, area derivative, volume derivative.
Nerve Theorem

[Lesay 1946]
Nerve Theorem

\[ D_r(x) = \text{Nerve} \{ B_r(x) \cap V(x) \mid x \in X \}. \]
Nerve Theorem

\[ D_r(X) = \text{Nerve} \{ B_r(x) \cap V(x) \mid x \in X \}. \]

/ covering of \( \bigcup_{x \in X} B_r(x) \) with convex sets
Nerve Theorem

\[ D_r(X) = \text{Nerve} \left\{ B_r(x) \cap V(x) \mid x \in X \right\}. \]

\[ \text{covering of } \bigcup_{x \in X} B_r(x) \text{ with convex sets} \]

\[ \Rightarrow D_r(X) \text{ and } \bigcup_{x \in X} B_r(x) \text{ have same homotopy type} \]
I  BIO GEOMETRY
II  WRAP
III  PERSISTENCE
IV  EXPECTATION
COLLAPSES

(elem.) collapse
Collapses

(elem.) collapse
Collapses

(elem.) collapse

interval

\([L, U] = \{L \leq Q \leq U\}\)
Gen. Discrete Morse Function

gen. discrete vector field = partition into intervals
admits generalized discrete Morse function if acyclic
Gen. Discrete Morse Function

\[ \text{gen. discrete vector field} \quad = \quad \text{partition into intervals} \]

admits generalized discrete Morse function if acyclic

[Forman 1998]
Gen. Discrete Morse Function

gen. discrete vector field = partition into intervals
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Generalized Discrete Morse Function

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[Forman 1998]
Gen. Discrete Morse Function

gen. discrete vector field = partition into intervals
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[Forman 1998]
Wrap Complex

lower set of critical simplex, \( Q_t \)
Wrap Complex

lower set of critical simplex, \( Q_b \)

wrap complex for radius \( r \) is

\[
\text{Wrap}(r) = \bigcup_{Q \in Q_b} Q \quad \text{if} \quad R(Q) \leq r
\]

[E. 1996]
INTERFACES [Ban, E., Rudolph 2005]
INTERFACES [BAN, E., RUDOLPH 2005]
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INTERFACES [BAN, E., RUDOLPH 2005]
I  BioGeometry
II  Wrap
III  Persistence
IV  Expectation
Betti #s in $\mathbb{R}^3$: $eta_0 = \# \text{components}$

$eta_1 = \# \text{tunnels}$

$eta_2 = \# \text{voids}$
Betti #s in $\mathbb{R}^3$: $\beta_0 = \text{# components}$
$\beta_1 = \text{# tunnels}$
$\beta_2 = \text{# voids}$

vertex \[ \bullet \beta_0^{++} \]
Betti #s in $\mathbb{R}^3$:

- $\beta_0 = \#\text{components}$
- $\beta_1 = \#\text{tunnels}$
- $\beta_2 = \#\text{voids}$

Vertex: $\bullet \beta_{0++}$

Edge: $\beta_{i--}$, $\beta_{i++]$
Betti #s in $\mathbb{R}^3$: $\beta_0 = \# \text{components}$
$\beta_1 = \# \text{tunnels}$
$\beta_2 = \# \text{voids}$

**Vertex**

**Edge**

**Triangle**
**Betti #s**

in $\mathbb{R}^3$:
- $\beta_0$ = # components
- $\beta_1$ = # tunnels
- $\beta_2$ = # voids

- **Vertex**
- **Edge**
- **Triangle**
- **Tetrahedron**
**Incremental Algorithm**

\[ \beta_0 = \beta_i = \ldots = \beta_n = 0; \]

for i = 1 to m do

\[ k = \dim Q_i; \]

if \( Q_i \) is k-cycle then \( \beta_i \)++

else \( \beta_i \)--

endif

endfor
Incremental Algorithm

\[ \beta_0 = \beta_1 = \ldots = \beta_n = 0; \]
for \( i = 1 \) to \( m \) do
  \[ k = \text{dim} \ Q_i; \]
  if \( Q_i \in k\text{-cycle} \) then \( \beta_i++ \) (birth)
  else \( \beta_{i-1}-- \) (death)
endif
endfor

