Constructing isotropic auto-covariance functions on graphs with Euclidean edges with respect to the shortest path distance and the resistance metric

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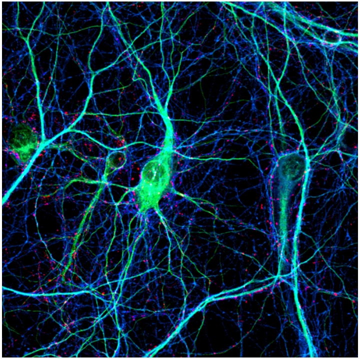
Dendrite networks of neurons (green lines):

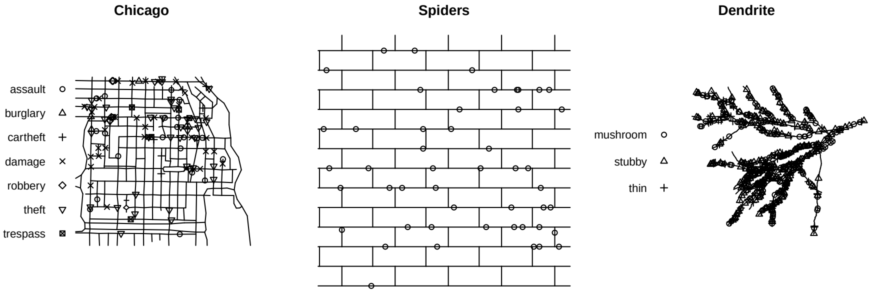


How do we construct an isotropic auto-covariance function C_o for the diameter Y (e.g. a GRF):

$$\mathrm{cov}(Y(u), Y(v)) = C_o(d(u,v))$$

and what should the metric d be?

Point patterns on linear networks:



How do we construct point processes with an isotropic (pseudo-stationary) pair correlation function

$$\mathrm{pcf}(u, v) = g_o(d(u, v))$$

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Need for a more general definition than linear networks

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Example (road networks):

- bridges and tunnels can generate networks which do not have a planar representation as a union of line segments in $\mathbf{R}^2$;
- varying speed limits or number of traffic lanes may require distances on line segments to be measured differently than their spatial extent.

Definition 1

A **graph with Euclidean edges** is a triple $\mathcal{G} = (\mathcal{V}, \mathcal{E}, \{\varphi_e\}_{e \in \mathcal{E}})$ s.t.

(a) **Graph structure**: $(\mathcal{V}, \mathcal{E})$ is a finite simple connected graph ($\mathcal{V}$ is finite; every pair of vertices is connected by a path; no multiple edges or loops).

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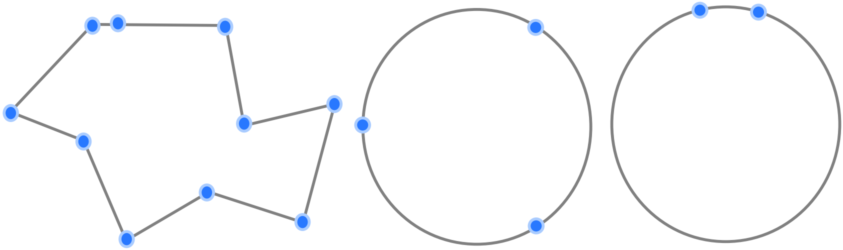
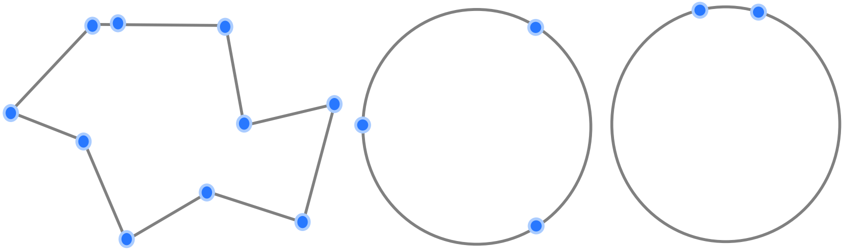
(d) **Distance consistency**: If $e = \{u, v\} \in \mathcal{E}$, then

$$d_{\mathcal{V}}(u, v) = \operatorname{len}(e) := \overline{e} - \underline{e}$$

where $d_{\mathcal{V}}$ is the standard shortest-path weighted graph metric with edge weights given by $\operatorname{len}(e)$ for $e \in \mathcal{E}$.



