The accumulated persistence function, a useful functional summary statistic for topological data analysis

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The case of a point cloud - Delaunay complex filtration

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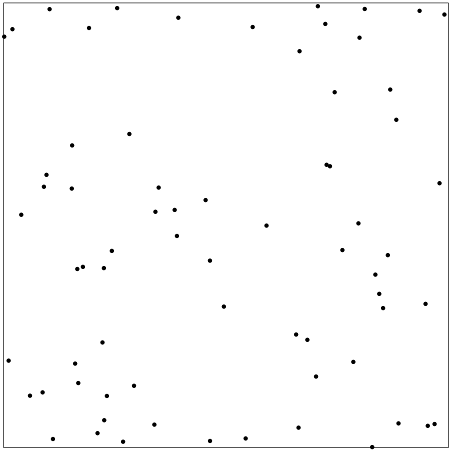

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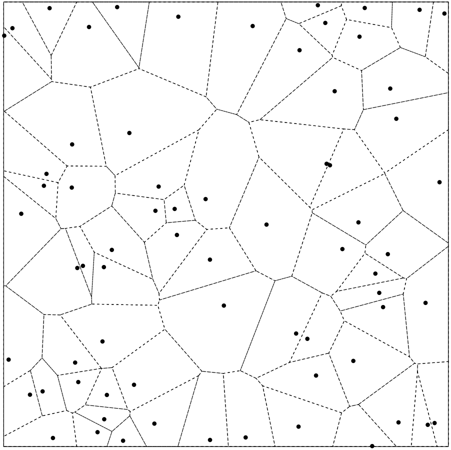

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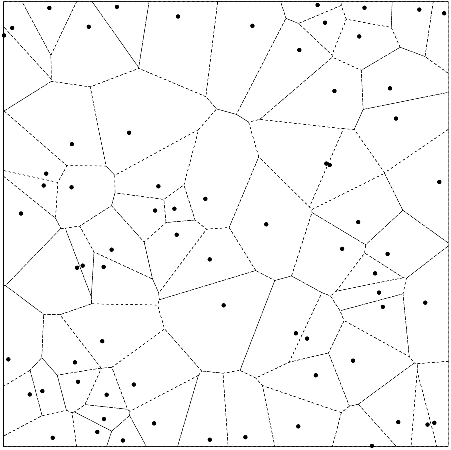

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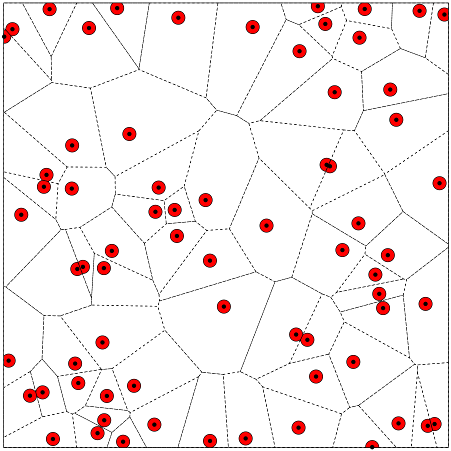

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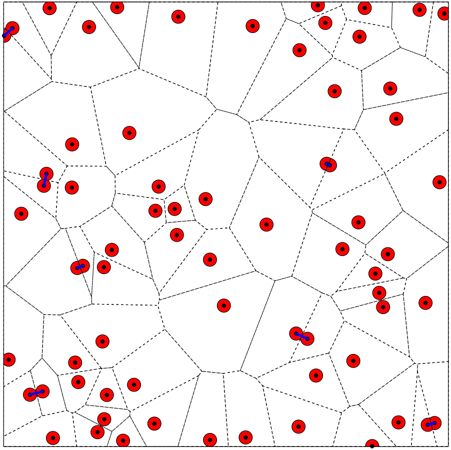

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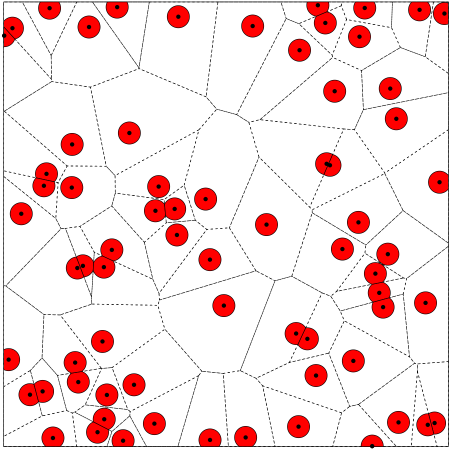

