

Generative modelling of multivariate geometric extremes using normalising flows

Lambert De Monte¹

Joint work with Raphaël Huser², Ioannis Papastathopoulos¹, Jordan Richards¹



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Very broad overview

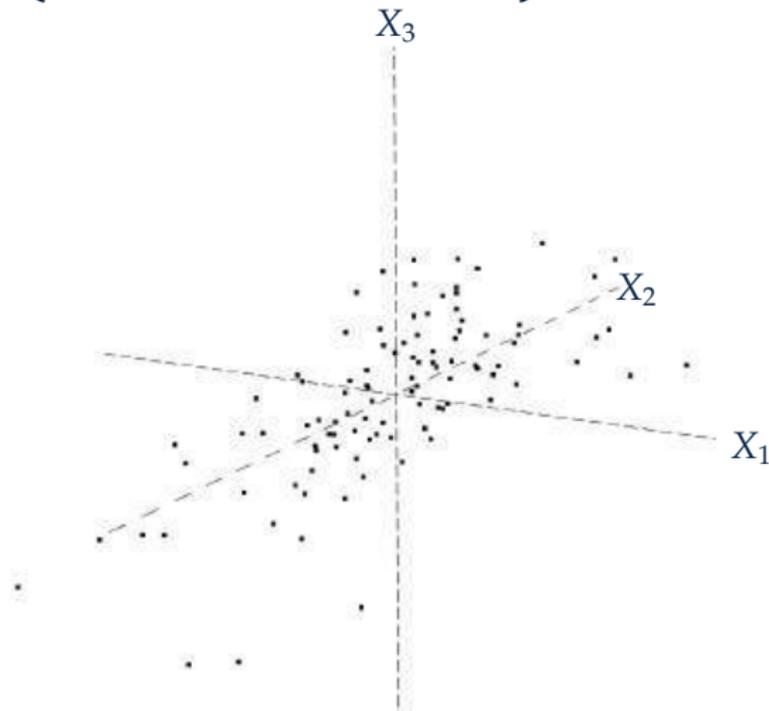
- 1 Geometric extreme value theory
- 2 Statistical inference
- 3 Simulation study
- 4 An application to low and high wind speeds

Limit sets

Let $X_1, X_2, \dots \in \mathbb{R}^d$ be iid draws from \mathbb{P}_X with standard Laplace marginal distributions, and

$$N_n := \left\{ \frac{X_1}{\log(n)}, \dots, \frac{X_n}{\log(n)} \right\}$$

$n = 100$

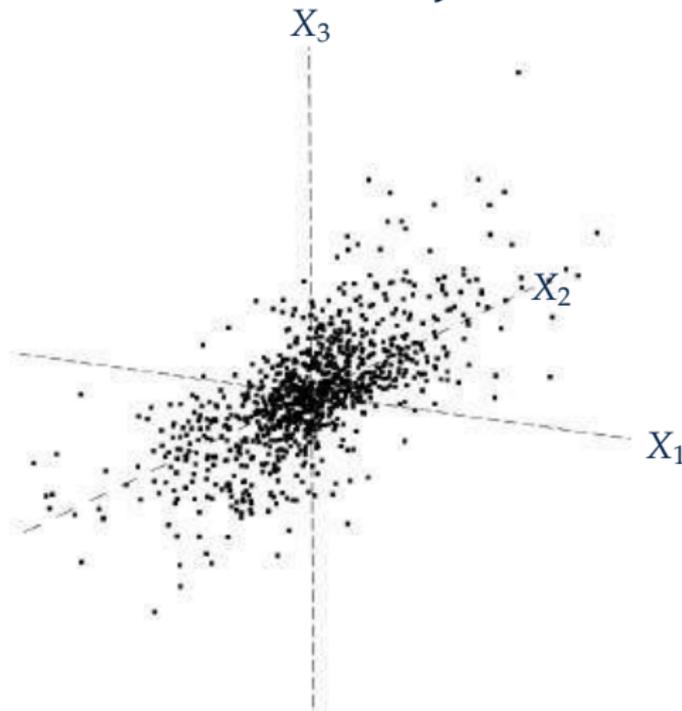


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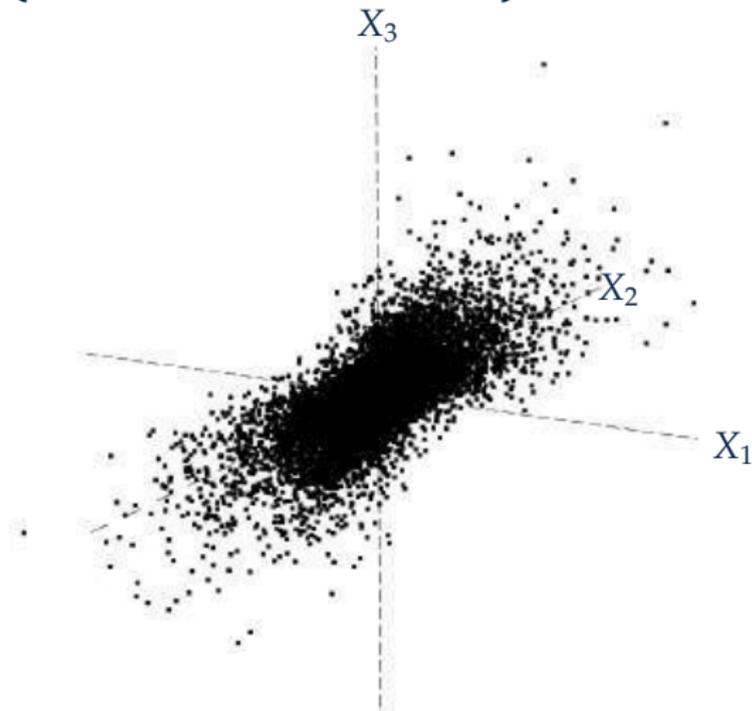


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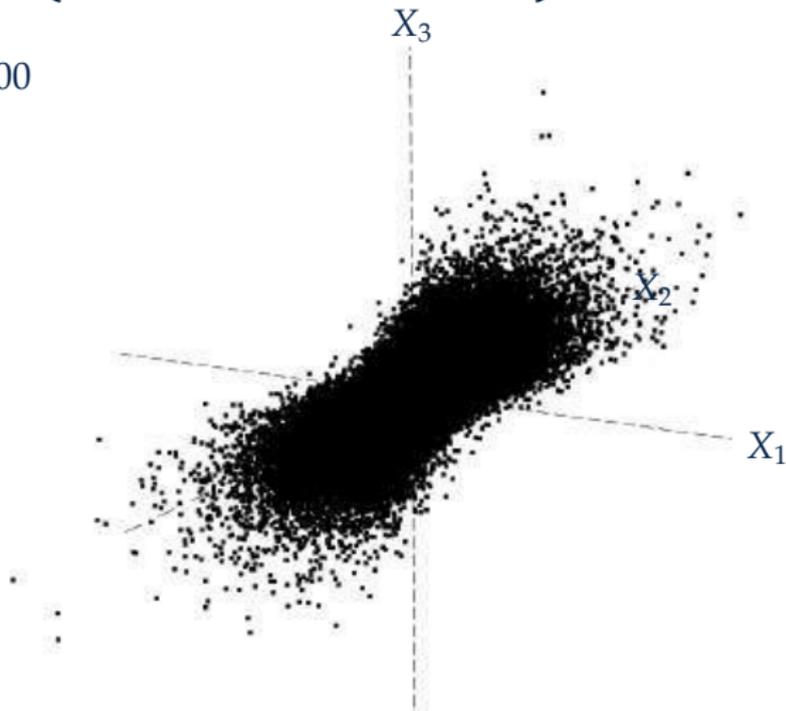


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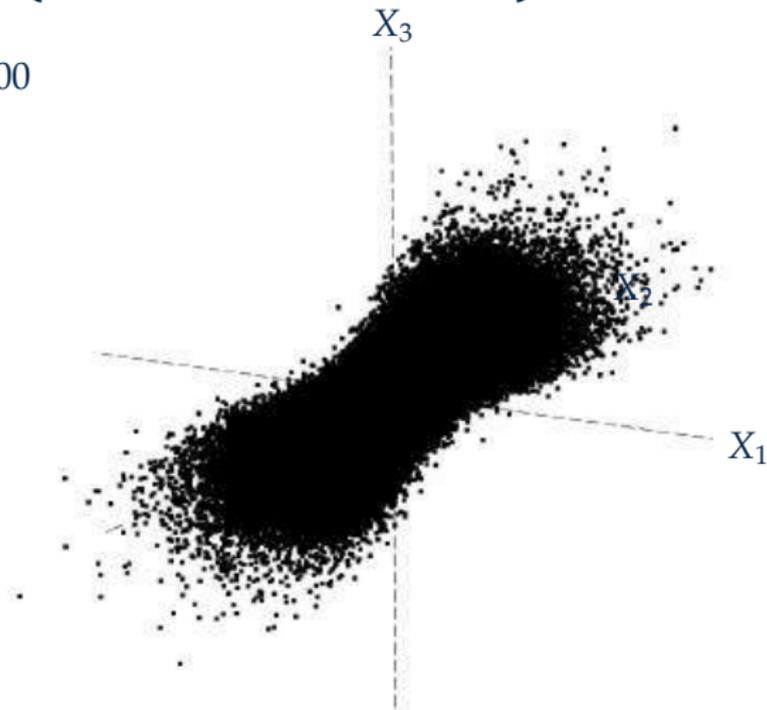


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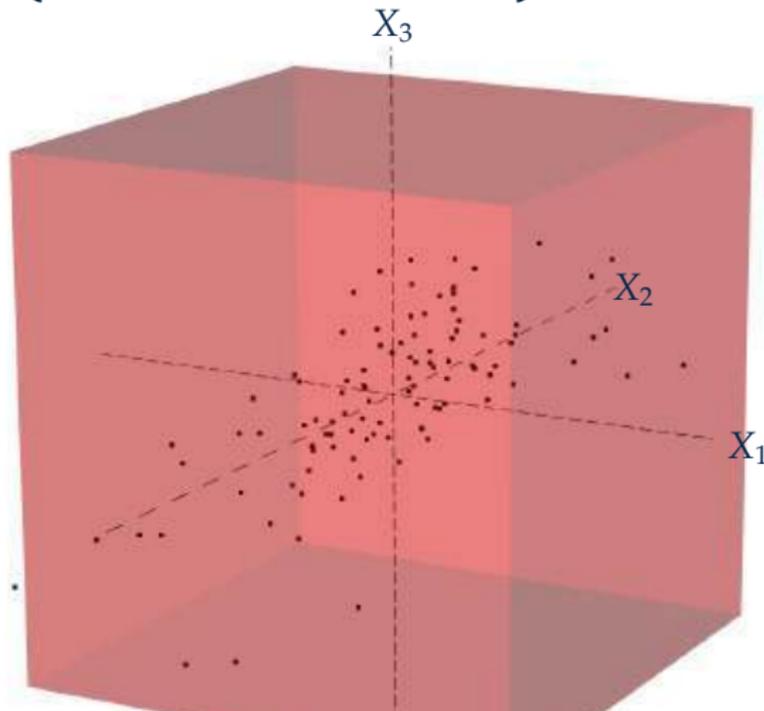


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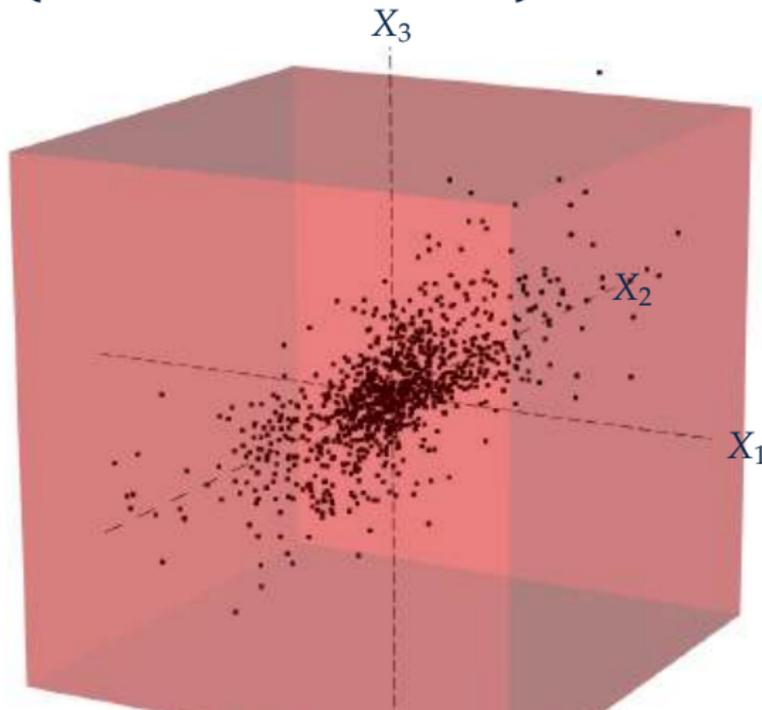


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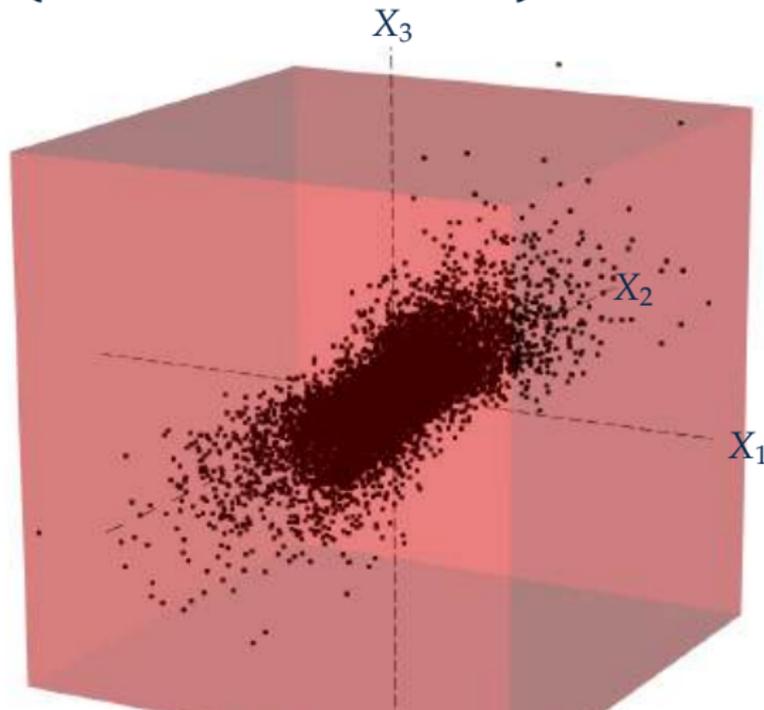