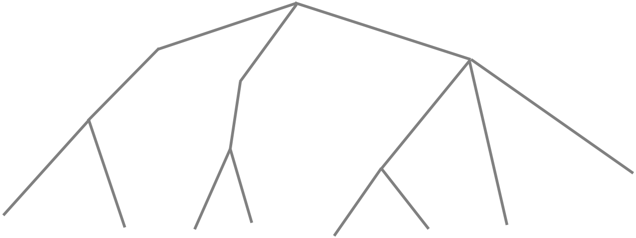
The two graphs on the left are graphs with Euclidean edges (the blue dots represent the vertices, the grey lines (as subsets of $\mathbf{R}^2$) represent the edges, and edge coordinates are given by arc-length.)



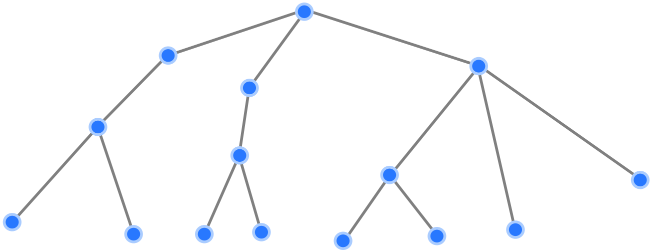
The two graphs on the left are graphs with Euclidean edges (the blue dots represent the vertices, the grey lines (as subsets of $\mathbf{R}^2$) represent the edges, and edge coordinates are given by arc-length.)

However, the right most graph is **not** a graph with Euclidean edges: there are multiple edges; and distance consistency is violated.

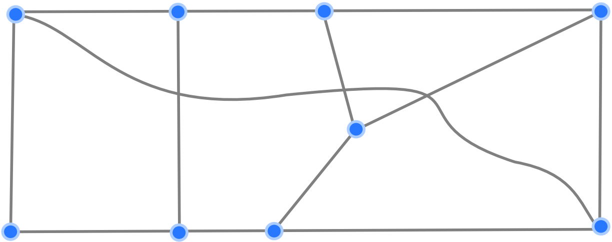
A linear network...



A linear network... is clearly a graph with Euclidean edges



A graph with Euclidean edges which is not a linear network (has no planar representation):



Definition 2 (Geodesic metric)

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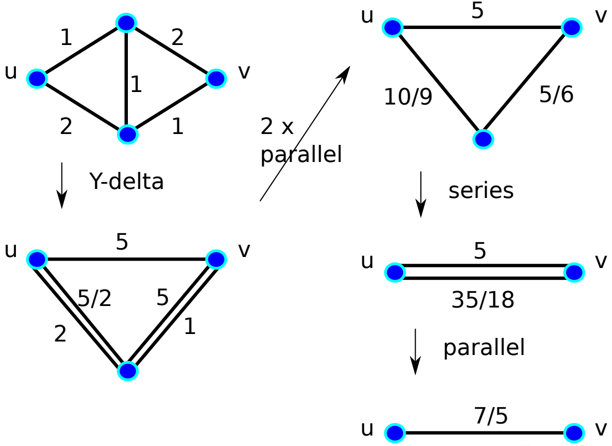
As soon argued, we want in addition another metric related to electrical network theory...

Electrical network

Definition from physics: For a finite (or countable) graph with each edge representing a resistor, the **resistance** between nodes u and v is the voltage drop from u to v when a current of one ampere flows from u to v.



Definition 3 (Extension of resistance distance on $\mathcal{V}$ to $\mathcal{G}$)

Define the resistance metric as the variogram of an auxiliary random field $Z_{\mathcal{G}}$:

$$d_R(u, v) := \mathrm{var}(Z_{\mathcal{G}}(u) - Z_{\mathcal{G}}(v)) \qquad u, v \in \mathcal{G},$$

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  - on each edge by linear interpolation;
- $Z_e(u) = B_e(\varphi_e(u))$ if $u \in e$, where B_e is an independent Brownian bridge defined over $[\underline{e}, \overline{e}]$, and $Z_e(u) = 0$ if $u \notin e$.

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Theorem 1 $d_R(u, v)$ is a metric which is an extension of the classic (effective) resistance metric when viewing $\mathcal{G}$ as an electrical network over nodes $\mathcal{V}$ and with resistors given by $\mathrm{len}(e)$ for $e \in \mathcal{E}$.

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Theorem 3 $d_R(u, v)$ is invariant to splitting edges and to merging edges at degree two vertices.