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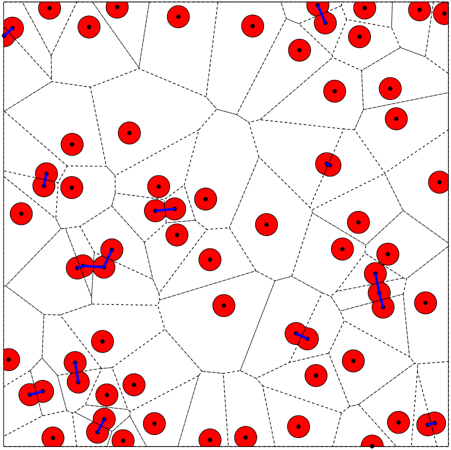

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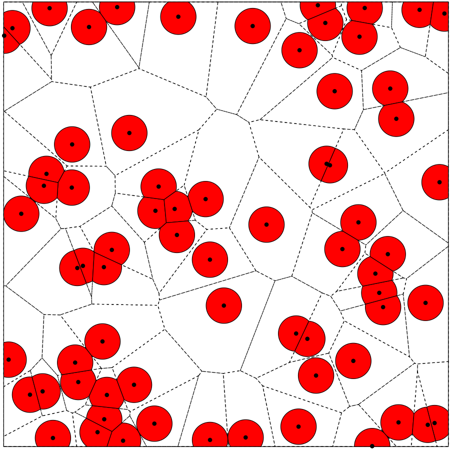

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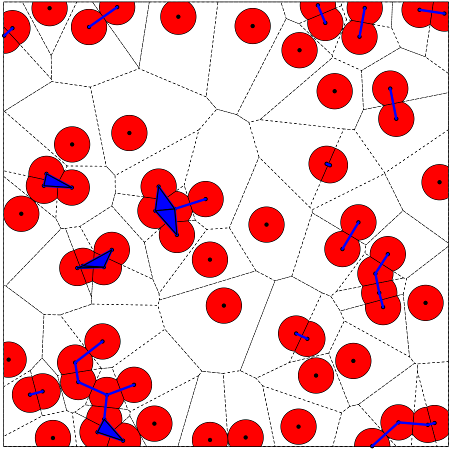

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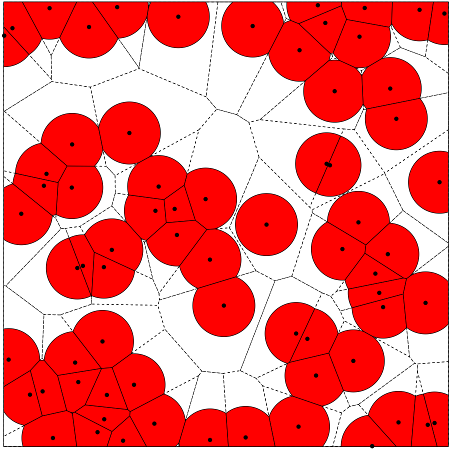

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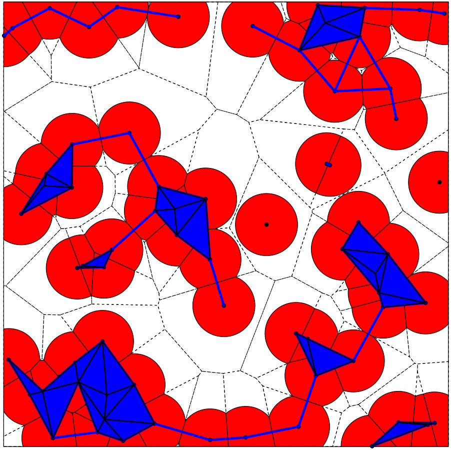

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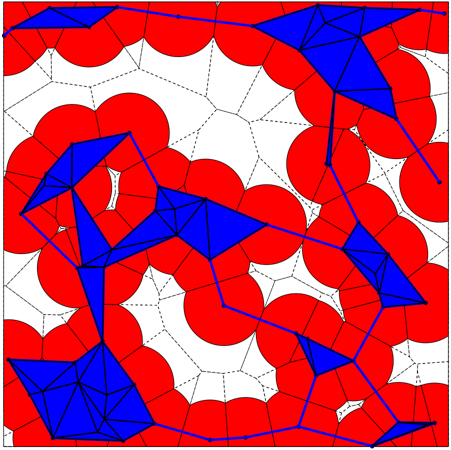