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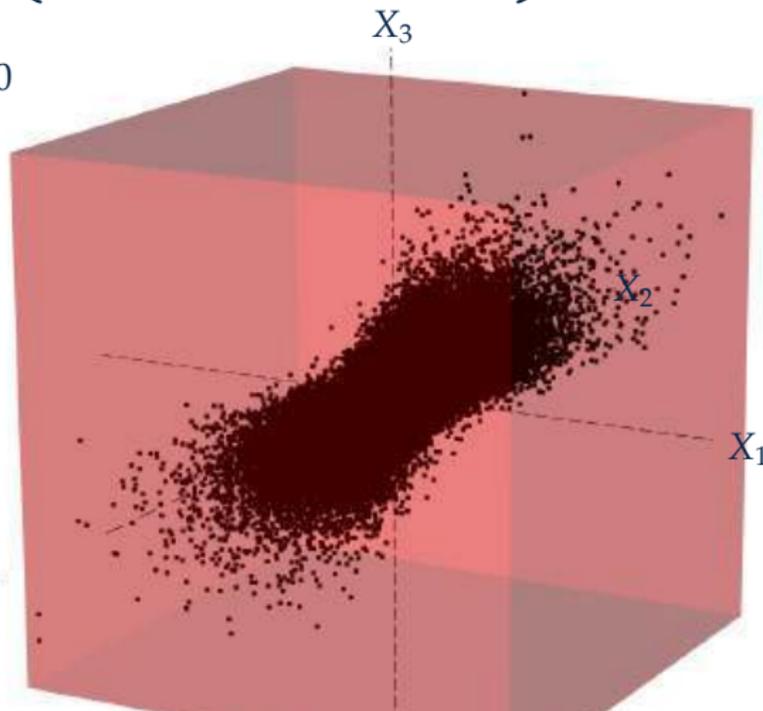


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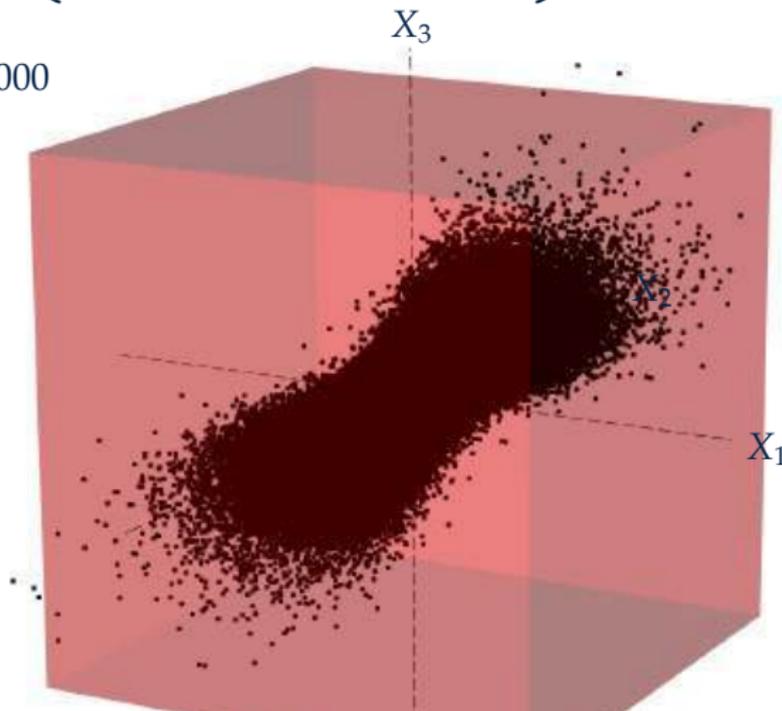


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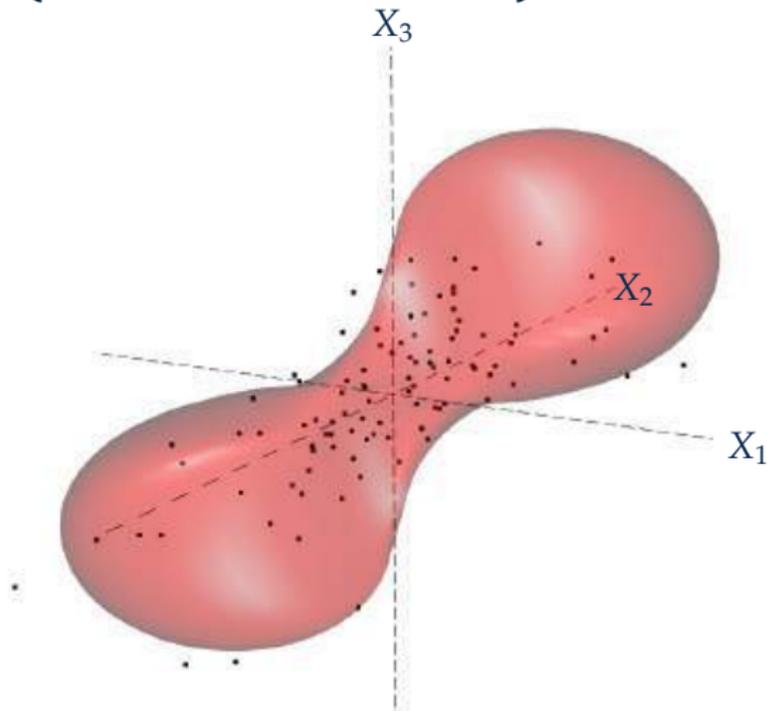


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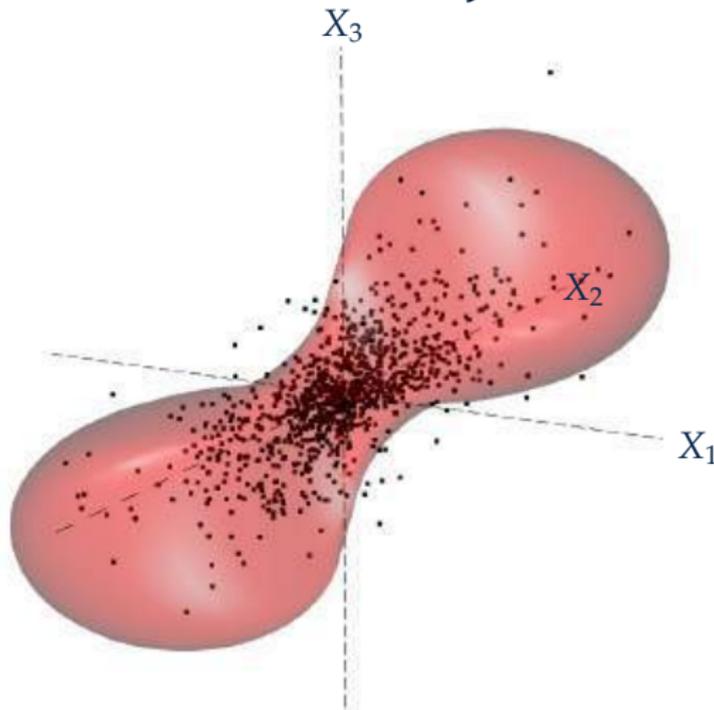


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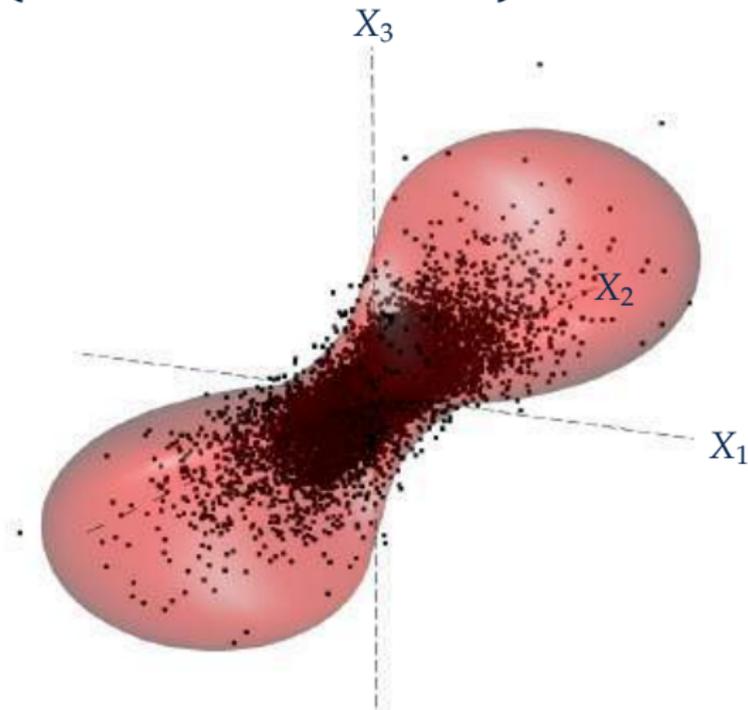


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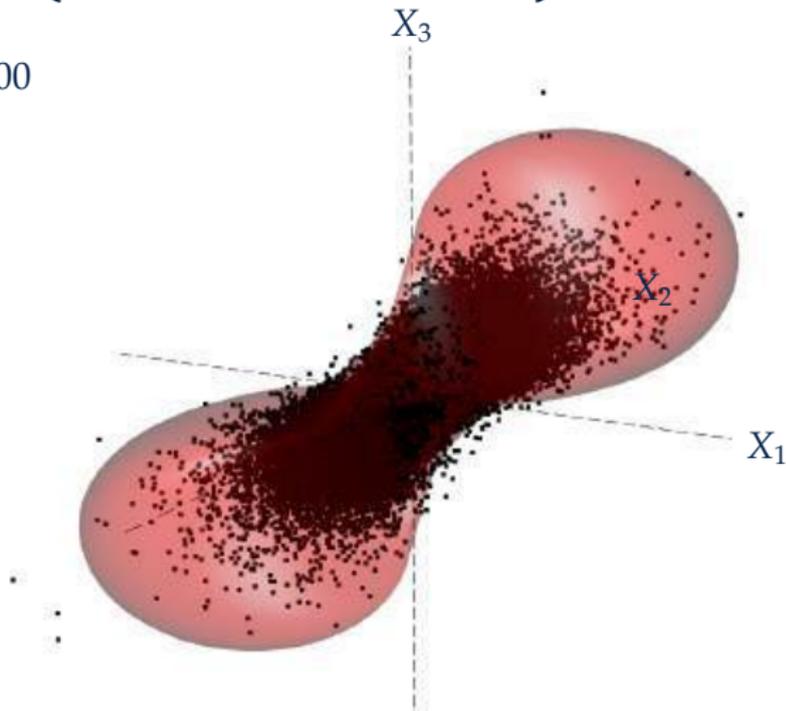


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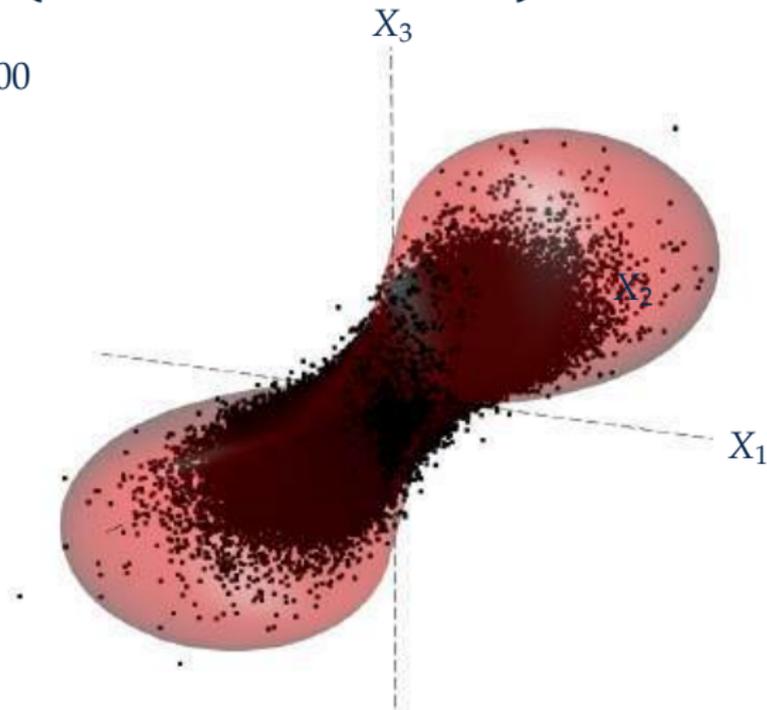


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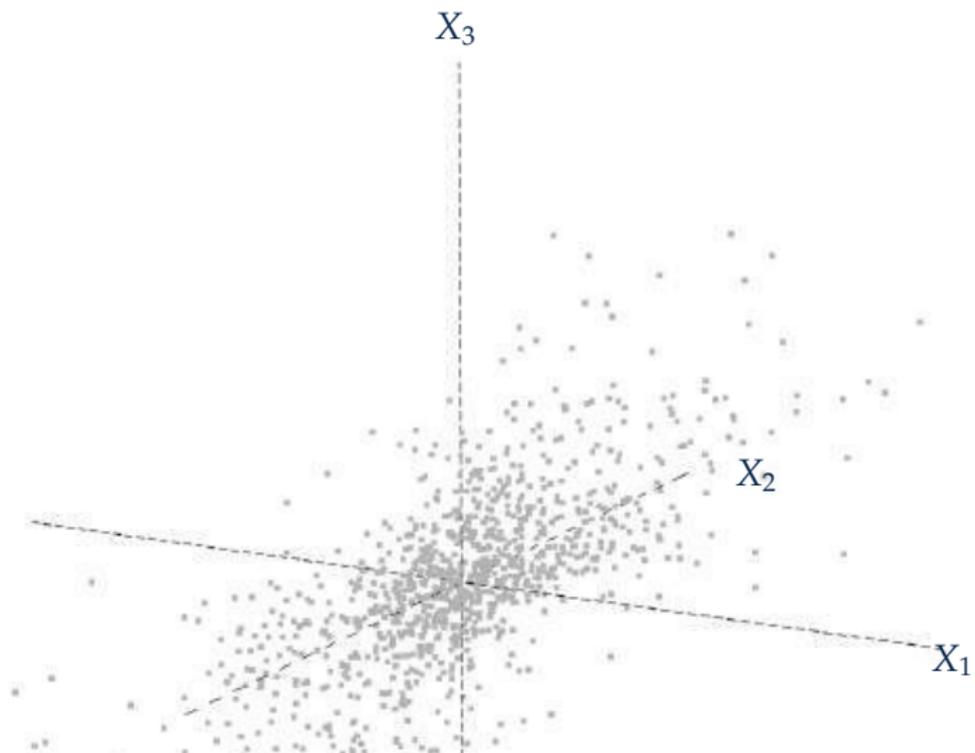
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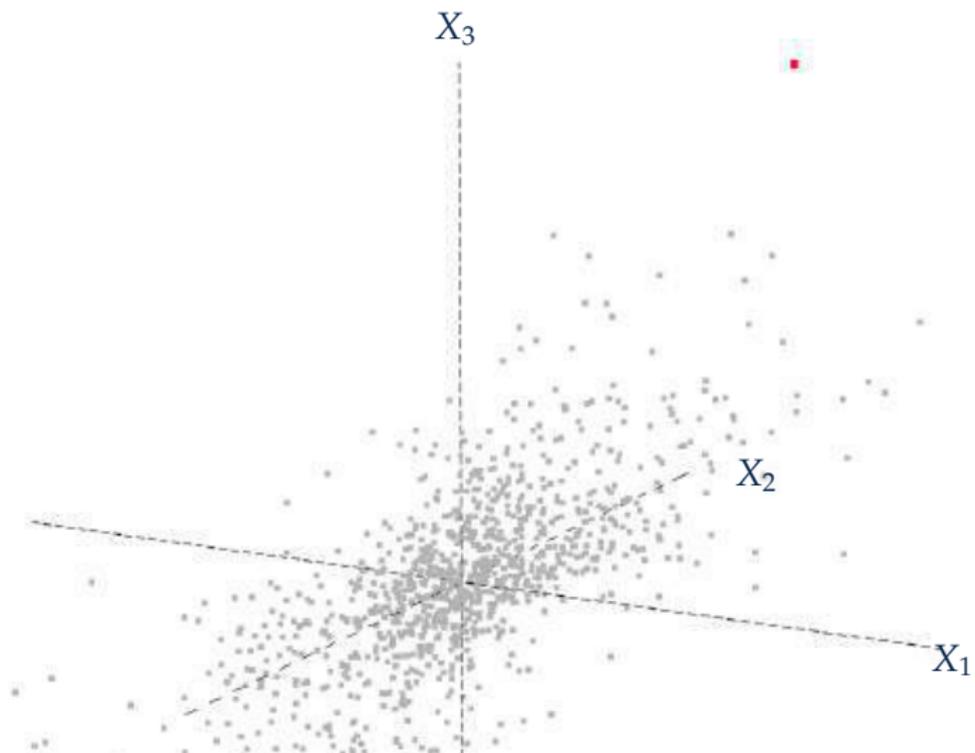
Very broad overview – A directional statistics approach

