Statistical analysis for the Johnson-Mehl germination-growth model

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The main idea

• Studying the Johnson-Mehl germination-growth model in \mathbb{R}^d .



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- Studying the Johnson-Mehl germination-growth model in \mathbb{R}^d .
- Estimating parameters of specific parametric models for the conditional intensity by maximum likelihood.



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- Studying the Johnson-Mehl germination-growth model in \mathbb{R}^d .
- Estimating parameters of specific parametric models for the conditional intensity by maximum likelihood.
- Model checking by new functional summary statistics related to the inhomogeneous K- function and to the Palm distribution of the typical Johnson-Mehl cell.



- Outline

Outline of Topics

- 1 Johnson-Mehl germination-growth Model
- 2 First and second-order properties
- Sunctional summary statistics and non-parametric estimation
- Parametric Models
- 5 Likelihood Analysis
- 6 A case study: Neurotransmitter data



└─ Johnson-Mehl germination-growth Model

Definition

• $\Phi \equiv \{(x_i, t_i)\} \subset \mathbb{R}^d \times [0, \infty)$: Primary process, a space-time Poisson process with intensity function $\kappa(t)$.



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- Time T((x,t),y)

 $T((x,t),y)=t+\|x-y\|/v,\quad (x,t)\in \mathbb{R}^d\times [0,\infty) \text{ and } y\in \mathbb{R}^d.$



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• New points and cells form and grow only in uncovered space.



└─ Johnson-Mehl germination-growth Model

Definition(cont.)

• Growth ceases for each cell whenever and wherever it touches a neighbouring cell.



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Figure: The Johnson-Mehl model for times (a) t=1, (b) t=3, and (c) t=7 $\,$



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└─ Johnson-Mehl germination-growth Model

Definition(cont.)

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- $\Psi = \{(x_i, t_i) \in \Phi : T_j(x_i) > t_i \text{ for all } (x_j, t_j) \in \Phi\}.$



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Figure: Thinned and unthinned points of a germination-growth process

Johnson-Mehl and Voronoi tessellation

• If the points of Φ all arrive at exactly the same time, the Johnson-Mehl tessellation reduces to a Voronoi tessellation.



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Figure: Voronoi tessellation; cells are convex polyhedra. J-M tessellation: cells here are non-convex sets with curved boundaries



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Historical point of view

• J-M germination-growth model well studied from a probabilistic point of view, with the pioneering work by Kolmogorov (1937) and Johnson and Mehl (1939)



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- The statistical aspects?



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First and second-order properties

First-order properties

 $\bullet\,$ The intensity of Ψ is given by

$$\rho(t) = \exp\left(-\int \int_{C(0,t)} \kappa(s) \,\mathrm{d}x \,\mathrm{d}s\right) \kappa(t)$$



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Figure: Cone generated by (x_1, t_1) (Red colored area) and by the thinned point (Blue+Red colored area)



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First and second-order properties

Stationarity of Ψ

• For which choice of κ , ρ is constant?



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- For which choice of κ , ρ is constant?
- Suppose d = 1,

$$\rho(t) = \exp\left(-2v \int_0^t (t-s)\kappa(s) \mathrm{d}s\right)\kappa(t). \tag{1}$$



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• By (1) we have obtained a second-order non-linear differential equation with solution

$$\kappa(t) = \frac{c_1}{\cos^2(c_2 t + c_3)},$$
(2)

 c_1, c_2 and c_3 are constants (and $c_2t + c_3 \neq k\pi/2, k \in \mathbb{Z} \setminus \{0\}$)

Second-order properties

• Let $(x,s) \neq (y,t)$ in $\mathbb{R}^d \times [0,\infty)$ with distance r = ||x - y||, (x,s) and (y,t) are in Ψ , if T((x,s),y) > t and T((y,t),x) > s, or r > v|s - t|.