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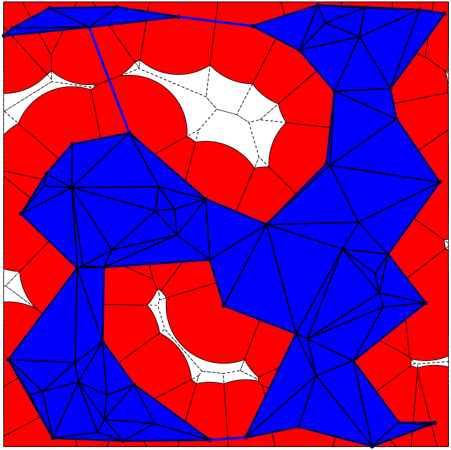

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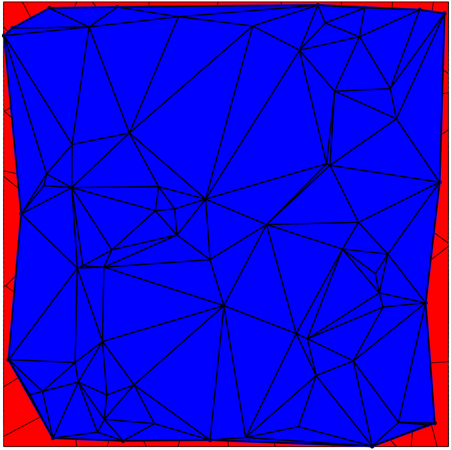

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Main tool in persistent homology: Persistence diagram

- For dimension $k = 0, 1, \ldots$, a persistent diagram consists of points (b_i, d_i) representing as r varies connected components ($k = 0$), holes ($k = 1$), etc. appearing at $r = b_i$ (birth) and disappearing at $r = d_i$ (death),
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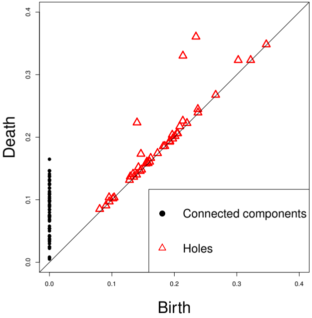

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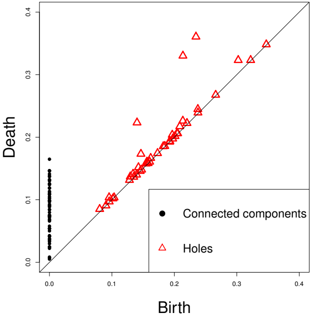

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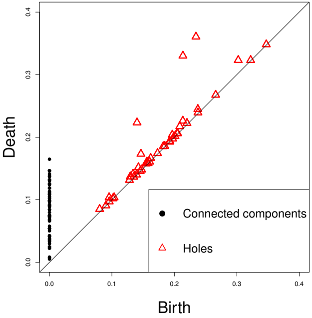

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- Two-dim. alternatives: persistent landscape (Bubenik, 2015: sequence of 1-dim. functions).
- One-dim. alternatives provide selected information: Bubenik's dominant function λ_1; the silhoutte (Chazal et al., 2013: a weighted average of Bubenik's functions); kernel estimate of the intensity function for the persistent diagram (Chen et al., 2015).

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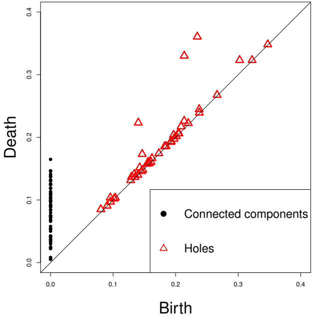
- $(b_i, d_i) \leftrightarrow (m_i, l_i)$, where $m_i = \frac{b_i+d_i}{2}$ is the meanage and $l_i = d_i - b_i$ is the lifetime.