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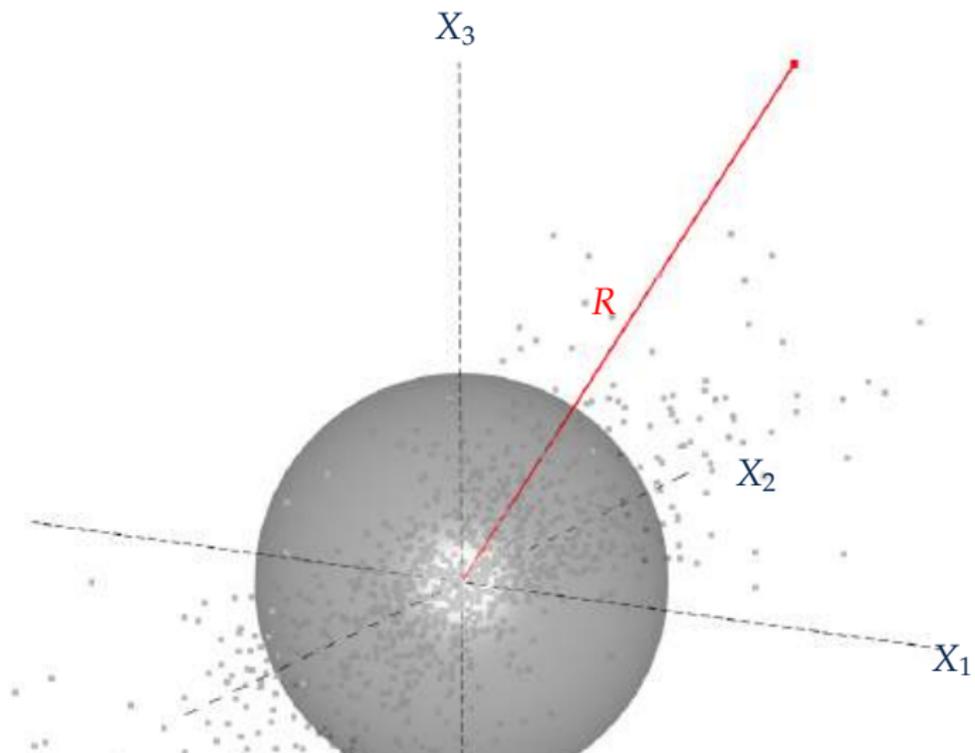
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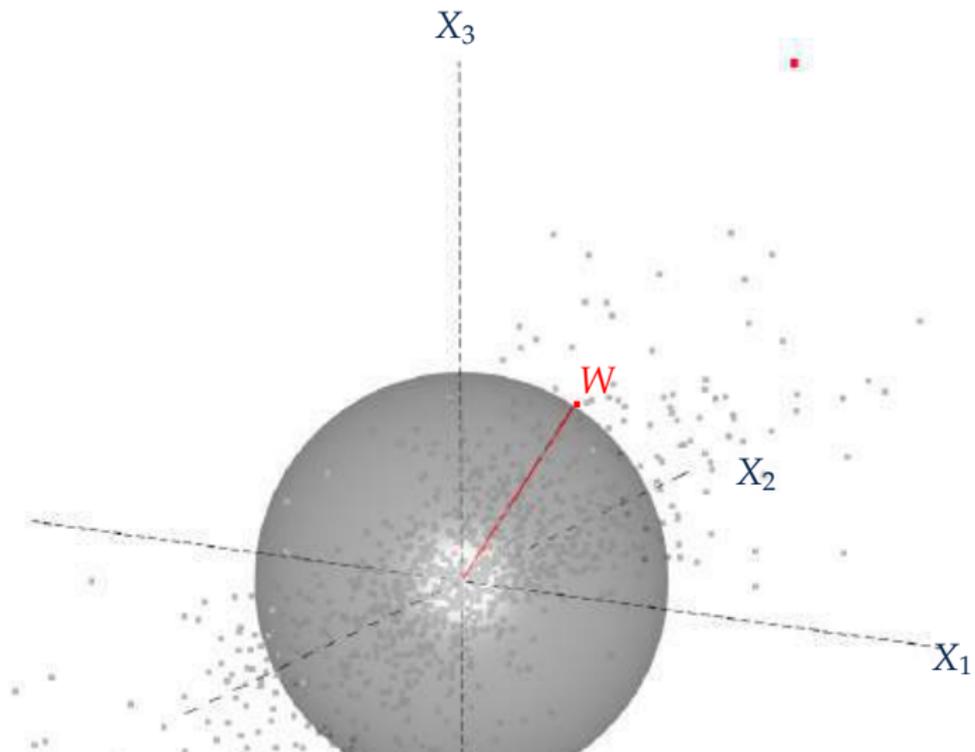
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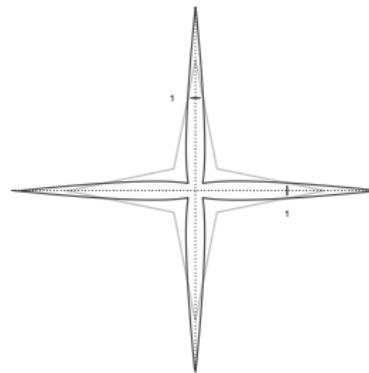
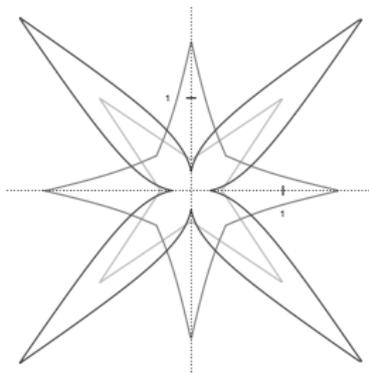
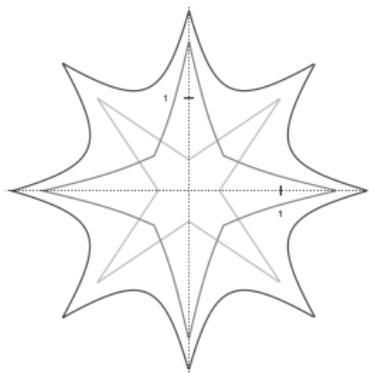
Starshaped sets ★ – A basis for our model construction

- A set $\mathcal{B} \in \mathbb{R}^d$ is starshaped if there exists a set $\ker(\mathcal{B}) \subseteq \mathcal{B}$ such that for $x \in \ker(\mathcal{B})$ and for all $y \in \mathcal{B}$, the segment $[x : y] \in \mathcal{B}$.

- A set $\mathcal{B} \in \star$ is in one-to-one correspondence with a radial function

$$r_{\mathcal{B}}(w) = \sup\{\lambda \in \mathbb{R} : \lambda w \in \mathcal{B}\}, \quad w \in \mathbb{S}^{d-1}.$$

- Starshaped sets admit algebraic operations via their radial functions:



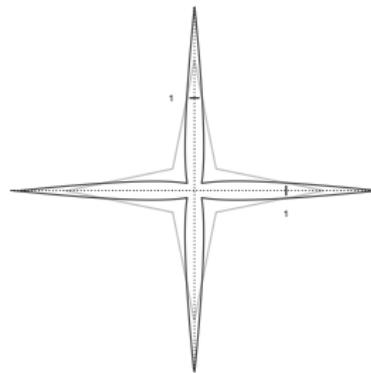
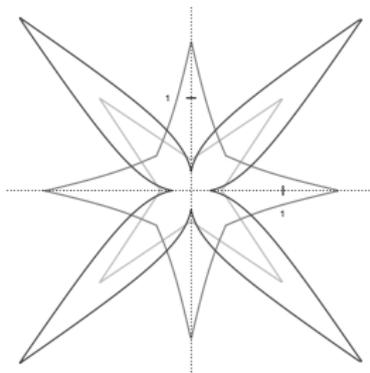
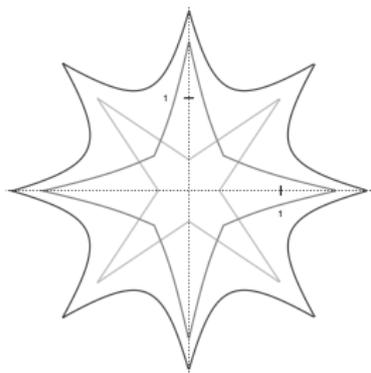
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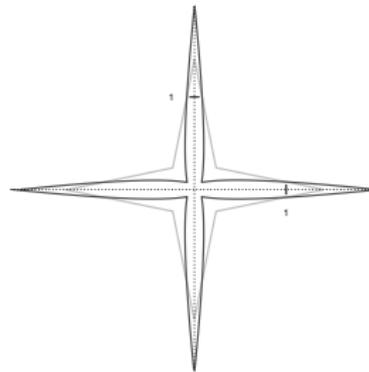
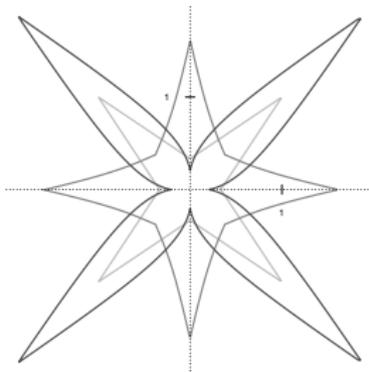
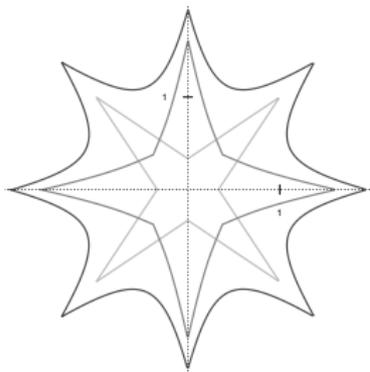
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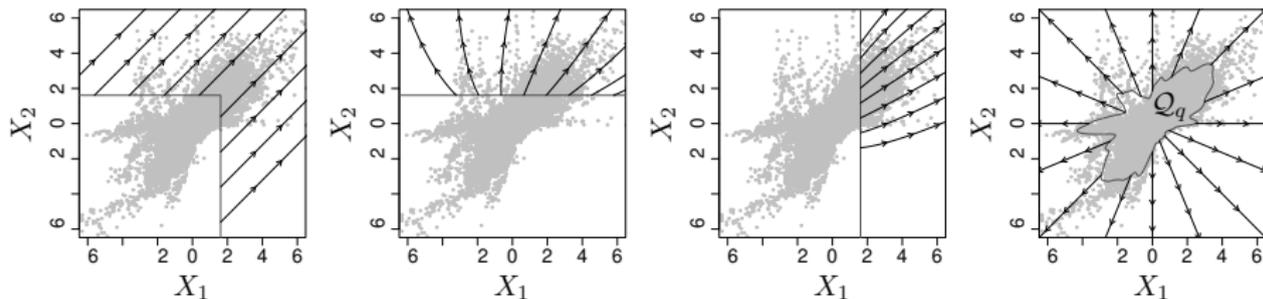
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Geometric multivariate EVT: Motivation

- Interest in gaining more insight into the (extremal) **dependence structure** of a random vector $\mathbf{X} = (X_1, \dots, X_d) \in \mathbb{R}^d$.
- Extrapolating beyond the range of observed data:



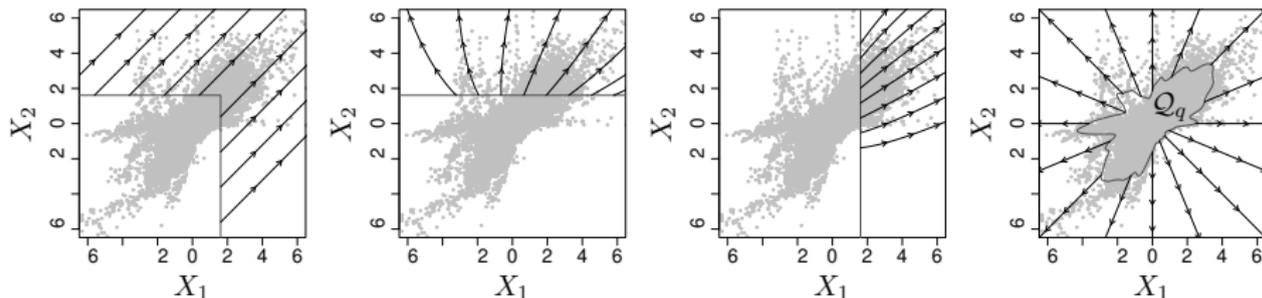
Directions along which MEVT frameworks allow extrapolation to tail regions: (a) MRV, (b) and (c) conditional extremes, (d) geometric extremes.