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- Second-order product density $\rho^{(2)}((x,s),(y,t)) = \rho_0^{(2)}(r,s,t) = \rho_0^{(2)}(r,t,s).$



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- $\bullet\,$ Using the Slivnyak-Mecke's formula, the second-order product density of Ψ is given by

$$\rho_0^{(2)}(r,s,t) = \kappa(s)\kappa(t)\mathbf{1}[r > v|s-t|] \exp\left(-\int_0^{\max\{s,t\}} \kappa(u)V_{\cup}(r,s-u,t-u)\,\mathrm{d}u\right).$$



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Second-order properties

• The pair correlation function is given by

$$g(r, s, t) = \mathbf{1}[v|s - t| < r < v(s + t)] \exp\left(-\int_{0}^{(s+t-r/v)/2} \kappa(u) V_{\cap}(r, s - u, t - u) \,\mathrm{d}u\right) + \mathbf{1}[r > v(s + t)].$$



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•
$$V_{\cap}(r, s-u, t-u) = V(b(x, v(s-u)) \cap b(y, v(t-u))).$$



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$$V_{\cap}(r, s - u, t - u) = V(b(x, v(s - u)) \cap b(y, v(t - u))).$$

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$$V_{\cap} > 0 \iff u < (s + t - r/v)/2$$
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Since g(r, s, t) is not a function of r and s - t only. Therefore, Ψ is not second-order intensity-reweighted stationary.



$$V_{\cap}(r,s-u,t-u)$$

•
$$V_{\cup}(r, s - u, t - u) = \omega_d [v(s - u)]_+^d + \omega_d [v(t - u)]_+^d - V_{\cap}(r, s - u, t - u)$$



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 $V_{\cap}(r,s-u,t-u)$



volume of a d-dimensional hyper-spherical cap:

$$V_d(l,h) = \frac{1}{2} \frac{\pi^{d/2}}{\Gamma(1+d/2)} r^d I_{(2lh-h^2)/l^2}((d+1)/2, 1/2)$$
$$I_c(a,b) = \frac{1}{B(a,b)} \int_0^c u^{a-1} (1-u)^{b-1} du \quad \text{with } B(a,b) = \frac{\Gamma(a)\Gamma(b)}{\Gamma(a+b)}$$



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$$\begin{split} V_{\cap}(r,s-u,t-u) &= V_d\left(v(s-u),\frac{[v(t-u)]^2 - (r-v(s-u))^2}{2r}\right) \\ &+ V_d\left(v(t-u),\frac{[v(s-u)]^2 - (r-v(t-u))^2}{2r}\right) \end{split}$$



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Inhomogeneous K-function-like summary statistics and their Non-parametric Estimation

• For R > 0, define

$$K_1(R) = E \sum_{i \neq j} \frac{1 \left[x_i \in W, \ v(t_i + t_j) < \|x_i - x_j\| \le R \right]}{|W|\rho(t_i)\rho(t_j)}$$



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$$K_{2}(R) = \mathbf{E} \sum_{i \neq j} \frac{\mathbf{1} \left[x_{i} \in W, \ \|x_{i} - x_{j}\| \leq v(t_{i} + t_{j}), \ \|x_{i} - x_{j}\| \leq R \right]}{|W|\rho(t_{i})\rho(t_{j})}$$



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An unbiased estimator of K₁(R):

$$\hat{K}_1(R) = \sum_{i \neq j} \frac{\mathbf{1} \left[x_i \in W, \; x_j \in W, \; v(t_i + t_j) < \|x_i - x_j\| \le R \right]}{|W| \rho(t_i) \rho(t_j) w(x_i, \|x_i - x_j\|)}$$



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Summary statistics based on the characteristics for the typical Johnson-Mehl cell

• The Palm distribution of the typical cell ${\mathscr C}$ is defined by

$$\zeta |W| P(\mathscr{C} \in F) = \mathbb{E} \sum_{i} \mathbf{1} \left[T_j(x_i) > t_i \; \forall j \neq i, x_i \in W, \; C_i - x_i \in F \right]$$



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- Let *o* denote the origin.