Persistence diagram



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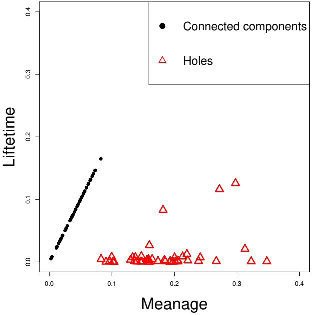

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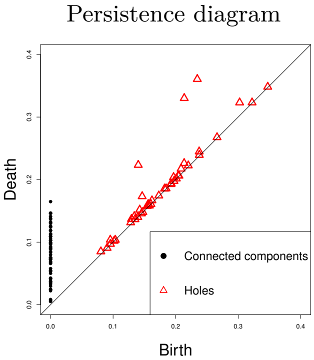
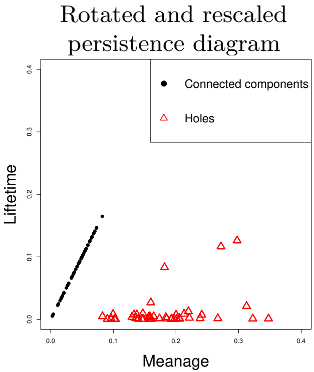




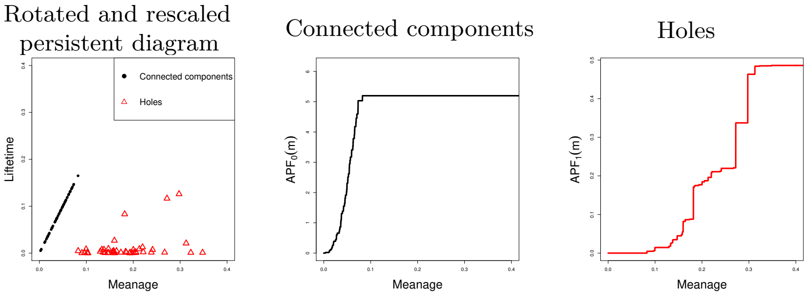
NB: For each dimension k, $\mathrm{PD}_k \leftrightarrow \mathrm{RRPD}_k$
(where $k = 0$ if connected components are considered, $k = 1$ if holes, $k = 2$ if voids...).

A new functional summary statistic

The **accumulated persistence function** for k-dimensional topological features:

$$\mathrm{APF}_k(m) = \sum_i c_i l_i 1(m_i \leq m), \quad m \geq 0.$$

Example:



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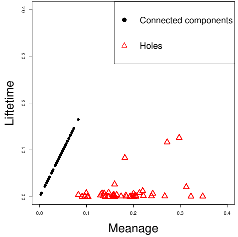
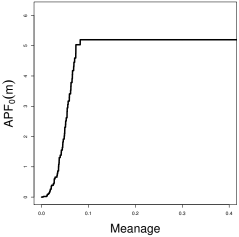
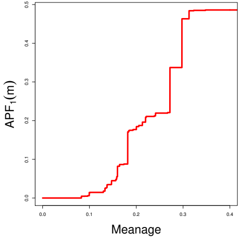


Connected components



Holes



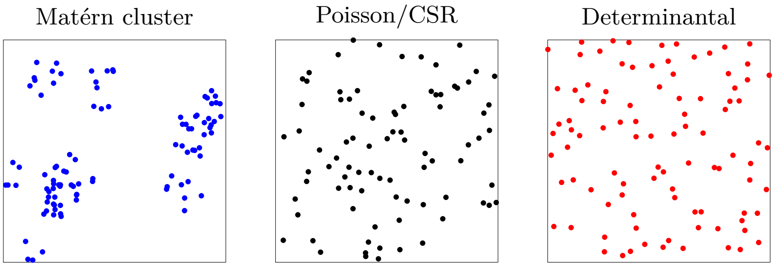
Under mild conditions, $\mathrm{RRPD}_k \leftrightarrow \mathrm{APF}_k$.

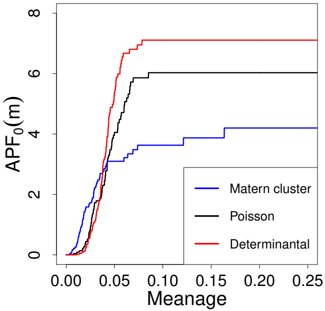
NB: APF_k is a 1-dim. function! Apply methods from functional data analysis...