- Effectively, we want to study the random variable

$$(R, W) \mid \{R \notin \mathcal{Q}_q\}.$$

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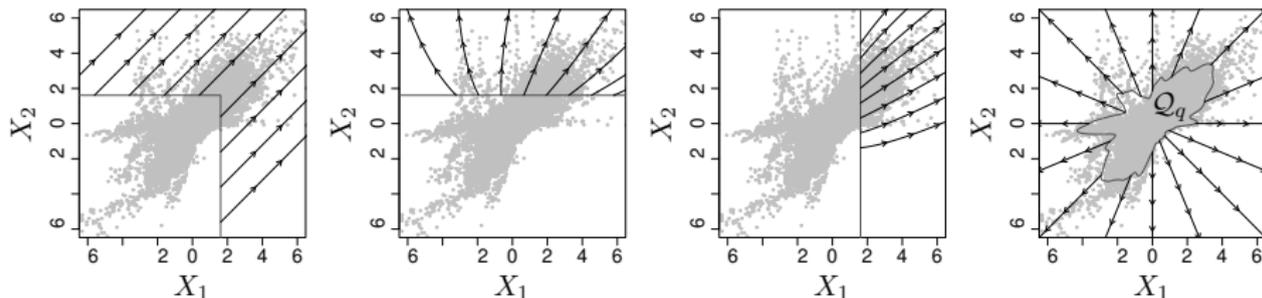
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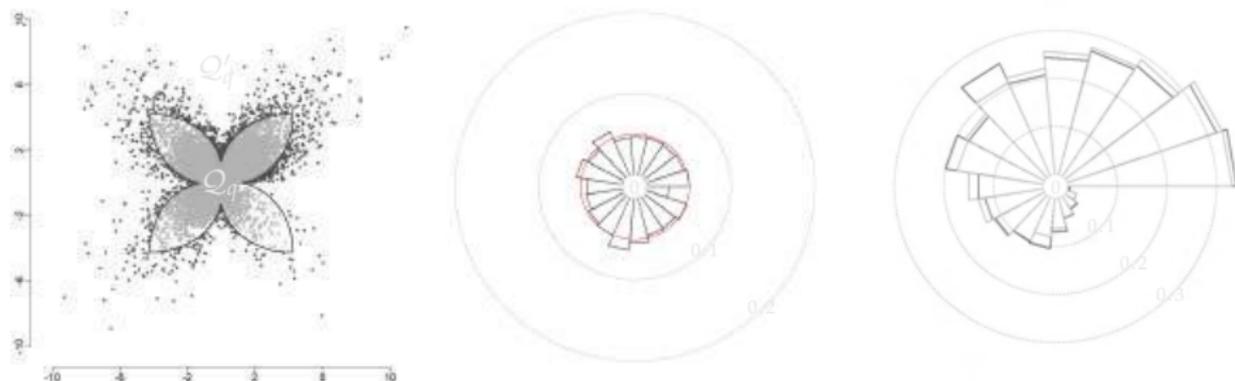
The quantile set Q_q

- We let Q_q via the q -th quantile of $R \mid W = w$, that is, it satisfies

$$\mathbb{P}[R \leq r_{Q_q}(w) \mid W = w] = q, \quad \text{for all } w \in \mathbb{S}^{d-1}.$$

- Q_q then satisfies that

$$\mathbb{P}[X \notin Q_q] = 1 - q, \quad \text{and} \quad W \mid \{X \notin Q_q\} \stackrel{d}{=} W.$$



Left: Independent samples ($n = 2 \times 10^4$) from a bivariate distribution having true quantile set $Q_{0.95}$, boundary $\partial Q_{0.95}$ (solid black line) and complement $Q'_{0.95}$. **Centre:** Empirical proportion of exceedances binned by angular regions with true exceedance probability (0.05) in red. **Right:** Circular histogram of the density of all sampled angles (light grey) and of exceedance angles (dark grey) with concentric circles denoting density level sets.

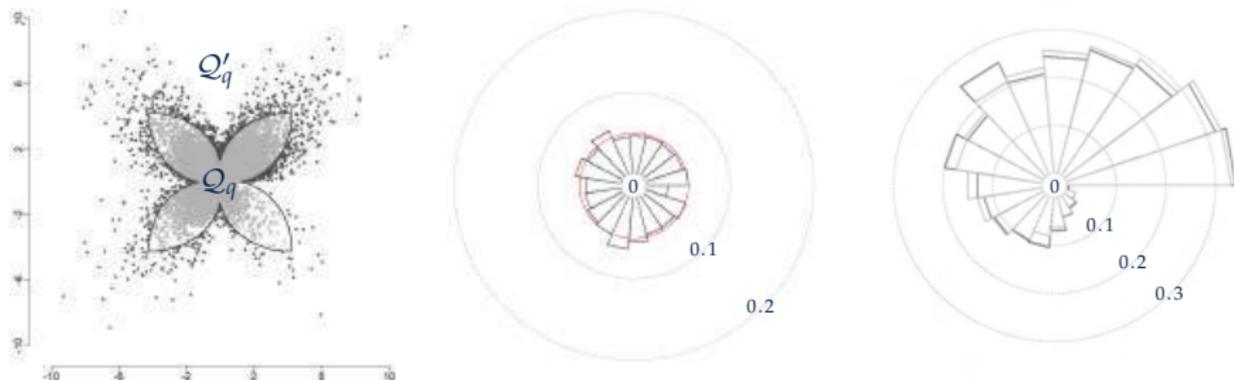
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- Note that the event $\{X = RW \notin \mathcal{Q}_q\}$ corresponds to $\{R > r_{\mathcal{Q}_q}(\mathbf{W})\}$.
- Further, Papastathopoulos et al. (2023) show conditions under which there exist a starshaped set G such that

$$\left(\frac{R - r_{\mathcal{Q}_q}(\mathbf{W})}{r_G(\mathbf{W})}, \mathbf{W} \right) | \{R > r_{\mathcal{Q}_q}(\mathbf{W})\} \xrightarrow{d} (Z, V), \quad \text{as } q \rightarrow 1, \quad (1)$$

where $Z \sim \text{Exp}(1)$, $V \sim \mathbb{P}_{\mathbf{W}}$.

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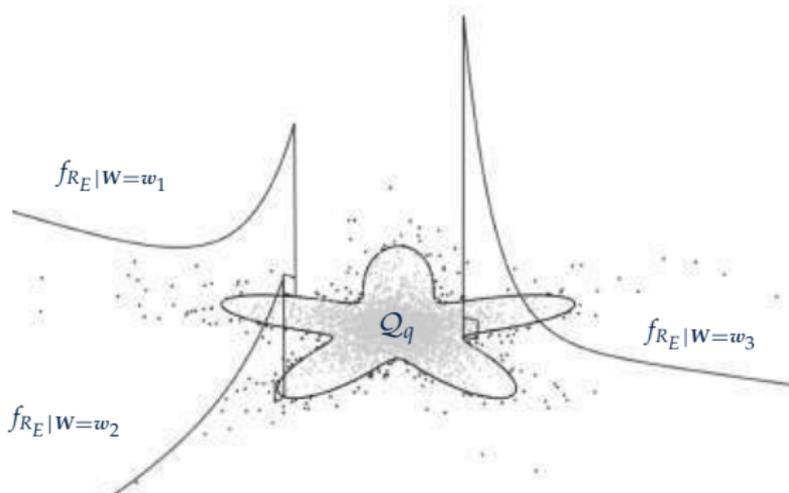
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Exceedances of Q_q

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PROPOSED MODELS

Links between parameters and models

Under appropriate convergence conditions¹, it can be shown that the quantile set \mathcal{Q}_q is asymptotically ($q \rightarrow 1$) a scale multiple of the scaling/limit set \mathcal{G} , that is,

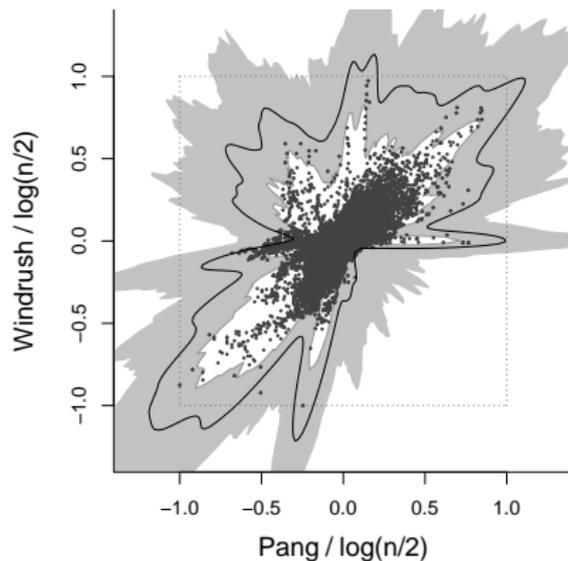
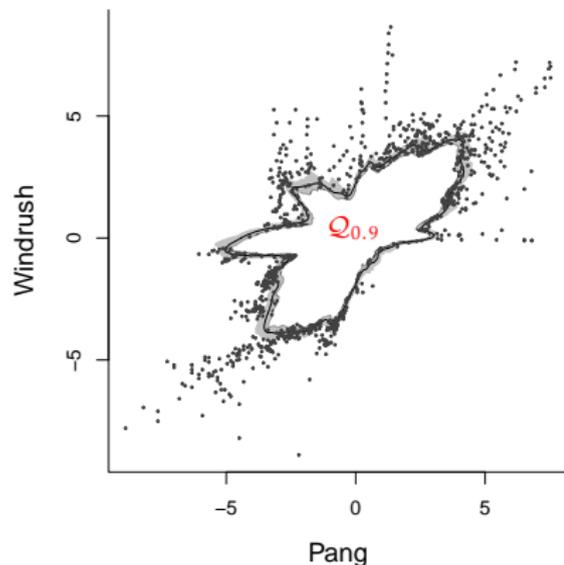
$$\mathcal{Q}_q \approx \alpha_q \mathcal{G}, \quad \alpha_q > 0, \quad \text{as } q \rightarrow 1$$

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If the density of X is homothetic with respect to $r_{\mathcal{G}}^{-1}$, that is,

$$f_{\mathbf{X}}(\mathbf{x}) = f_0(r_{\mathcal{G}}^{-1}(\mathbf{x})), \quad \mathbf{x} \in \mathbb{R}^d,$$

then \mathcal{G} and \mathcal{W} can be linked¹ through

$$r_{\mathcal{W}}(\mathbf{w}) = f_{\mathcal{W}}(\mathbf{w}) = \frac{r_{\mathcal{G}}(\mathbf{w})^d}{d|\mathcal{G}|}, \quad \mathbf{w} \in \mathbb{S}^{d-1}.$$

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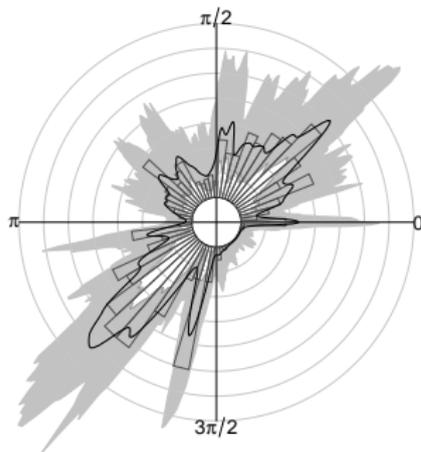
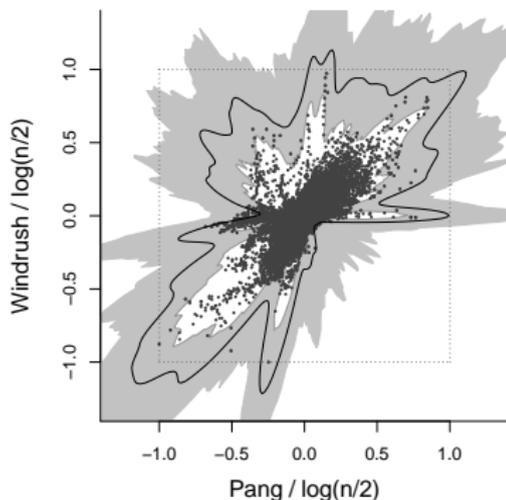
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- Any positive function $r_{\mathcal{B}}$ defined on \mathbb{S}^{d-1} can be written as

$$r_{\mathcal{B}}(\boldsymbol{w}) = \beta_{\mathcal{B}} f_{\mathcal{B}}(\boldsymbol{w}), \quad \boldsymbol{w} \in \mathbb{S}^{d-1},$$

for a **constant** $\beta_{\mathcal{B}} = \int_{\mathbb{S}^{d-1}} r_{\mathcal{B}}(\boldsymbol{w}) d\boldsymbol{w}$ and **density** $f_{\mathcal{B}}$ integrating to 1 on \mathbb{S}^{d-1} .

- Using the links $\mathcal{G}-\mathcal{Q}_q$ and $\mathcal{G}-\mathcal{W}$, we can formulate a statistical model

$$r_{\mathcal{Q}_q}(\boldsymbol{w}) = \beta_{\mathcal{Q}_q} f_{\mathcal{W}}(\boldsymbol{w})^d \text{ and } r_{\mathcal{G}}(\boldsymbol{w}) = \beta_{\mathcal{G}} f_{\mathcal{W}}(\boldsymbol{w})^d, \quad \boldsymbol{w} \in \mathbb{S}^{d-1}.$$

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Proposed models

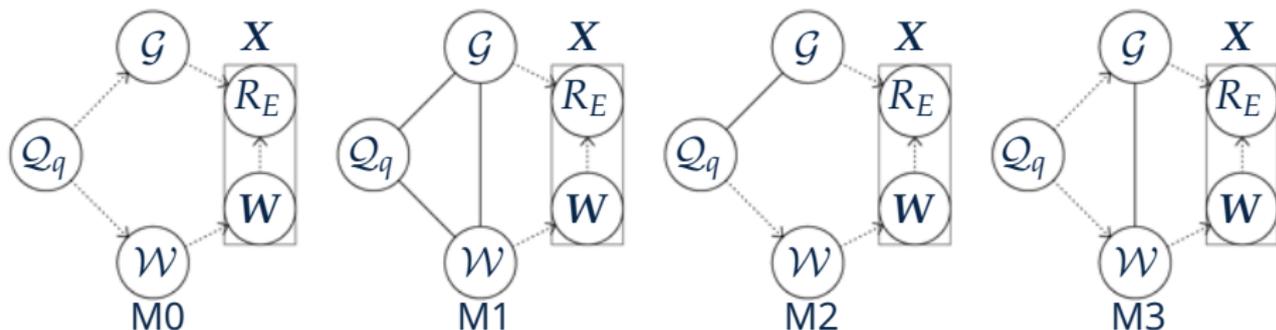
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- We introduce a **deformation set** \mathcal{D} with radial function $f_{\mathcal{D}} : \mathbb{S}^{d-1} \rightarrow [0, \infty)$.
- We can then **weaken the equality assumptions** of models M1, M2, and M3 via

$$r_{\mathcal{Q}_q}(w) = \beta_q f_{\mathcal{D}}(w) f_G(w), \quad w \in \mathbb{S}^{d-1},$$

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$$r_G(w) = \beta_G \{f_{\mathcal{D}}(w) f_W(w)\}^{1/d}, \quad w \in \mathbb{S}^{d-1},$$

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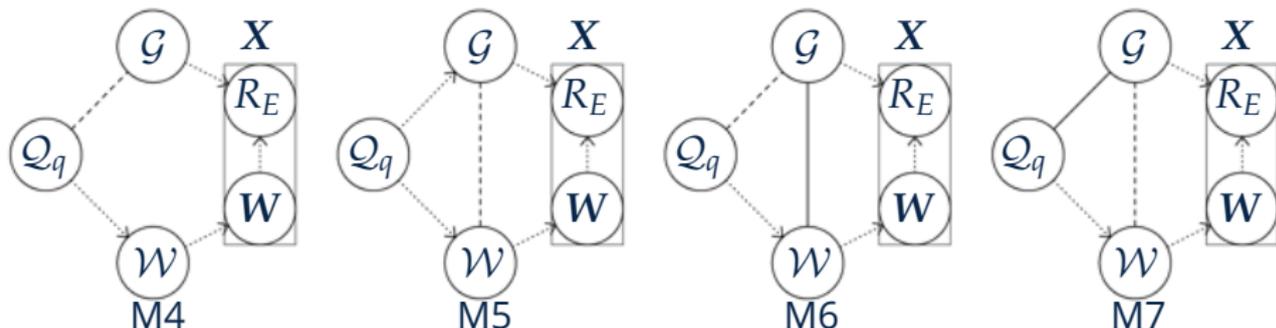
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- Models M4 to M7 are identifiable as is, but we impose penalisation on \mathcal{D} .

STATISTICAL INFERENCE

Normalising flows¹ and density estimation²

- A **normalising flow** (NF) learns a **transformation** mapping a random variable $Y \in \mathcal{Y}$ with unknown distribution to that of a known, base variable $Z \in \mathcal{Z}$.