 $C(o,t|\Phi) = \{y \in \mathbb{R}^d: T((o,t),y) \leq T((x_j,t_j),y) \text{ for all } (x_j,t_j) \in \Psi\}$



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• Hence, by Slivnyak-Mecke formula

$$P(\mathscr{C} \in F) = \int P\left(T_j(o) > t \; \forall j, \; C((o,t)|\Phi) \in F\right) \kappa(t) \, \mathrm{d}t/\zeta$$



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Johnson-Mehl germination-growth model

-Functional summary statistics and non-parametric estimation

Palm distribution of the typical shortest nucleus-boundary distance R

• In the Johnson-Mehl case, the distribution function for R is

$$D(r) = P(R \le r) = 1 - \iint P\left(\Phi \cap H(t, r) = \emptyset\right) \kappa(t) \, \mathrm{d}x \, \mathrm{d}t/\zeta, \quad r > 0,$$



Johnson-Mehl germination-growth model

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$$H(t,r) = \{(y,u) \in \mathbb{R}^d \times [0,t] : \|y\| \le 2r + v(t-u)\}$$
$$\cup \{(y,u) \in \mathbb{R}^d \times (t,t+r/v] : v(t-u) \le \|y\| \le 2r + v(t-u)\}.$$



Figure: Example of the region H(t, r).



Palm distribution of the typical shortest nucleus-boundary distance ${\cal R}$

 In the Voronoi case, 2R is just the typical nearest-neighbor distance for the nuclei.



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Johnson-Mehl germination-growth model

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Figure: Shortest boundary distance: Vorronoi tessellation (left panel), and Johnson-Mehl tessellation (right panel)



Johnson-Mehl germination-growth model

- Functional summary statistics and non-parametric estimation

Palm distribution of the typical shortest nucleus-boundary distance R

• In the Voronoi case, 2R is just the typical nearest-neighbor distance for the nuclei.



Figure: Shortest boundary distance: Vorronoi tessellation (left panel), and Johnson-Mehl tessellation (right panel)

• By ignoring edge effects, a ratio unbiased non-parametric estimate of ${\cal D}(r)$ is

$$\hat{D}(r) = \frac{1}{|W|} \sum_{i} \frac{\mathbf{1} \left[T_j(x_i) > t_i \; \forall j \neq i, x_i \in W, \; R_i \leq r \right]}{\hat{\zeta}},$$



Johnson-Mehl germination-growth i

Model M1

• M1:
$$\kappa(t) = \alpha t^{\beta-1}$$
 where $\alpha > 0, \beta > 0$.



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- From a probabilistic point of view Johnson-Mehl tessellations under model M1 have been studied in:



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- In Horálek (1988, 1990) for d = 3, and in more detail and for any $d \ge 1$ in Møller (1992, 1995).

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- In Horálek (1988, 1990) for d = 3, and in more detail and for any $d \ge 1$ in Møller (1992, 1995).
- From a statistical point of view in: only paper is Quine and Robinson (1992). They considered only the one-dimensional case d = 1 and the time-homogeneous case, β = 1.



Model M2

• M2:
$$\kappa(t) = \frac{\alpha \gamma^{\beta}}{\Gamma(\beta)} t^{\beta-1} \exp(-\gamma t)$$
 where $\alpha > 0, \beta > 0, \gamma > 0.$



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Model M2

- M2: $\kappa(t) = \frac{\alpha \gamma^{\beta}}{\Gamma(\beta)} t^{\beta-1} \exp(-\gamma t)$ where $\alpha > 0, \ \beta > 0, \ \gamma > 0.$
- Source of this model: Bennett and Robinson (1990)



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Model M2

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$$\kappa(t) = \frac{\alpha \gamma^{\beta}}{\Gamma(\beta)} t^{\beta-1} \exp(-\gamma t)$$
 where $\alpha > 0, \ \beta > 0, \ \gamma > 0.$

- Source of this model: Bennett and Robinson (1990)
- This model has been used by Thomson et al. (1995), Holst et al. (1996) and in a series of papers by Chiu and coworkers to analysis neurotransmitter data-set, see Chiu et al. (2003) and the refrences therein.



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- Chiu (1995) studied the limiting distribution of the time of completion for Johnson-Mehl model within a bounded region.



