New developments for a geometric approach to multivariate extremal inference

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### Multivariate Extreme Value Theory (MEVT)

• Interested in  $Pr(\boldsymbol{X} \in B)$  for  $\boldsymbol{X} \in \mathbb{R}^d$ .



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- Interested in  $Pr(\boldsymbol{X} \in B)$  for  $\boldsymbol{X} \in \mathbb{R}^d$ .
- B not in range of data

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### MEVT: Multivariate Regular Variation

► Suppose 
$$\boldsymbol{X}_{E} = (X_{E,1}, \dots, X_{E,d})^{\top}$$
,  $X_{E,j} \sim \text{Exp}(1)$ .

▶ Perform *extrapolation*:  $Pr(\mathbf{X}_E \in B) \approx e^{-t} Pr(\mathbf{X}_E \in B - t)$ 

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- de Haan (1970), has drawbacks...



### 🖤 MEVT: Hidden Regular Variation

• Introduce  $\eta$  to correct tail decay.

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### MEVT: Hidden Regular Variation

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- ▶ Perform *extrapolation*:  $Pr(\mathbf{X}_{E} \in B) \approx e^{-t/\eta} Pr(\mathbf{X}_{E} \in B t)$
- Ledford and Tawn (1997), also has drawbacks...



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• Given 
$$\boldsymbol{X} = (X, Y)$$
, model  $Y|X > x$ , x large

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$$\boldsymbol{X} = (X, Y)$$
, model  $Y|X > x$ , x large

Heffernan and Tawn (2004)

Relies on false working assumption

$$\left. \frac{Y - lpha x}{x^{eta}} \right| X > x \sim \mathcal{N}(0, 1)$$

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- Complicated inference for d > 2.
- Doesn't capture complex dependence structures.
- Requires prior knowledge of dependence structure.



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### Timit sets and gauge functions

# ▶ $X_1, ..., X_n \stackrel{\text{iid}}{\sim} f_{X_E}$ , *d*-dimensional, Exponential(1) margins.

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### 🖤 Limit sets and gauge functions

X<sub>1</sub>,..., X<sub>n</sub> <sup>iid</sup> <sup>∼</sup> f<sub>X<sub>E</sub></sub>, d-dimensional, Exponential(1) margins.
 If not in Exponential(1) margins, can standardize using

$$egin{aligned} & X_{E,j} = F_E^{-1} \left( F_{X_j}(X_j) 
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► Scaled sample clouds \$\left\{\frac{\mathbf{X}\_1}{\log n}, \ldots, \frac{\mathbf{X}\_n}{\log n}\right\}\$ converge onto a limit set,  $G := \left\{\mathbf{x} \in \mathbb{R}^d \ \begin{smallmatrix} g(\mathbf{x}) \le 1 \right\}$$ 

as  $n \rightarrow \infty$  (Balkema and Nolde, 2010).

### Timit sets and gauge functions

► The gauge function, g : ℝ<sup>d</sup> → ℝ, is 1-homogeneous and is obtained through:

$$g(\mathbf{x}) = \lim_{t \to \infty} \frac{-\log f_{\mathbf{X}_E}(t\mathbf{x})}{t}$$

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Nolde (2014); Nolde and Wadsworth (2022) use g to describe extremal dependence properties.



$$f_{\mathsf{Gauss.}}(\boldsymbol{z}) = rac{1}{\sqrt{2\pi \left|\boldsymbol{\Sigma}
ight|}} \exp\left\{-rac{1}{2} \boldsymbol{z}^{ op} \boldsymbol{\Sigma}^{-1} \boldsymbol{z}
ight\}$$

$$g(\mathbf{x}) = \lim_{t \to \infty} \frac{-\log f_{\mathbf{X}_E}(t\mathbf{x})}{t}$$
$$= \left(\mathbf{x}^{1/2}\right)^\top \mathbf{\Sigma}^{-1} \mathbf{x}^{1/2}$$

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f=d=3 Gaussian,  $ho_{12}=0.5$ ,  $ho_{13}=0.2$ ,  $ho_{23}=0.8$ 

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$$f_{\mathsf{Fr\acute{e}chet}}(oldsymbol{z}) = \exp\left\{-\left(\sum_{j=1}^{d} z_{j}^{-1/ heta}
ight)^{ heta}
ight\}$$

$$g(\mathbf{x}) = \lim_{t \to \infty} \frac{-\log f_{\mathbf{X}_{\mathcal{E}}}(t\mathbf{x})}{t}$$
$$= \frac{1}{\theta} \sum_{j=1}^{d} x_j + \left(1 - \frac{d}{\theta}\right) \min\{x_1, \dots, x_d\}$$

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d = 2 Logistic,  $\theta = 0.5$ 



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d = 2 Logistic,  $\theta = 0.5$ 



# Texample: Asymmetric logistic

Let 
$$\mathcal{D} = \{1, \ldots, d\}$$
 and  $P(\mathcal{D}) =$  power set of  $\mathcal{D}$ .

$$f_{\mathsf{Gumbel}}(\boldsymbol{z}) = \exp\left\{-\sum_{\boldsymbol{c}\in P(\mathcal{D})}\gamma_{\boldsymbol{c}}\left(\sum_{j=1}^{d}z_{j}^{-1/\theta_{\boldsymbol{c}}}\right)^{\theta_{\boldsymbol{c}}}
ight\}$$

$$g(\mathbf{x}) = \lim_{t \to \infty} \frac{-\log f_{\mathbf{X}_E}(t\mathbf{x})}{t}$$
  
= very complicated!