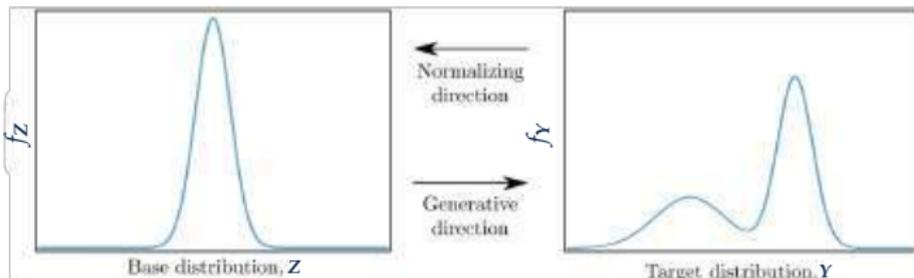


Figure 1 of Kobyzev et al. (2021)

¹Tabak & Vanden-Eijnden (2010), ²Dinh et al. (2015)

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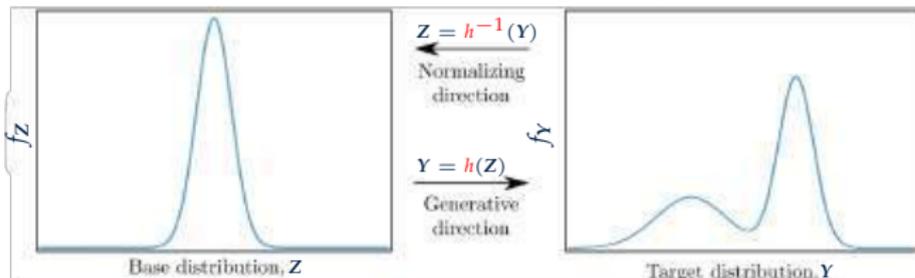


Figure 1 of Kobyzev et al. (2021)

- Assuming Y admits a density on \mathcal{Y} , this problem can be phrased as aiming to infer a (bijective and differentiable) transformation function h such that

$$f_Y(\mathbf{y}) = f_Z\{h^{-1}(\mathbf{y})\} \left| \frac{\partial h^{-1}(\mathbf{y})}{\partial \mathbf{y}} \right|, \quad \mathbf{y} \in \mathcal{Y}.$$

In practice, h is modelled as a composition of many simple bijective transformations h_1, \dots, h_k , i.e. $h = h_1 \circ h_2 \circ \dots \circ h_k$.

¹Tabak & Vanden-Eijnden (2010), ²Dinh et al. (2017)

A map from the hypersphere to the hypercylinder

- Transform the observations and models from \mathbb{S}^{d-1} to a cylindrical space \mathbb{C}^{d-1} (by abuse of notation).

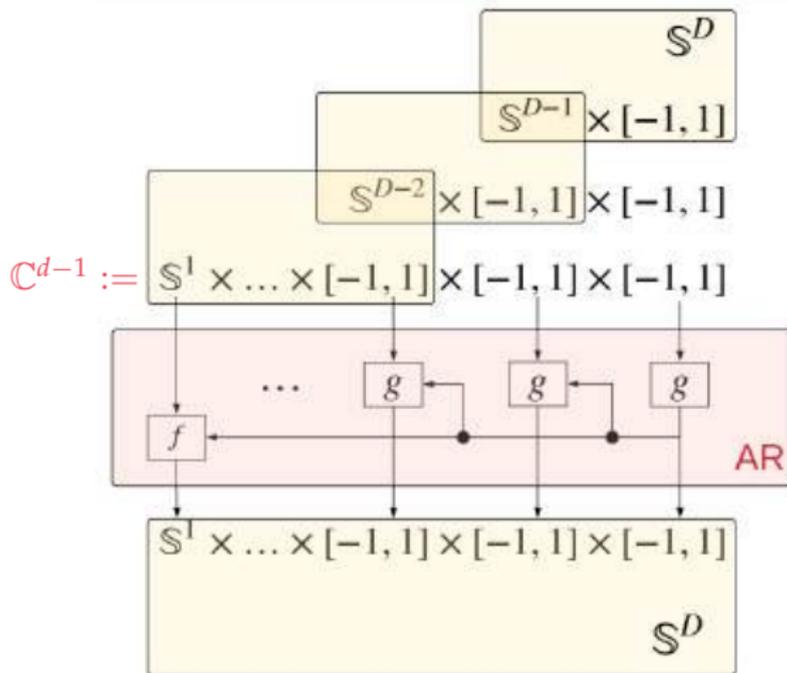
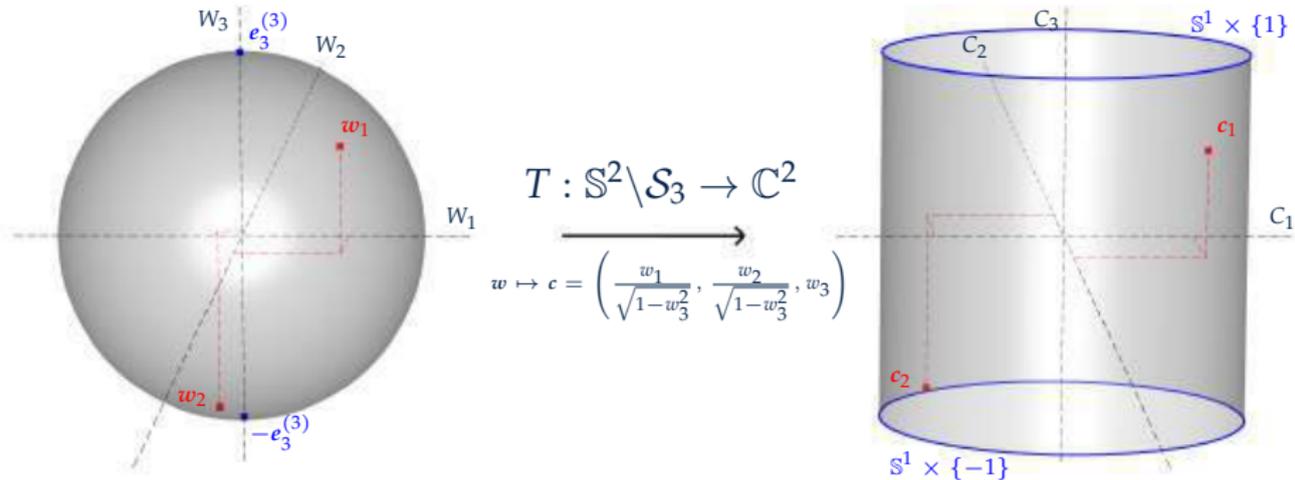


Figure 6 of Rezende et al. (2020)

A map from the hypersphere \mathbb{S}^2 to the hypercylinder \mathbb{C}^2



A model for PDFs and positive functions on \mathbb{S}^{d-1}

- It follows from the map T that a target PDF $f_B : \mathbb{S}^{d-1} \setminus \mathcal{S}_d \rightarrow [0, \infty)$, describing the **shape of a starshaped set** $B \in \mathbb{R}^d$ a.e., can be written as

$$f_B(w) = f_Y(T(w)) |\partial T(w) / \partial w|, \quad w \in \mathbb{S}^{d-1} \setminus \mathcal{S}_d,$$

for a target PDF f_Y defined on \mathbb{C}^{d-1} .

- Using the NFs formulation, f_B can in turn be modelled in terms of a **known base PDF** $f_Z : \mathbb{C}^{d-1} \rightarrow [0, \infty)$ and a **normalising flow** h_B as

$$f_B(w) = f_Z\{h_B^{-1}(T(w))\} \left| \frac{\partial h_B^{-1}(T(w))}{\partial T(w)} \right| \left| \frac{\partial T(w)}{\partial w} \right|, \quad w \in \mathbb{S}^{d-1} \setminus \mathcal{S}_d,$$

where $|\partial T(w) / w|$ is the Jacobian of the recursive transformation T .

- Further, a model for any **positive/radial function** r_B of a starshaped set B – such as the quantile set \mathcal{Q}_q or the scaling set \mathcal{G} – can be obtained via

$$r_B = \beta_B f_B$$

where f_B is as above, and $\beta_B > 0$ is a coefficient to be learned alongside the NF h_B .

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- It follows from the map T that a target PDF $f_{\mathcal{B}} : \mathbb{S}^{d-1} \setminus \mathcal{S}_d \rightarrow [0, \infty)$, describing the **shape of a starshaped set** $\mathcal{B} \in \mathbb{R}^d$ a.e., can be written as

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- Using the NFs formulation, $f_{\mathcal{B}}$ can in turn be modelled in terms of a **known base PDF** $f_Z : \mathbb{C}^{d-1} \rightarrow [0, \infty)$ and a **normalising flow** $h_{\mathcal{B}}$ as

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where $f_{\mathcal{B}}$ is as above, and $\beta_{\mathcal{B}} > 0$ is a coefficient to be learned alongside the NF $h_{\mathcal{B}}$.

¹Stimper et al. (2023)

A GRADIENT DESCENT APPROACH

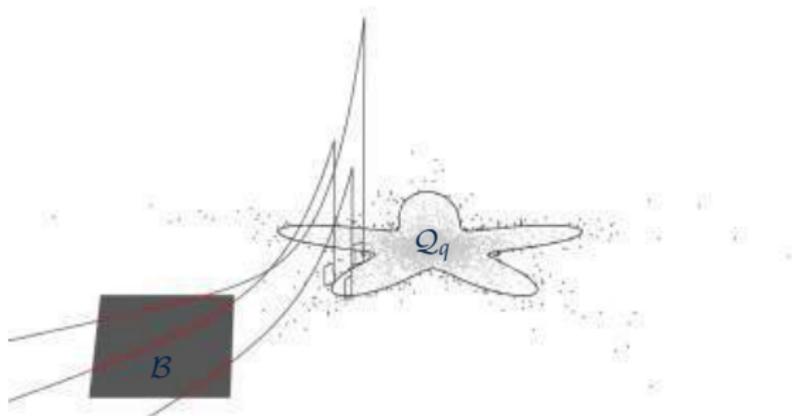
A PyTorch¹ implementation² of NFs and composite loss minimisation via the Adam optimiser³

¹Paszke et al. (2019), ²Stimper et al. (2023), ³Kingma & Ba (2017)

PROBABILITY ESTIMATION

- For any Borel set $\mathcal{B} \in \mathbb{R}^d \setminus \mathcal{Q}_q$,

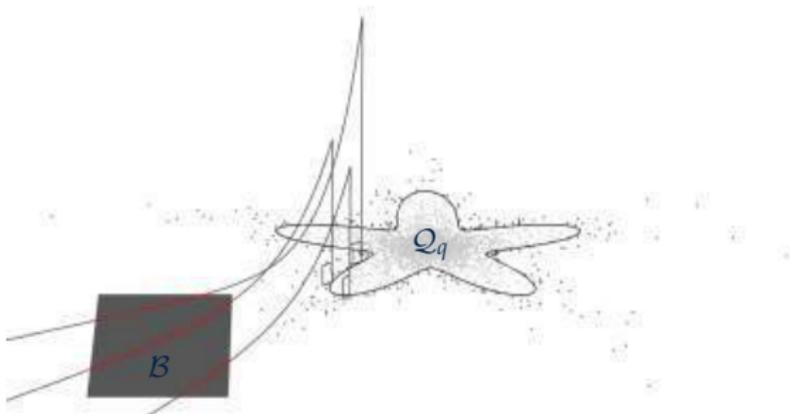
$$\mathbb{P}[X \in \mathcal{B} \mid X \notin \mathcal{Q}_q] = \int_{\mathbb{S}^{d-1}} \int_{\mathcal{B} \cap]0:w)} \frac{1}{r_G(\boldsymbol{w})} \exp \left\{ -\frac{r - r_{\mathcal{Q}_q}(\boldsymbol{w})}{r_G(\boldsymbol{w})} \right\} f_{\boldsymbol{W}}(\boldsymbol{w}) dr d\boldsymbol{w}.$$



- For any Borel set $\mathcal{B} \in \mathbb{R}^d \setminus \mathcal{Q}_q$, we use the **Monte Carlo integration**

$$\mathbb{P}[X \in \mathcal{B} \mid X \notin \mathcal{Q}_q] \stackrel{\text{P}}{\leftarrow} \frac{1}{m} \sum_{i=1}^m \int_{\mathcal{B} \cap]0:w_i)} \frac{1}{r_{\mathcal{G}}(w_i)} \exp \left\{ -\frac{r - r_{\mathcal{Q}_q}(w_i)}{r_{\mathcal{G}}(w_i)} \right\} dr, \quad n \rightarrow \infty.$$

where $w_1, \dots, w_m \sim f_W$.

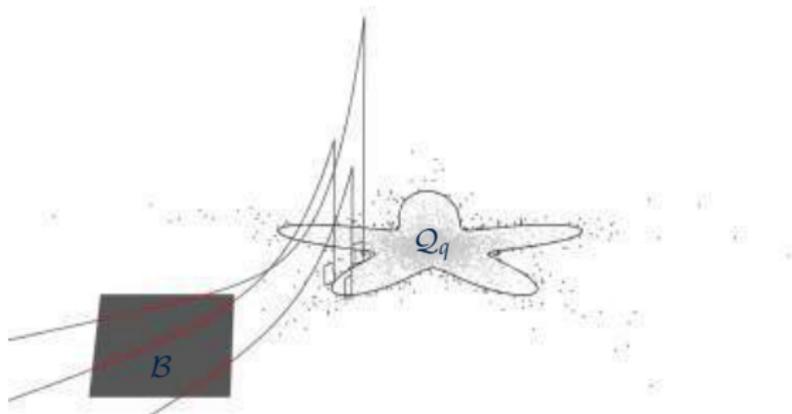


- The integral is **exact** provided one knows all radial entry and exit points of \mathcal{B} .
- The collection $w_1, \dots, w_m \sim f_W$ is sampled **fast** using the **generative direction** of the NF.