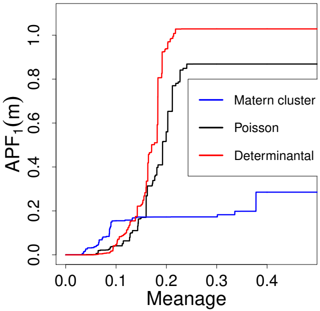
Applications

- A single APF:
  - Transfer confidence region for the persistence diagram to the APF
  - Extreme rank envelope
- A sample of APFs:
  - Functional boxplot
  - Confidence region for the mean of APFs
- Two or more samples of APFs:
  - Two-sample test
  - Clustering
  - Supervised classification

APFs for aggregated, completely random or regular point clouds







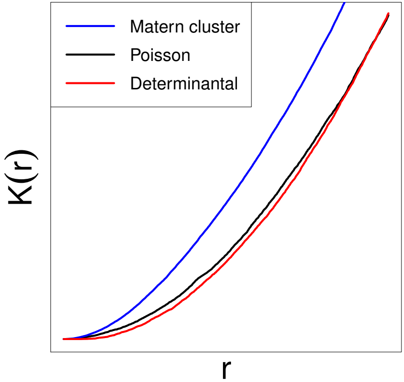
Classical functional summary functions for aggregated, completely random or regular point clouds

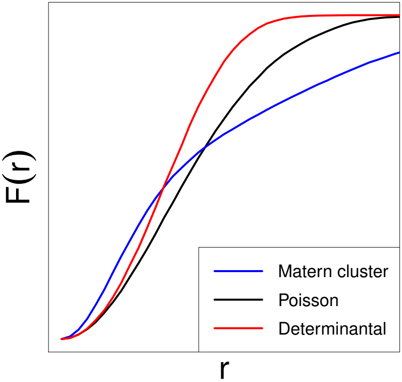
- Ripley's K-function for a stationary point process $X \subset \mathbb{R}^2$:

$$K(r) = \frac{\mathrm{E}\left[\text{“Number of further points in } B(0,r)\text{”} \,|\, 0 \in \mathbf{X}\right]}{\mathrm{E}\left[\text{“Number of points per unit area”}\right]}, \quad r \geq 0.$$

- The empty space function:

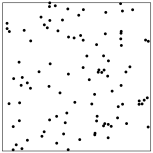
$$F(r) = \mathrm{P}\left(\mathbf{X} \cap B(0,r) \neq \emptyset\right), \quad r \geq 0.$$



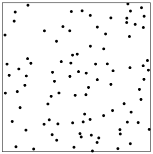


Extreme rank envelope test for CSR

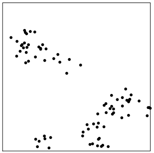
CSR: Poisson process



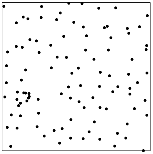
Inhibition: DPP



Aggregation: Matérn cluster



Baddeley-Silverman cell process



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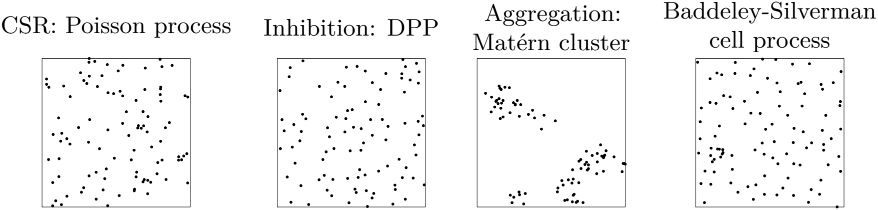
Extreme rank envelope test for CSR



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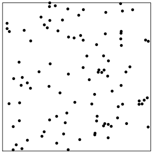

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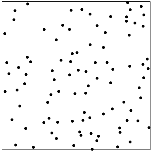

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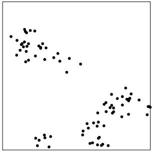

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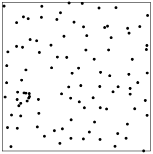

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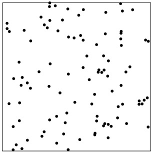

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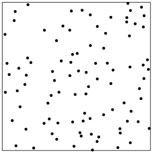

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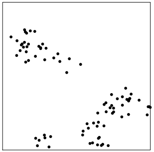

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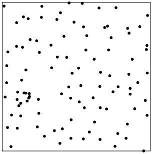