One main result (reproducible Hilbert space embedding)

Definition 4 For an arbitrary chosen origin $u_o \in \mathcal{V}$, let $\mathcal{F}$ be the class of functions $f : \mathcal{G} \mapsto \mathbf{R}$ continuous with respect to d_G s.t. for all $e \in \mathcal{E}$, the restriction of f to e, f_e, is absolutely continuous and $f_e' \in L^2([\underline{e}, \overline{e}])$. Define

$$\langle f, g \rangle_{\mathcal{F}} := f(u_o)g(u_o) + \sum_{e \in \mathcal{E}(\mathcal{G})} \int_{\underline{e}}^{\overline{e}} f_e'(t) g_e'(t) \, \mathrm{d}t, \qquad f, g \in \mathcal{F}.$$

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$$= \sup_{f \in \mathcal{F}} \left\{ |f(u) - f(v)|^2 : \|f\|_{\mathcal{F}} \leq 1 \right\}.$$

Another main result (Hilbert space embedding)

Definition 5 If (X, d) is a distance space, then C_o is an **isotropic auto-covariance function on** (X, d) iff $C_o(d(x, y))\colon X \times X \mapsto \mathbf{R}$ is p.s.f.

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To obtain isotropic auto-covariance functions on $(\mathcal{G}, d_R)$ and $(\mathcal{G}, d_G)$, we use certain Hilbert space embeddings, including

Theorem 5 $(\mathcal{G}, d_G) \overset{\sqrt{\cdot}}{\hookrightarrow} H$

and based on deep results of von Neumann and Schoenberg from the 1930's and 1940's...

Yet another main result — for the resistance metric!

Theorem 6 For $\sigma^2, \beta > 0$, we have parametric families of isotropic auto-covariance functions on $(\mathcal{G}, d_R)$:

- **Power exponential covariance function:**

$$C_o(s) = \sigma^2 \exp\left(-\beta s^{\alpha}\right), \quad \alpha \in (0, 1].$$

- **Generalized Cauchy covariance function:**

$$C_o(s) = \sigma^2 \left(\beta s^{\alpha} + 1\right)^{-\xi/\alpha}, \quad \alpha \in (0, 1], \ \xi > 0.$$

- **The Matérn covariance function:**

$$C_o(s) = \sigma^2 \frac{\left(\beta s\right)^{\alpha} K_{\alpha}\left(\beta s\right)}{\Gamma(\alpha) 2^{\alpha - 1}}, \quad \alpha \in (0, 1/2].$$

- **The Dagum covariance function:**

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Each C_o is strictly p.d. and completely monotonic.

For the geodesic metric!

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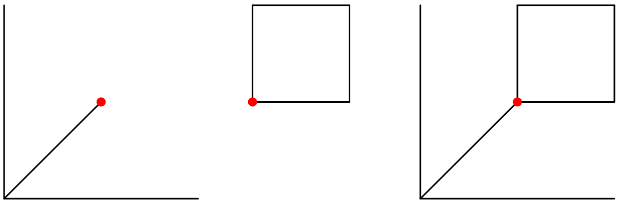
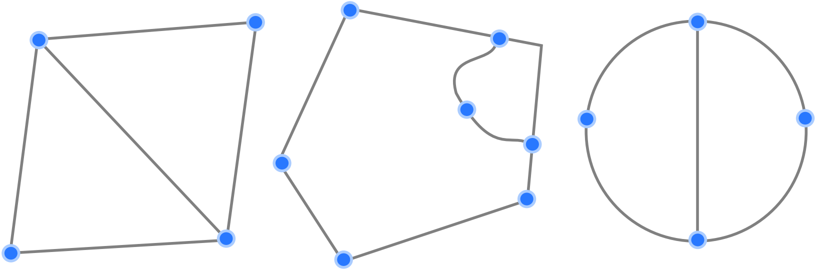


Forbidden graph for the geodesic metric

Theorem 8 If $\mathcal{G}$ has three paths which have common endpoints but are otherwise pairwise disjoint, then $\exists\beta > 0$ s.t. $s \mapsto \exp(-\beta s)$ $(s \geq 0)$ is **not** an isotropic auto-covariance function on $(\mathcal{G}, d_G)$.



Some other results

Theorem 9 Let C_o be one of the functions given in (I)-(IV) in Theorem 6 but with α outside the parameter range ($\alpha > 1$ in (I), (II), or (IV), and $\alpha > 1/2$ in (III)). Then there exists a star-shaped graph with Euclidean edges $\mathcal{G}$ s.t. $s \mapsto \exp(-\beta s)$ ($s \geq 0$) is an isotropic auto-covariance function on $(\mathcal{G}, d_G)$, but C_o is **not** an isotropic covariance function on $(\mathcal{G}, d_G)$.

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NB: I Theorems 9 and 10, "$(\mathcal{G}, d_G)$" can be replaced by "$(\mathcal{R}, d_G)$".

Simulations of LGCPs using exponential auto-covariance functions:

Given a realisation of a GRF Y on $\mathcal{G}$ with exponential auto-covariance function, simulate a Poisson process with intensity function $\exp(Y)$.