- For any Borel set $\mathcal{B} \in \mathbb{R}^d \setminus \mathcal{Q}_q$, we use the **Monte Carlo integration**

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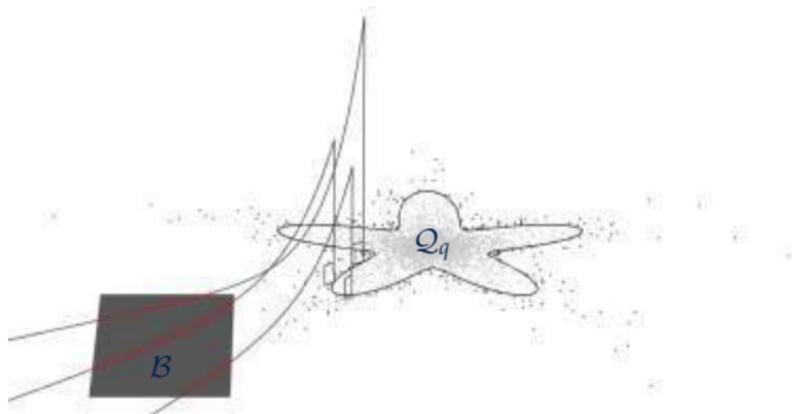


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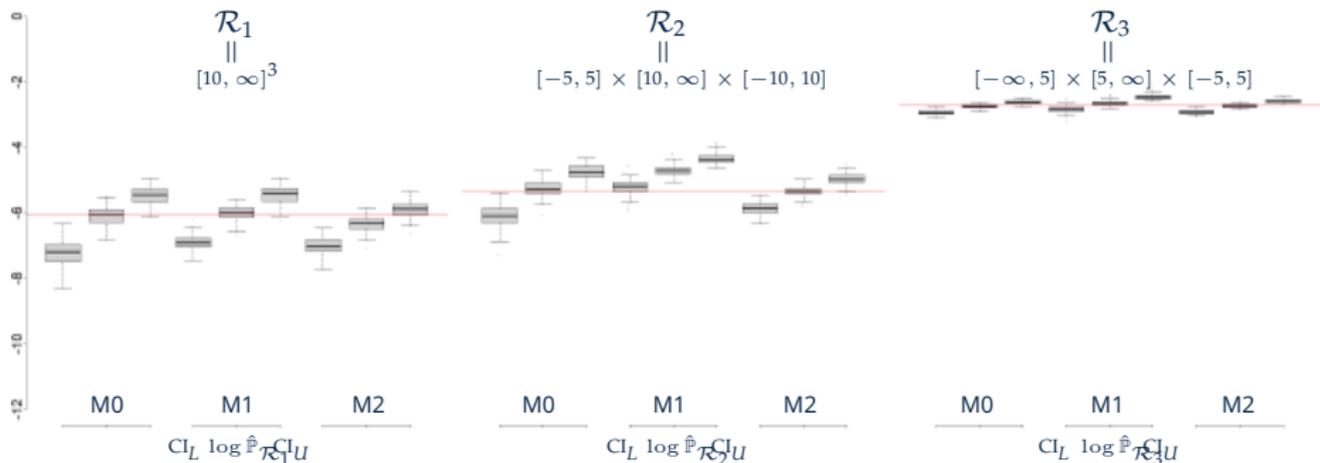
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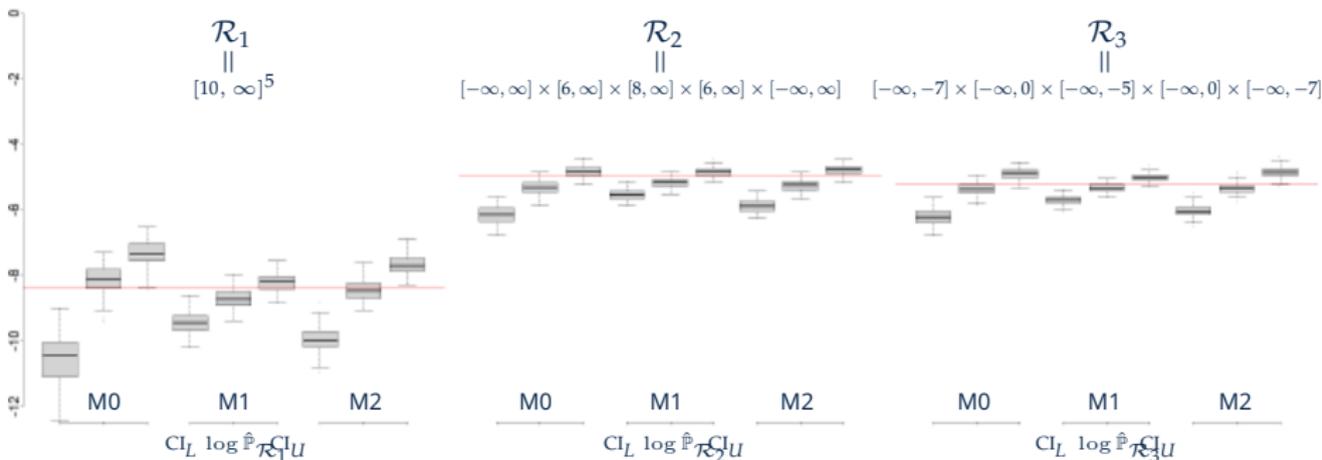
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Simulation study results – 3 dimensions



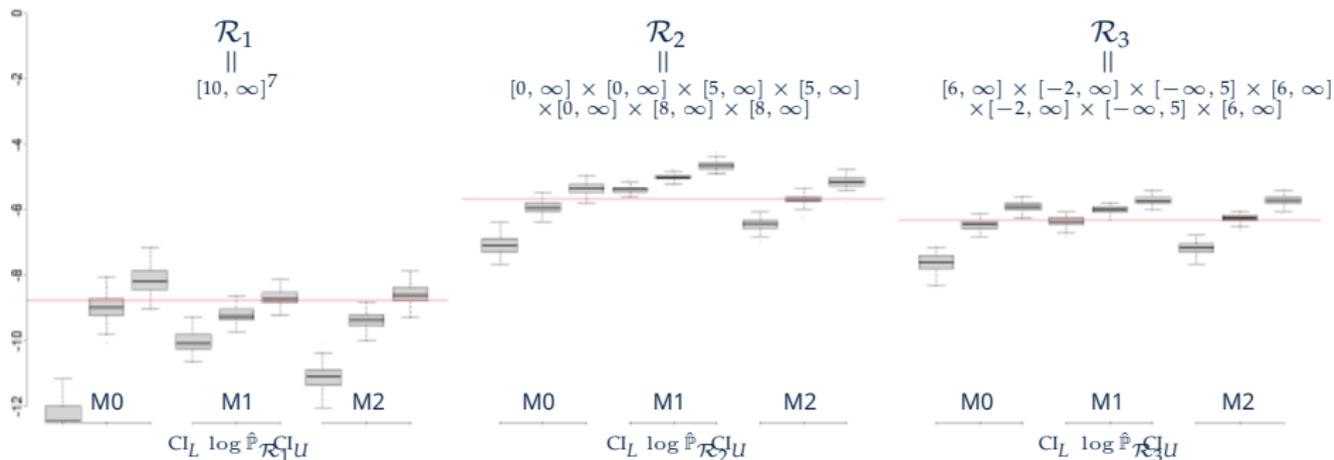
Boxplots of 100 estimated log-probabilities and associated lower- and upper-bounds of 95% bootstrap confidence intervals for the sets $\mathcal{R}_1, \mathcal{R}_2, \mathcal{R}_3 \in \mathbb{R}^3$. ($n = 10^4$).

Simulation study results – 5 dimensions



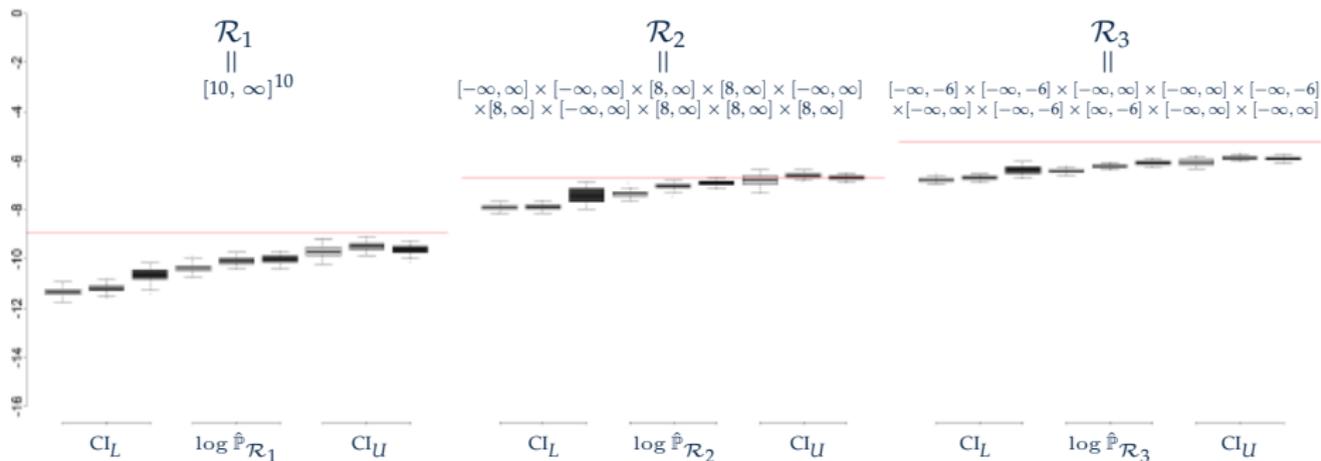
Boxplots of 100 estimated log-probabilities and associated lower- and upper-bounds of 95% bootstrap confidence intervals for the sets $\mathcal{R}_1, \mathcal{R}_2, \mathcal{R}_3 \in \mathbb{R}^5$. ($n = 10^4$).

Simulation study results – 7 dimensions



Boxplots of 100 estimated log-probabilities and associated lower- and upper-bounds of 95% bootstrap confidence intervals for the sets $\mathcal{R}_1, \mathcal{R}_2, \mathcal{R}_3 \in \mathbb{R}^7$. ($n = 10^4$).

Simulation study results – 10 dimensions

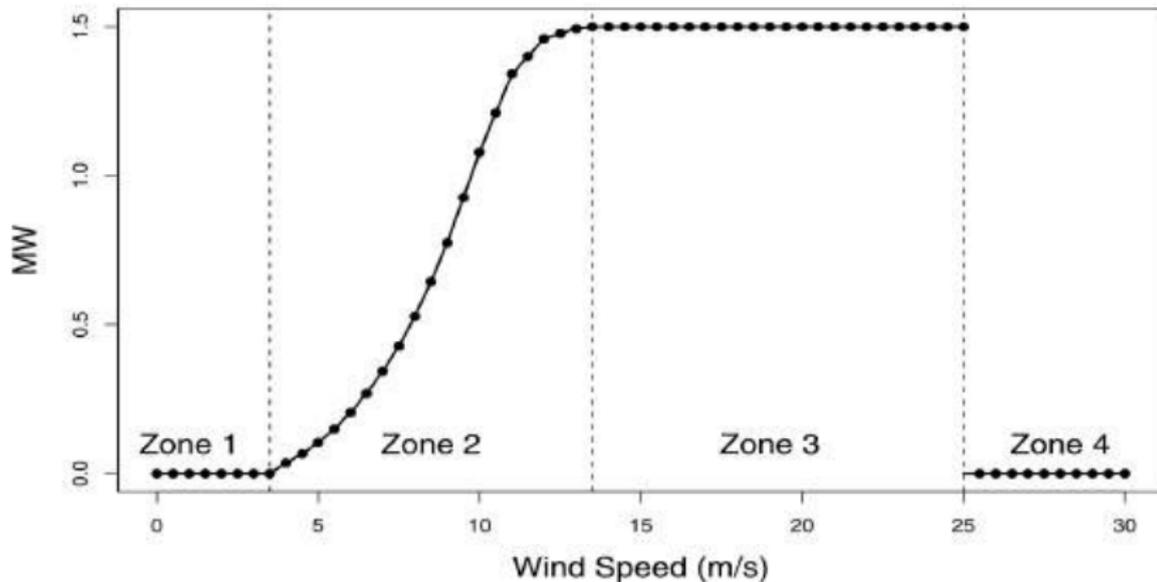


Boxplots of 100 estimated log-probabilities and associated lower- and upper-bounds of 95% bootstrap confidence intervals for the sets $\mathcal{R}_1, \mathcal{R}_2, \mathcal{R}_3 \in \mathbb{R}^{10}$. ($n = 5 \times 10^4, 10^5, 2 \times 10^5$).

LOW AND HIGH WIND SPEEDS

In relation to electricity production in the
Pacific Northwest, United States

GE 1.5 MW Power Curve



Scale-shape homogenisation

- Define the windspeed

$$X_{j,m,h}^o$$

at station j in month m of the year and hour h .

Scale-shape homogenisation

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- We assume¹

$$X_{j,m,h}^o \sim \text{Weibull}(\lambda_{j,m,h} = s_{j,1}(m) + s_{j,2}(h), \kappa_{j,m,h} = s_{j,3}(m) + s_{j,4}(h)), \quad (3)$$

where s denotes a cubic cyclic spline on $m \in \{1, \dots, 12\}$ or $h \in \{0, \dots, 23\}$.

¹Elliott et al. (2004)

Scale-shape homogenisation

- Define the windspeed

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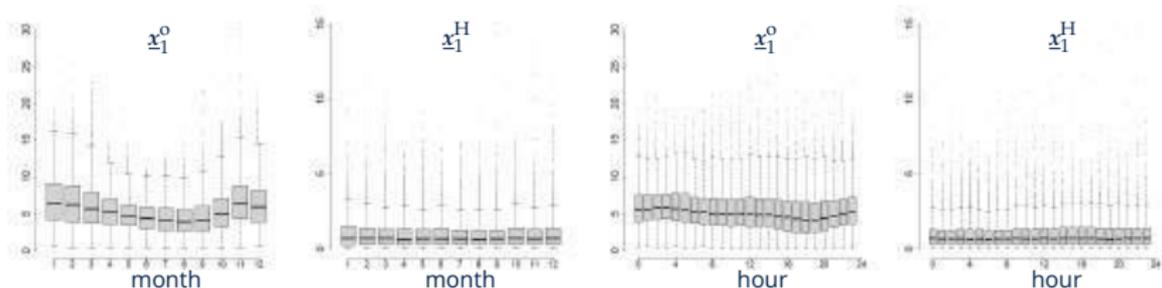
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where s denotes a cubic cyclic spline on $m \in \{1, \dots, 12\}$ or $h \in \{0, \dots, 23\}$.