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Functional summary statistics for model M1

• The intensity function: $\rho(t) = \exp\left(-\alpha \omega_d v^d t^{\beta+d} B(\beta, d+1)\right) \alpha t^{\beta-1}$



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Figure: Behavior of $\rho(t)$ for model M1 with d = 2 and $\alpha = v = 1$, when $\beta = 0.5$ (solid line), $\beta = 1$ (dashed line), $\beta = 2$ (dotted line), and $\beta = 3$ (dot-dashed line).



Image: A image: A

Pair correlation function under model M1

- For d = 1, $V_{\cap}(r, s u, t u) = v(s + t 2u) r$.
- The pair correlation function:

$$g(r, s, t) = 1[r > v|s - t|] \exp\left(\frac{\alpha(v(\beta + 1) + \beta)}{\beta(\beta + 1)2^{\beta}}(s + t - r/v)^{\beta + 1}\right)$$



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• Shortest nucleus-boundary distance distribution function

$$P(R \le r) = 1 - \int \exp\left(\frac{-2\alpha}{\beta} \left(2r(t+r/v)^{\beta} + \frac{v}{\beta+1}t^{\beta+1}\right)\right) \alpha t^{\beta-1} dt/\zeta$$



Functional summary statistics for model M2

The intensity function:

$$\rho(t) = \exp\left(-2\alpha v \left(t\Gamma(t;\beta,\gamma) - \frac{\beta}{\gamma}\Gamma(t;\beta+1,\gamma)\right)\right) \frac{\alpha\gamma^{\beta}}{\Gamma(\beta)} t^{\beta-1} \exp(-\gamma t) \quad \text{if } d = 1$$



Functional summary statistics for model M2

The intensity function:

$$\rho(t) = \exp\left(-2\alpha \upsilon \left(t\Gamma(t;\beta,\gamma) - \frac{\beta}{\gamma}\Gamma(t;\beta+1,\gamma)\right)\right) \frac{\alpha\gamma^{\beta}}{\Gamma(\beta)} t^{\beta-1} \exp(-\gamma t) \quad \text{if } d = 1$$



Figure: Behavior of $\rho(t)$ for model M2 with d = 2, $\alpha = v = \gamma = 1$, $\beta = 0.5$ (solid line), $\beta = 1$ (dashed line), $\beta = 2$ (dotted line) and $\beta = 3$ (dot-dashed line).


Parametric Models

Pair correlation function under model M2

• For d = 1 and v|s - t| < r < v(s + t).



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• Shortest nucleus-boundary distance distribution function:

$$\begin{split} P(R \leq r) &= 1 - \int \exp\left(-2\alpha \left(2r\Gamma(t+\frac{r}{v};\beta,\gamma) + v\Gamma(t;\beta,\gamma)(t-\frac{\beta+1}{\gamma})\right) \\ &\times \frac{\alpha\gamma^{\beta}}{\Gamma(\beta)} t^{\beta-1} \exp(-\gamma t) \,\mathrm{d}t/\zeta. \end{split}$$



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Likelihood when Φ is defined on $W \times [0, \infty)$

• Assume d = 1 and let $\kappa = \kappa_{\theta}$ depends on a parameter θ , e.g., $\theta = (\alpha, \beta) \in [0, \infty)^2$ in case of M1 or $\theta = (\alpha, \beta, \gamma) \in [0, \infty)^3$ in case of M2.



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- For a finite version of $\Psi, \, \Psi_W,$ defined on $W\times [0,\infty)$ the conditional intensity function is

 $\lambda(x,t|\mathcal{H}_t)\,\mathrm{d}t = \mathbf{1}[T_i(x) > t\;\forall\, t_i < t\;\;\mathrm{with}\;(x_i,t_i) \in \Psi_W]\,\mathcal{K}(\mathrm{d}t), \quad (x,t) \in W \times [0,\infty),$

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• A realisation $\Psi_1 = \{(x_1, t_1), \dots, (x_n, t_n)\}$ has been given.