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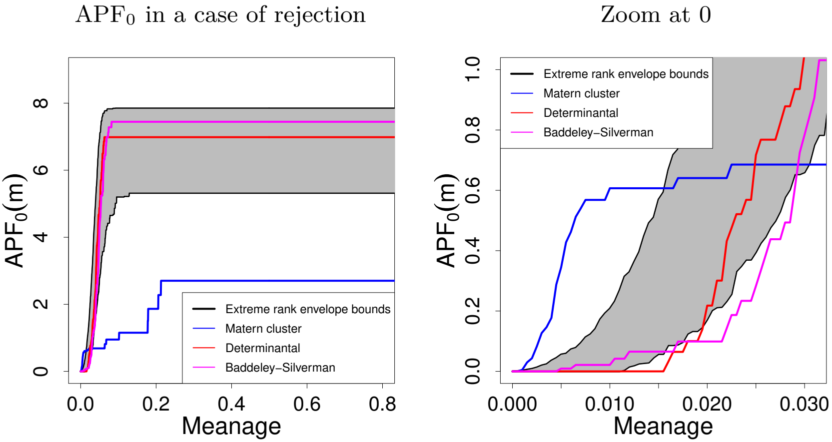
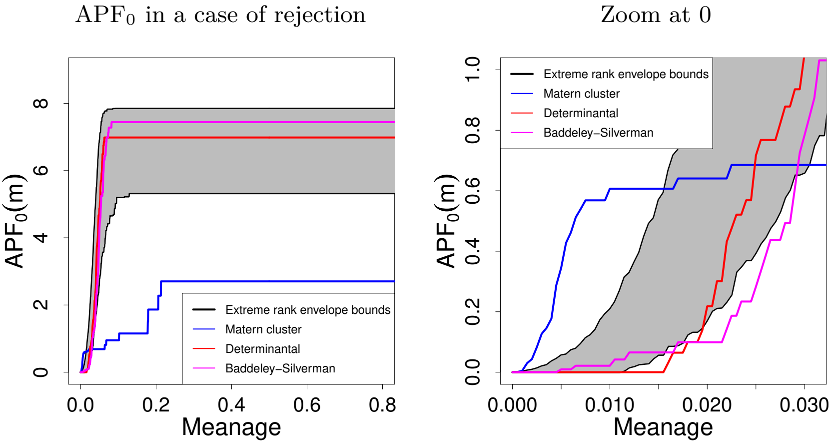
- We repeated all this 500 times.

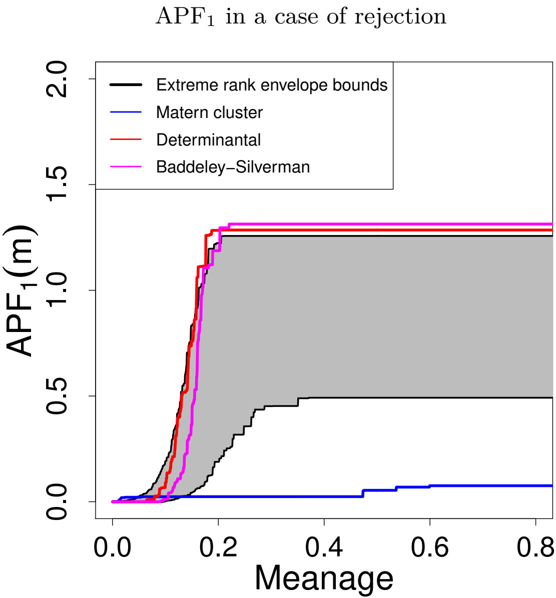
Extreme rank envelope for APF_0





NB: Small lifetimes are not noise but of particular importance!

Extreme rank envelope for APF_1



Test for CSR using different functional summary statistics

Percentage of simulated point patterns rejected by the 95%-extreme rank envelope test.

	Poisson		Determinantal		Matérn cluster		Baddeley-Silverman	
	$\rho = 100$	$\rho = 400$	$\rho = 100$	$\rho = 400$	$\rho = 100$	$\rho = 400$	$\rho = 100$	$\rho = 400$
APF_0	3.6	4	77.4	100	100	100	45.6	99.6
APF_1	3.8	4.6	28.2	57.8	100	100	65.8	100
$\hat{K}$	3.4	2.8	97.4	100	100	100	52.4	50.2
$\hat{F}$	2.2	0.8	29.8	48.8	100	100	60.8	100
APF_0, APF_1, $\hat{K}$, $\hat{F}$	4.5	5	99	100	100	100	65	100

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- Excellent detection for cluster model.
- Decent detection for Baddeley-Silverman cell process.
- The power increases with the number of points and by combining all summary statistics.