- We fit the model using `evgam`² and apply $X_{j,m,h}^H := (X_{j,m,h}^o / \hat{\lambda}_{j,m,h})^{\hat{\kappa}_{j,m,h}}$



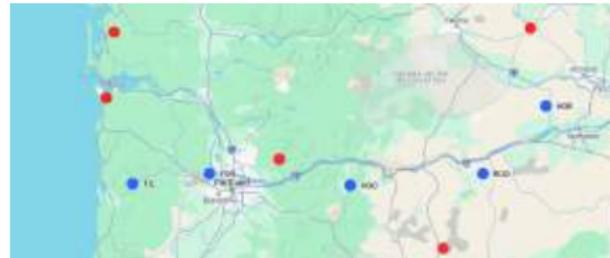
¹Elliott et al. (2004), ²Youngman (2022)

Analysis of station configurations – January at 18:00



(a) Minimises probability of no production

Analysis of station configurations – January at 18:00

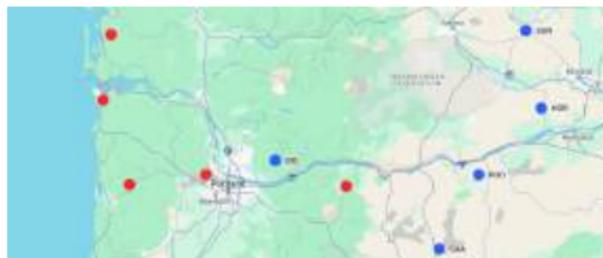


(a) Minimises probability of no production (b) Maximises probability of no production

Analysis of station configurations – January at 18:00

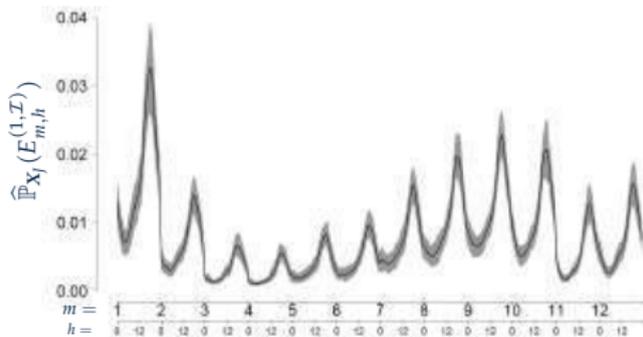


(a) Minimises probability of no production (b) Maximises probability of no production

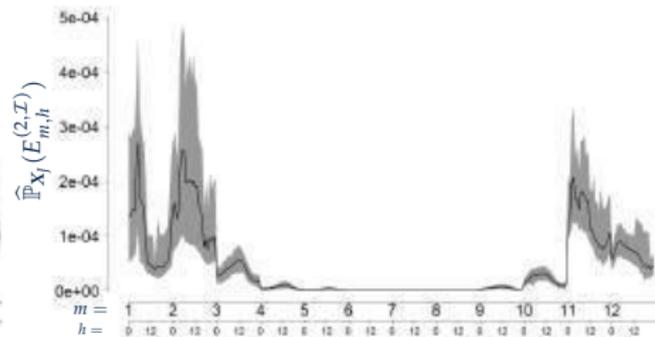


(c) Maximises probability of full production

Analysis of seasonality of power production – configuration (a)



Month m , Hour h



Month m , Hour h

Configuration (a): Minimises probability of no production

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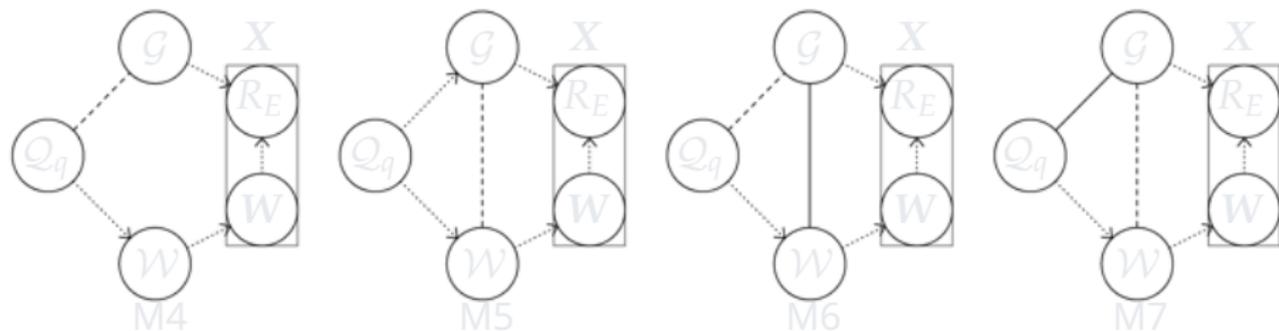
Proposed models

- We introduce a **deformation set** \mathcal{D} with radial function $f_{\mathcal{D}} : \mathbb{S}^{d-1} \rightarrow [0, \infty)$.
- We can then **weaken the equality assumptions** of models M1, M2, and M3 via

$$r_{Q_q}(w) = \beta_{qf} f_{\mathcal{D}}(w) f_G(w), \quad w \in \mathbb{S}^{d-1},$$

and

$$r_G(w) = \beta_G \{f_{\mathcal{D}}(w) f_W(w)\}^{1/d}, \quad w \in \mathbb{S}^{d-1},$$



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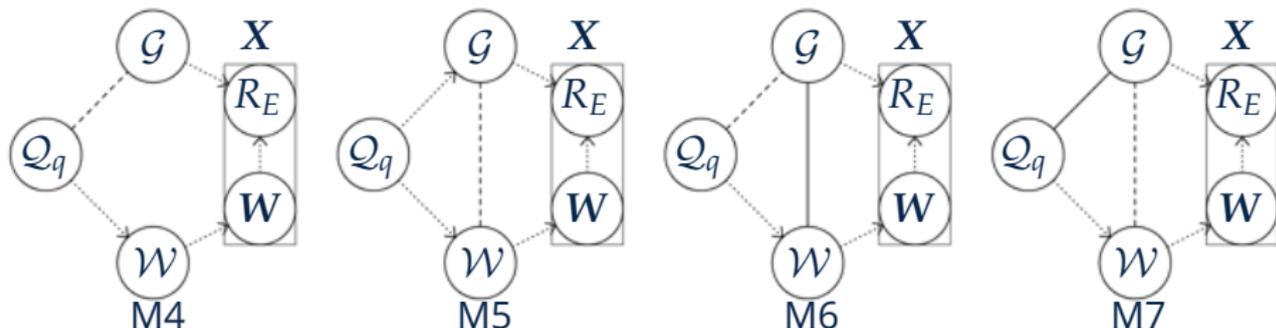
Proposed models

- We introduce a **deformation set** \mathcal{D} with radial function $f_{\mathcal{D}} : \mathbb{S}^{d-1} \rightarrow [0, \infty)$.
- We can then **weaken the equality assumptions** of models M1, M2, and M3 via

$$r_{Q_q}(w) = \beta_q f_{\mathcal{D}}(w) f_{\mathcal{G}}(w), \quad w \in \mathbb{S}^{d-1},$$

and

$$r_{\mathcal{G}}(w) = \beta_{\mathcal{G}} \{f_{\mathcal{D}}(w) f_{\mathcal{W}}(w)\}^{1/d}, \quad w \in \mathbb{S}^{d-1},$$



- Models M4 to M7 are identifiable as is, but I discuss this further in the next section if there are no questions!

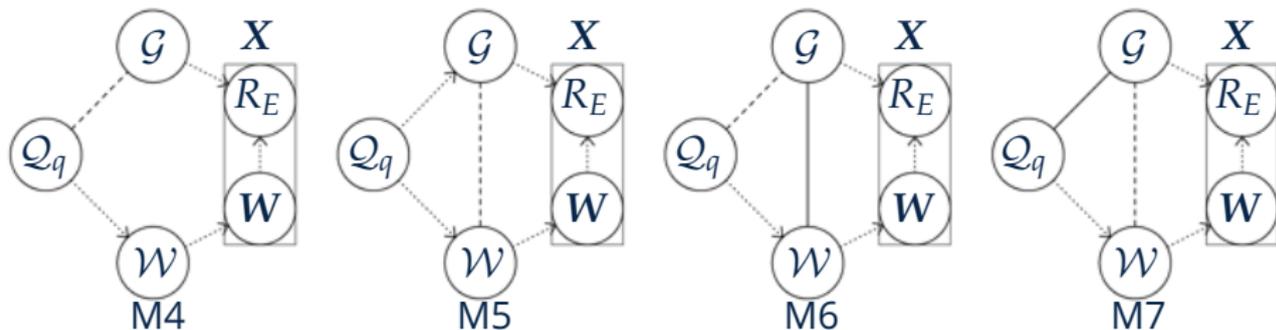
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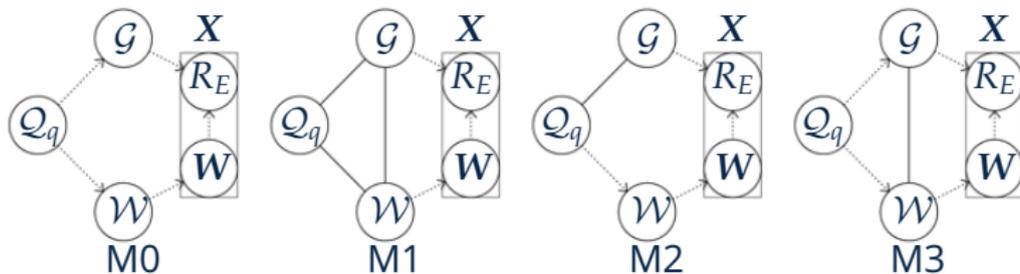
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Model fitting via loss minimisation

- Recall models M0 to M3:

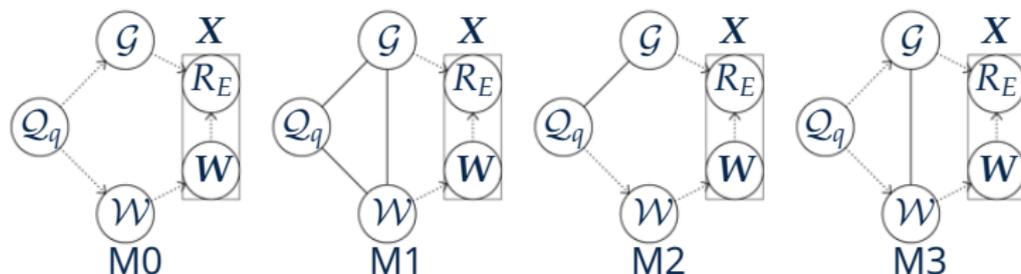


- Model M0 is fitted by sequentially minimising the losses
for Q_q .

$$L_{Q_q}(\theta_G, \theta_W, \theta) = \frac{1}{n} \sum_{i=1}^n \max \left\{ (1-\alpha) \left[|x_i| - \theta_G / \alpha, \left(\frac{x_i}{|x_i|} \right) \right], \alpha \left[|x_i| - \theta_W / \alpha, \left(\frac{x_i}{|x_i|} \right) \right] \right\}$$

Model fitting via loss minimisation

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$$\mathcal{L}_{Q_q}(\beta_{Q_q}, f_{Q_q}; \mathbf{x}) = \frac{1}{n} \sum_{i=1}^n \max \left\{ (1-q) \left[\|x_i\| - \beta_{Q_q} f_{Q_q} \left(\frac{x_i}{\|x_i\|} \right) \right], q \left[\|x_i\| - \beta_{Q_q} f_{Q_q} \left(\frac{x_i}{\|x_i\|} \right) \right] \right\}.$$

- for G :

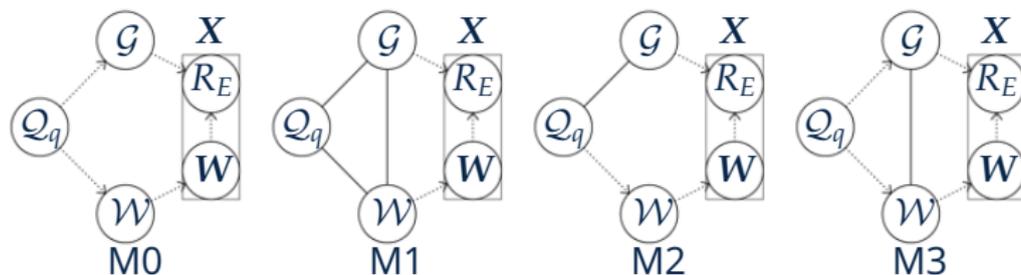
$$\mathcal{L}_G(\beta_G, f_G; r_{Q_q}, \mathbf{x}) = -\frac{1}{\#\mathcal{E}} \sum_{i \in \mathcal{E}} \log \left[\{\beta_G f_G(x_i / \|x_i\|)\}^{-1} \exp \left\{ -\frac{\|x_i\| - r_{Q_q}(x_i / \|x_i\|)}{\beta_G f_G(x_i / \|x_i\|)} \right\} \right].$$

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$$\mathcal{L}_W(f_W; r_{Q_q}, \mathbf{x}) = -\frac{1}{\#\mathcal{E}} \sum_{i \in \mathcal{E}} \log f_W(x_i / \|x_i\|).$$

Model fitting via loss minimisation

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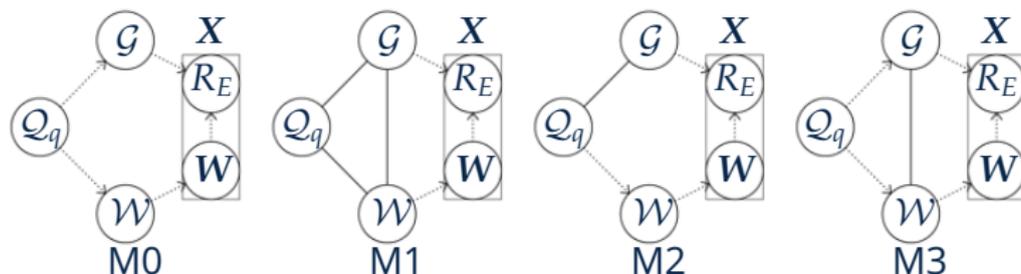
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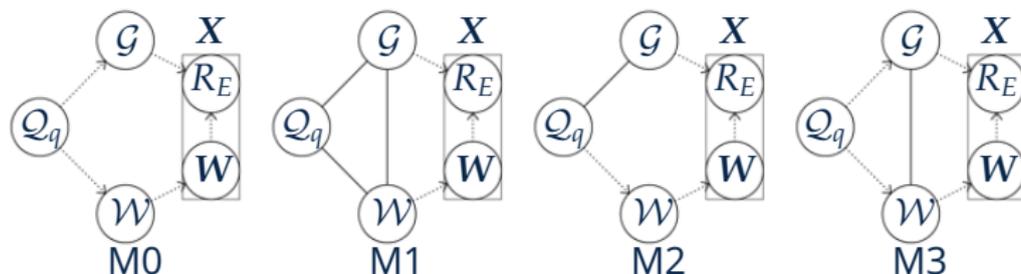
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Model fitting via loss minimisation

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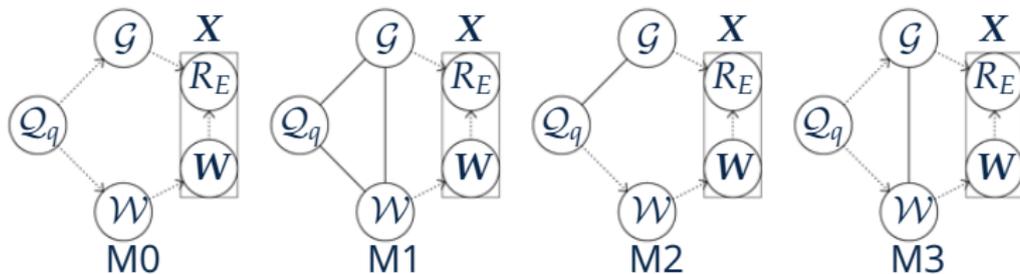
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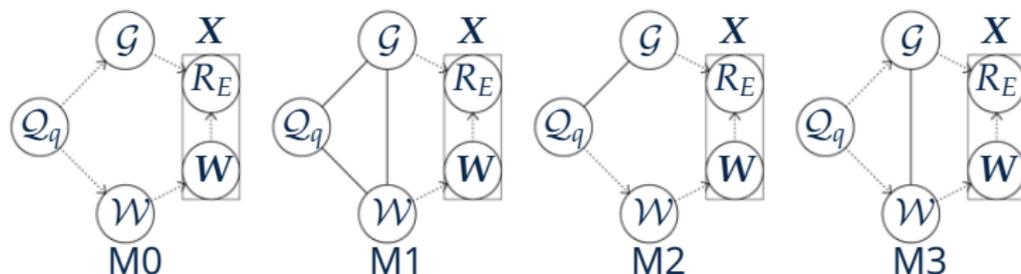
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- Model M1 is fitted by sequentially minimising the loss $\mathcal{L}_{Q_q, G, W}(\beta_{Q_q}, \beta_G, f_W; \underline{x}) = \mathcal{L}_{Q_q}(\beta_{Q_q}, f_W^{1/d}; \underline{x}) + \lambda[\mathcal{L}_G(\beta_G, f_W^{1/d}; \beta_{Q_q} f_W^{1/d}, \underline{x}) + \mathcal{L}_W(f_W; \beta_{Q_q} f_W^{1/d}, \underline{x})]$.
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- Comments on M2 and M3.