[DeFonado, E. 1995]
Number of Tunnels
Persistence

... \rightarrow H(X_{i-1}) \rightarrow H(X_i) \rightarrow ... \rightarrow H(X_{j-1}) \rightarrow H(X_j) \rightarrow ...
Persistence

\[ \ldots \rightarrow H(X_{i-1}) \rightarrow H(X_i) \rightarrow \ldots \rightarrow H(X_{j-1}) \rightarrow H(X_j) \rightarrow \ldots \]
Persistence

\[ \ldots \rightarrow H(X_{i-1}) \rightarrow H(X_i) \rightarrow \ldots \rightarrow H(X_{j-1}) \rightarrow H(X_j) \rightarrow \ldots \]

\( \alpha \) is born at \( X_i \)
PERSISTENCE

\[ \ldots \rightarrow H(X_{i-1}) \rightarrow H(X_i) \rightarrow \ldots \rightarrow H(X_{j-1}) \rightarrow H(X_j) \rightarrow \ldots \]

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\( \alpha \) is born at \( x_i \) and dies entering \( x_j \)
Persistence

\[ \ldots \rightarrow H(X_{i-1}) \rightarrow H(X_i) \rightarrow \ldots \rightarrow H(X_{j-1}) \rightarrow H(X_j) \rightarrow \ldots \]

\( \alpha \) is born at \( X_i \) and dies entering \( X_j \)

[E., Letsches, Zamorodian 2000]
Stability of persistence.
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Stability

Bottleneck distance between two diagrams is length of longest edge in minimizing matching: $W_{bo}(\text{Dgm}(f), \text{Dgm}(g))$
Stability

Bottleneck distance between two diagrams is length of longest edge in minimizing matching: $\omega_0(Dgm(f), Dgm(g))$

Thm. $\omega_0(Dgm(f), Dgm(g)) \leq \|f-g\|_\infty$.

[Cohen-Steiner, E, Harer 2007]
I  BioGeometry
II  Wrap
III  Persistence
IV  Expectation
Poisson Point Process
(with density $\lambda > 0$ in $\mathbb{R}^n$)

1. #pts in disjoint sets are independent
2. $E[\#\text{pts in } B] = \lambda |B|$
Poisson Point Process
(with density $\gamma > 0$ in $\mathbb{R}^n$)

1. $\#$pts in disjoint sets are independent
2. $E[\#\text{pts in } B] = \gamma \| B \|$

$TP[\#\text{pts in } B = k] = \frac{(\gamma \| B \|)^k}{k!} e^{-\gamma \| B \|}$. 
Poisson Point Process
(with density \( g > 0 \) in \( \mathbb{R}^n \))

1. \#pts in disjoint sets are independent

2. \( E[\#pts \text{ in } B] = g \|B\| \)

\[
P[\#pts \text{ in } B = k] = \frac{(g\|B\|)^k}{k!} e^{-g\|B\|}.
\]

Points are in general position with prob. 1.
Expectations in $\mathbb{R}^n$

$X$ chosen from PPP with density $g > 0$ in $\mathbb{R}^n$.

$\Omega \subseteq \mathbb{R}^n$, $l = \dim L$, $k = \dim U$. 
**Expectations in $\mathbb{R}^n$**

$x$ chosen from PPP with density $g > 0$ in $\mathbb{R}^n$.

$\Omega \subseteq \mathbb{R}^n; \quad l = \dim L, \quad k = \dim U.$

**Thm.** For $0 \leq l \leq k \leq n$ there is a constant $C_{\ell,k}^n$ such that

$$\mathbb{E}[\# \text{int}_{\ell,k} \text{ in } \Omega \text{ with } r_D \leq r] = \frac{x(k, q_{\ell,n} r^n)}{\Gamma(k)} \cdot C_{\ell,k}^n \cdot g \|\Omega\|.$$
**Expectations in $\mathbb{R}^n$**

$X$ chosen from PPP with density $g > 0$ in $\mathbb{R}^n$.