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- A realisation $\Psi_1 = \{(x_1, t_1), \dots, (x_n, t_n)\}$ has been given.
- The likelihood function is

$$L(\theta, v; \Psi_1) = \left[\prod_{i=1}^n \kappa_\theta(t_i)\right] \exp\left(-\iint_{W \times [0,\infty)} \mathbf{1}[T_i(x) \ge t \; \forall t_i < t, i \in \{1, \dots, n\}] \kappa_\theta(t) \, \mathrm{d}x \, \mathrm{d}t_i\right),$$

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Likelihood when Φ is defined on $W \times [0, \infty)$

• $\{(x,t) \in W \times [0,\infty), \mathbf{1}(.) = 1\}$ is given by $A = \{(x,t) : x \in W, 0 \le t \le T_i(x) \text{ if } x \in C_i\},\$



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Figure: Example of the region A (shaded region) when n = 2.



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Thus

$$L(\theta, v; \Psi_1) = \left[\prod_{i=1}^n \kappa_\theta(t_i)\right] \exp\left(-\iint_A \kappa_\theta(t) \, \mathrm{d}x \, \mathrm{d}t\right).$$

Likelihood when Φ is defined on $\mathbb{R} \times [0,\infty)$

Assume x₁ < ... < x_n and condition on x₁ and x_n to avoid the effect of Φ points outside the observation window W on the shape of region A.



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- Assume x₁ < ... < x_n and condition on x₁ and x_n to avoid the effect of Φ points outside the observation window W on the shape of region A.
- Then the likelihood of observing Ψ_1 given (x_1, t_1) and (x_n, t_n) is

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A case study: Neurotransmitter data

Release of neurotransmitter at the neuromuscular junction

 The neuronal axon terminal at the neuromuscular junction has branches consisting of strands containing many randomly scattered sites.



A case study: Neurotransmitter data

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- The neuronal axon terminal at the neuromuscular junction has branches consisting of strands containing many randomly scattered sites.
- An action potential triggers the release of neurotransmitters to the synapse as the synaptic vesicles diffuse into the cellular membrane.



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Release of neurotransmitter at the neuromuscular junction

- The neuronal axon terminal at the neuromuscular junction has branches consisting of strands containing many randomly scattered sites.
- An action potential triggers the release of neurotransmitters to the synapse as the synaptic vesicles diffuse into the cellular membrane.
- Each quantum released is assumed to cause release of an **inhibitory substance** which diffuses along the terminal at **a constant rate preventing further releases in the inhibited region** (Bennett and Robinson (1990)).



Johnson-Mehl germination-growth model	
A case study: Neurotransmitter data	
Data	
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• The data sets contain the times and the amplitudes of release of all transmitters in a series of 800 experiments.



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- The range of releases is from 0 to 4. The frequencies of 0's,1's,... are 101, 387, 237, 66, 9, respectively.



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- 50 experiments with two identical amplitudes are ignored.
- Due to have the same range for the real data-sets and the simulated ones we assume W = 1. By multiplying the location values by 5 we obtain roughly uniform values on [0,1].
- Among the transformed data, four outliers above 1 are deleted.
- Finally, 746 experiments with 101 experiments with no germinated seed and 645 with at least one germinated seed are obtained. The frequencies of 1's, ..., 4's now being 387, 210, 45, 3, respectively.



A case study: Neurotransmitter data

Model checking

• Estimates: $\hat{\alpha} = 1.29$, $\hat{\gamma} = 13.3$, $\hat{\beta} = 5.36$, $\hat{v} = 0.018$.



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Figure: Left: Estimated K_1 -function for the data (solid line), and average and envelopes calculated from 39 simulations of the fitted model (dashed lines). Right: as left for K_2 -function.



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Figure: Left: Estimated K_1 -function for the data (solid line), and average and envelopes calculated from 39 simulations of the fitted model (dashed lines). Right: as left for K_2 -function.

• For all R values, \hat{K}_1 and \hat{K}_2 for the data is between the envelopes, so the plot is in favor of the fitted model.

A case study: Neurotransmitter data



• Estimating the parameters of model M1 by MLE



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└─A case study: Neurotransmitter data



- Estimating the parameters of model M1 by MLE
- Checking the fitted model by D(r)



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