Applications

- A single APF
  - Transfer confidence region for the persistence diagram to the APF
  - Extreme rank envelope
- A sample of APFs
  - Functional boxplot
  - Confidence region for the mean of APFs
- Two or more samples of APFs
  - Two-sample test
  - Clustering
  - Supervised classification

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- <u>**Aim:**</u> Test $\mathcal{H}_0$: $D_0 = E_0$.
- $\overline{A_{r_1}}$ and $\overline{A_{r_2}}$: the empirical mean of $A_1, \dots, A_{r_1}$ and $A_{r_1+1}, \dots, A_{r_1+r_2}$.
- $0 \le T_1 < T_2 < \infty$.
- $KS_{r_1,r_2} = \sqrt{\frac{r_1 r_2}{r_1 + r_2}} \sup_{m \in [T_1, T_2]} \left| \overline{A_{r_1}}(m) - \overline{A_{r_2}}(m) \right|.$

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- Large values are critical for $\mathcal{H}_0$.
- Problem: the asymptotic distribution of KS_{r_1,r_2} known but intractable.

  $\Rightarrow$ Bootstrap procedure.

Theorem

Assume that $\lambda \in (0,1)$ *such that* $r_1/r \to \lambda$ *as* $r \to \infty$. *Under mild conditions, using a bootstrap method where we resample* B *times,*

- *if* $\mathcal{H}_0$ *is true,*

$$\lim_{r\to\infty} \lim_{B\to\infty} \mathrm{P}\left(KS_{r_1,r_2} > \hat{q}_{\alpha}^{B}\right) = \alpha,$$

- *if* $\mathcal{H}_0$ *is not true and* $\sup_{m\in[T_1,T_2]} \left|\mathrm{E}\left\{A_{D_0} - A_{E_0}\right\}(m)\right| > 0,$

$$\lim_{r\to\infty} \lim_{B\to\infty} \mathrm{P}\left(KS_{r_1,r_2} > \hat{q}_{\alpha}^{B}\right) = 1.$$

Example: Brain artery trees dataset (Bendich *et al.*, 2016)

- Subjects: 46 women and 49 men. Each subject/tree graph has $\approx 10^5$ nodes.
- Bendich *et al.* (2016) wanted to capture how the arteries bend through space and to detect age and gender effects.
- The age effect was clearly revealed $\Rightarrow$ we focus on the gender effect.

Another example: Brain artery trees

Bendich *et al.* (2016) performed a permutation test based on the mean of the 100 largest lifetimes of each subject:

- When $k = 0$ (connected components), p-value of 10%.
- When $k = 1$ (holes), p-value of 3%.

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We distinguish between male and female subjects using our two-sample test statistic KS_{r_1,r_2} based on APF_ks.

- We consider two settings:
  - (A) We use only the 100 largest lifetimes as in Bendich *et al.* (2016).
  - (B) We use all topological features.

Example - Brain artery trees

Estimated p-values of the two-sample test statistic KS_{r_1,r_2}:

	APF_0		APF_1	
	$I = [0, 137]$	$I = [0, 60]$	$I = [0, 25]$	$I = [15, 25]$
Setting (A)	5.26	3.26	3.18	2.72
Setting (B)	7.67	3.64	20.06	1.83

- As in Bendich *et al.* (2016): Usually better results when $k = 1$ (holes). In comparison with Bendich *et al.* (2016), we see a very clear gender effect.
- Good detection when $k = 0$ (connected components). In contrast to Bendich *et al.* (2016), we see a clear gender effect.
- Problem with APF_1 on $I = [0, 25]$ partly dues to outliers (further studies required).

Conclusions:

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- We have successfully used it in various situations.
- E.g. in connection to the extreme rank envelope test and the corresponding plot.
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Perspectives:

- Define new spatial point process models based on their persistence diagrams.
- Use voids ($k = 2$) to study brain artery trees.

Paper available at arXiv:1611.00630.

Thank you for your attention.