$\Omega \subseteq \mathbb{R}^n$; $l = \text{dim } L$, $k = \text{dim } U$.

**Thm.** For $0 \leq l \leq k \leq n \exists$ constant $C_{l,k}^n$ such that

$$E[\# \text{int}_{l,k} \text{ in } \Omega \text{ with } r_D \leq r] = \frac{x(k, gn \pi^n)}{\Gamma(k)} \cdot C_{l,k}^n \cdot g \| \Omega \|.$$

[ E., Nikitenko, Reitzner 2016 ]
### Critical Simplices and Intervals

<table>
<thead>
<tr>
<th>$C_{e,l}^2$</th>
<th>$k = 0$</th>
<th>$1$</th>
<th>$2$</th>
<th>$C_{e,l}^3$</th>
<th>$k = 0$</th>
<th>$1$</th>
<th>$2$</th>
<th>$3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$l = 0$</td>
<td>$1$</td>
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<td>$l = 0$</td>
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<td>$1.21$</td>
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<td>$3.70$</td>
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<td>$1.85$</td>
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</table>

<table>
<thead>
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<th>$C_{e,l}^4$</th>
<th>$k = 0$</th>
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<th>$2$</th>
<th>$3$</th>
<th>$4$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$l = 0$</td>
<td>$1$</td>
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<tr>
<td>$1$</td>
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<td>$5.66$</td>
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<td>$3.55$</td>
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<td>$17.66$</td>
<td>$11.14$</td>
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<td></td>
<td>$15.40$</td>
<td>$14.22$</td>
<td>$4.74$</td>
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</tbody>
</table>
Delaunay Simplices

\[ E[\# \text{j-simplex in Del}] = D_j^n \cdot g \| \Omega \| \]

\[ D_j^n = \sum_{k=j}^{n} \sum_{\ell=0}^{j} (k-j) C_{\ell,k} \]
Delaunay Simplices

\[ E[\# j\text{-simple}. \text{ in } \Omega] = D^n_j \cdot \|\Omega\|. \]

\[ D^n_j = \sum_{k=j}^n \sum_{\ell=0}^{j} \binom{k-\ell}{j-\ell} C^n_{\ell,k} \]

<table>
<thead>
<tr>
<th>D^n_j</th>
<th>j = 0</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
</tr>
</thead>
<tbody>
<tr>
<td>n = 2</td>
<td>1</td>
<td>3</td>
<td>2</td>
<td></td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>1</td>
<td>7.76</td>
<td>13.53</td>
<td>6.76</td>
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</tr>
<tr>
<td>4</td>
<td>1</td>
<td>18.88</td>
<td>65.55</td>
<td>79.44</td>
<td>31.77</td>
</tr>
</tbody>
</table>

blue = [Miles 1970/71]
red = [E, Nikiforov, Reitnes 2016]
DEPENDENCE ON RADIUS intervals in $\mathbb{R}^2$
Dependence on Radius

intervals in \( \mathbb{R}^3 \)
DEPENDENCE ON RADIUS

intervals in $\mathbb{R}^4$
Dependence on Radius

Delaunay simplices in $\mathbb{R}^2$
DEPENDENCE ON RADIUS

Delaunay simplices in $\mathbb{R}^3$
DEPENDENCE ON RADIUS

Delaunay simplices in \( \mathbb{R}^4 \)
Three Points on Circle
Three Points on Circle
Three Points on Circle

\[ \text{area}(\triangle ABC) = a + b + c \]
Three Points on Circle

\[ \text{area}(ABC) = a + b + c \]

\[ -\text{area}(ABC) = -a + b + c \]
Three Points on Circle

\[ \text{area}(ABC) = a + b + c \]
\[ -A\overline{BC} = -a + b + c \]
\[ \overline{AB}C = a - b + c \]
\[ -A\overline{B}C = -a - b + c \]
\[ \overline{A}\overline{B}C = -a + b - c \]
\[ -A\overline{B}\overline{C} = -a - b - c \]
THANK YOU