Model fitting via loss minimisation

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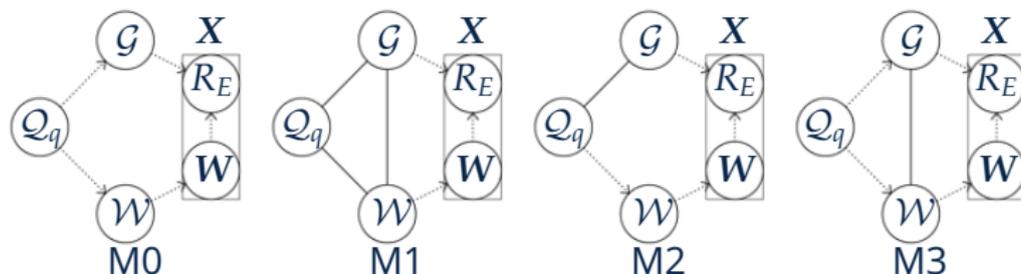
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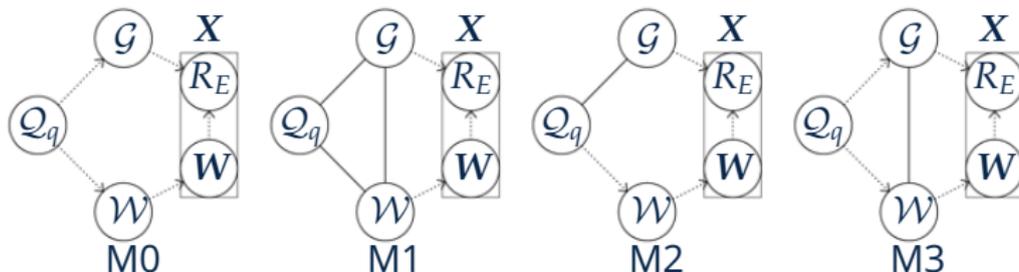
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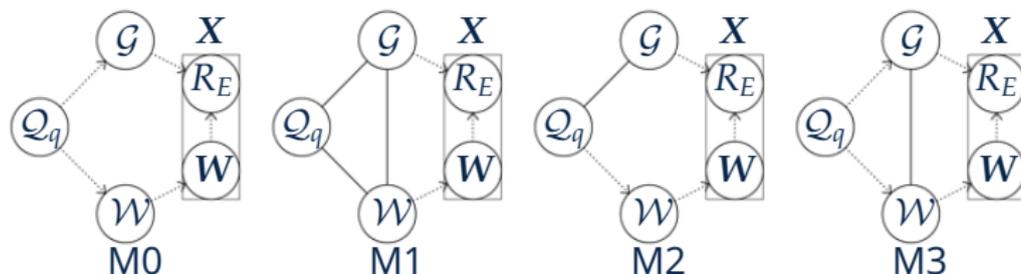
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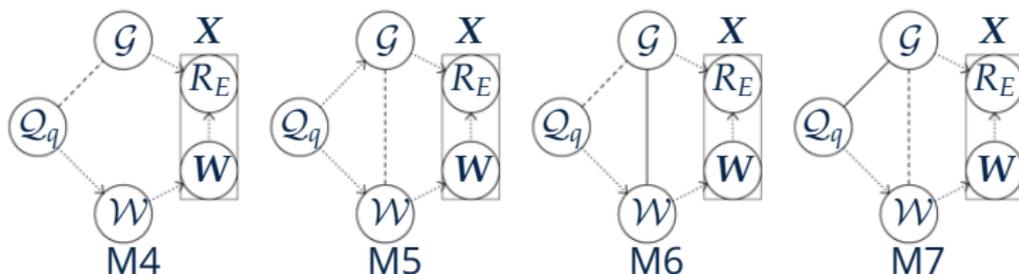
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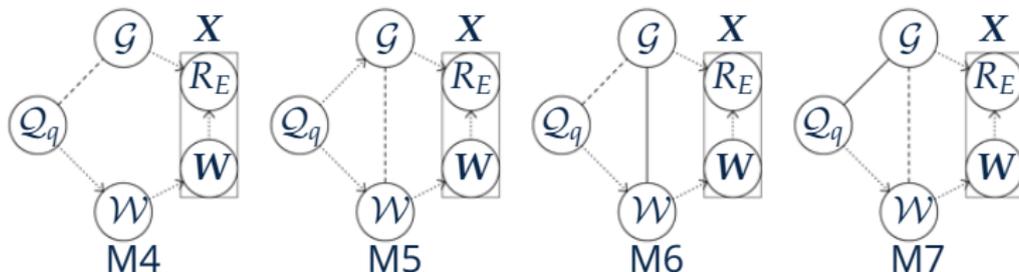
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- Model M4 to M7 require the same losses as their equivalent models with dashed edges replaced by solid edges.
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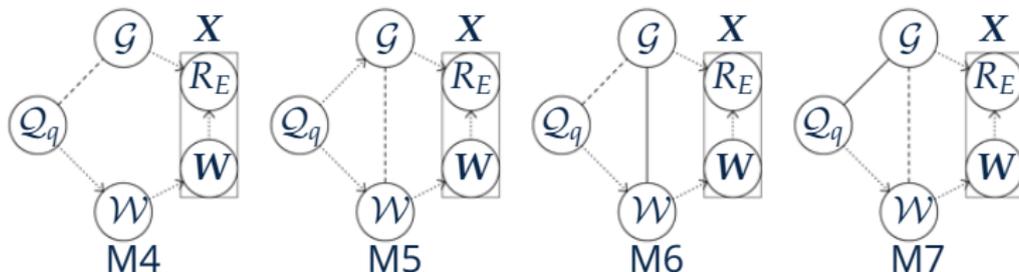
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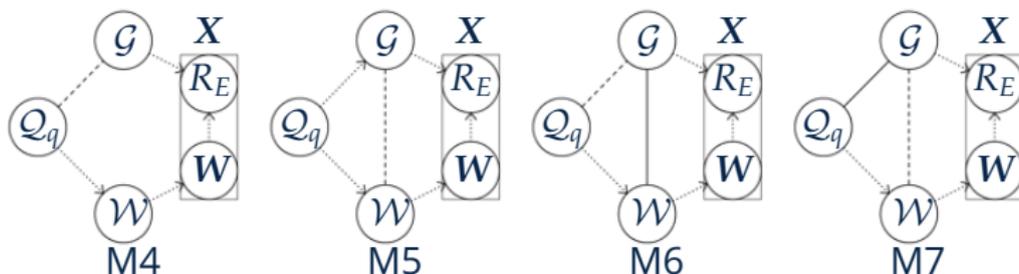
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Uniform-on- \mathbb{S}^{d-1} penalisation

- To devise the **uniform density on \mathbb{S}^{d-1}** , we consider $A_{d-1}(r)$ the hypervolume (or surface area) of the $(d-1)$ -sphere of radius r given by

$$A_{d-1}(r) = \frac{2\pi^{d/2}}{\Gamma(d/2)} r^{d-1}, \quad r \in (0, \infty),$$

where Γ denotes the gamma function.

- It follows that a PDF with uniform density on \mathbb{S}^{d-1} is given by

$$f_U(w) = 1/A_{d-1}(1)$$

for all $w \in \mathbb{S}^{d-1}$.

- Penalisation of $f_{\mathcal{D}}$ away from f_U can then be performed via the **Kullback-Leibler divergence** $D_{\text{KL}}[f_U||f_{\mathcal{D}}] = \int_{\mathbb{S}^{d-1}} \log[f_U(w)/f_{\mathcal{D}}(w)]f_U(w) dw$.
- In practice, this integral is approximated via **Monte Carlo integration** by sampling a large number m of directions u_1, \dots, u_m uniformly on \mathbb{S}^{d-1} and calculating

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Model assessment

- Under assumptions of uniform convergence on \mathbb{S}^{d-1} ,

$$F_{R|W} \left(\frac{R - r_{\mathcal{Q}_q^*}(W)}{r_{\mathcal{G}^*}(W)} \right)^{1/d} W \Big| \{R > r_{\mathcal{Q}_q^*}(W)\} \xrightarrow{d} \mathbf{u}_{B_1(0)}, \quad \text{as } q \rightarrow 1,$$

where $r_{\mathcal{Q}_q^*}$ and $r_{\mathcal{G}^*}$ are deterministic functions of $r_{\mathcal{Q}_q}$, $r_{\mathcal{G}}$, and f_W .

- We consider the stationary random point measure

$$P^* := \sum_{i=1}^n \delta \left[H_{W_i} \left(\frac{R_i - r_{\mathcal{Q}_q^*}(W_i)}{r_{\mathcal{G}^*}(W_i)} \right)^{1/d} W_i \right] \mathbb{1}_{R_i > r_{\mathcal{Q}_q^*}(W_i)}.$$

- We use an adapted version of the standard K -functions to assess if P^* is statistically distinguishable from a random point measure with constant intensity on $B_1(0)$.

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where $r_{\mathcal{Q}_q^*}$ and $r_{\mathcal{G}^*}$ are deterministic functions of $r_{\mathcal{Q}_q}$, $r_{\mathcal{G}}$, and f_W .

- We consider the stationary random point measure

$$P^* := \sum_{i=1}^n \delta \left[H_{\mathbf{W}_i} \left(\frac{R_i - r_{\mathcal{Q}_q^*}(\mathbf{W}_i)}{r_{\mathcal{G}^*}(\mathbf{W}_i)} \right)^{1/d} \mathbf{W}_i \right] \mathbb{1}_{R_i > r_{\mathcal{Q}_q^*}(\mathbf{W}_i)}.$$

- We use an adapted version of the standard K -functions to assess if P^* is statistically distinguishable from a random point measure with constant intensity on $B_1(\mathbf{0})$.

Model assessment – A random point measure approach

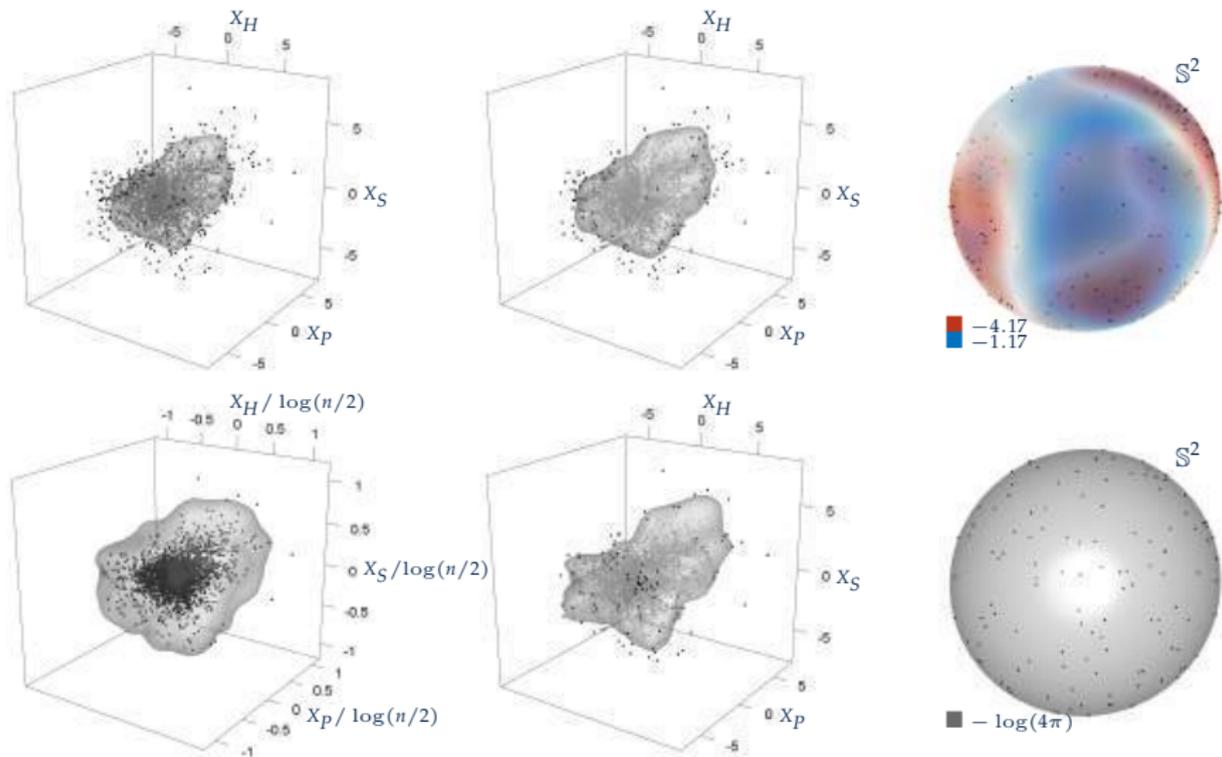


Figure from Papastathopoulos et al. (2023)

Model assessment – A random point measure approach

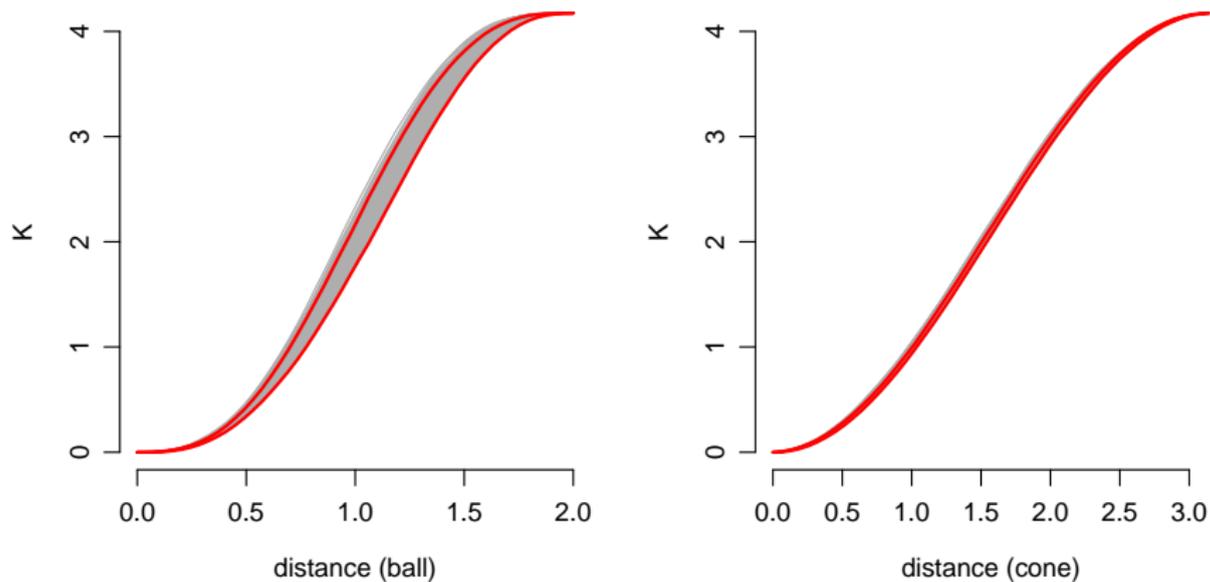


Figure from Papastathopoulos et al. (2023)