# 🗑 Example: Asymmetric logistic

• Example:  $\gamma_{\{1,...,d\}} = 1$ ,  $\gamma_c = 0$  otherwise.

$$g(\mathbf{x}) = \frac{1}{\theta_{\{1,...,d\}}} \sum_{j=1}^{d} x_j + \left(1 - \frac{d}{\theta_{\{1,...,d\}}}\right) \min\{x_1,\ldots,x_d\}$$

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# $\bigcirc d = 3$ Asymmetric logistic, variables $\{1, 2, 3\}$ large

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# Texample: Asymmetric logistic

• **Example:** 
$$\gamma_{\{1,2\}} = 1$$
,  $\gamma_{\{2,3\}} = 1$ ,  $\gamma_c = 0$  otherwise.

$$g(\mathbf{x}) = \min\left\{\frac{x_1 + x_2}{\theta_{\{1,2\}}} + \frac{x_3}{\theta_{\{2,3\}}} + \left(1 - \frac{2}{\theta_{\{1,2\}}}\right)\min(x_1, x_2) + \left(1 - \frac{1}{\theta_{\{2,3\}}}\right)\min(x_2, x_3), \\ \frac{x_2 + x_3}{\theta_{\{2,3\}}} + \frac{x_1}{\theta_{\{1,2\}}} + \left(1 - \frac{2}{\theta_{\{2,3\}}}\right)\min(x_2, x_3) + \left(1 - \frac{1}{\theta_{\{1,2\}}}\right)\min(x_1, x_2)\right\}$$

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d = 3 Asymmetric logistic, variables  $\{1, 2\}$  and  $\{2, 3\}$  large

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# How can we estimate *g* from data and use it for extremal statistical inference?



Consider

R

$$egin{aligned} &= \|oldsymbol{\mathcal{X}}_{\mathcal{E}}\|_1 \ &= \sum_{j=1}^d oldsymbol{\mathcal{X}}_{\mathcal{E},j} \end{aligned}$$

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Consider

$$R = \|\boldsymbol{X}_{E}\|_{1}$$
$$= \sum_{j=1}^{d} \boldsymbol{X}_{E,j}$$

$$\boldsymbol{W} = \boldsymbol{X}_{E} / \left\| \boldsymbol{X}_{E} \right\|_{1}$$

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 $r_q(oldsymbol{W}) = q^{ ext{th}}$  quantile of R given angle  $oldsymbol{W}$ 

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• Note that  $X_E = RW$ 

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$$R \in \mathbb{R}_+$$

$$oldsymbol{W}\in\mathcal{S}_{d-1}=\left\{oldsymbol{x}\in\mathbb{R}^d\ :\ \sum_{j=1}^d|x_j|=1
ight\}$$

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$$\lim_{t\to\infty}\frac{-\log f_{\boldsymbol{X}_E}(t\boldsymbol{x})}{t}=g(\boldsymbol{x})$$

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$$egin{aligned} -\log f_{oldsymbol{X}_E}(toldsymbol{x}) &\sim tg(oldsymbol{x}) \quad ; \quad t o \infty \ &= tg(oldsymbol{x}) \left[1+o(1)
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$$f_{\boldsymbol{X}_{E}}(t\boldsymbol{x}) = e^{-tg(\boldsymbol{x})[1+o(1)]}$$

$$f_{\boldsymbol{X}_E}(r\boldsymbol{w}) = e^{-rg(\boldsymbol{w})[1+o(1)]}$$

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$$f_{R,\boldsymbol{W}}(r,\boldsymbol{w}) = |\nabla r\boldsymbol{w}| f_{\boldsymbol{X}_{E}}(r\boldsymbol{w})$$
$$= r^{d-1} e^{-rg(\boldsymbol{w})[1+o(1)]}$$

$$f_{R|\boldsymbol{W}}(r \mid \boldsymbol{w}) = f_{R,\boldsymbol{W}}(r,\boldsymbol{w}) / f_{\boldsymbol{W}}(\boldsymbol{w})$$
$$\propto r^{d-1} e^{-rg(\boldsymbol{w})[1+o(1)]}$$

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$$f_{ ext{truncGamma}}\left(r\mid oldsymbol{w}
ight) = egin{camma}{c} rac{f_{ ext{Gamma}}\left(r;lpha,g(oldsymbol{w}; heta)
ight)}{ar{F}_{ ext{Gamma}}\left(r_q(oldsymbol{w});lpha,g(oldsymbol{w}; heta)
ight)} & ext{; } r > r_q(oldsymbol{w}) \ 0 & ext{; } r \leq r_q(oldsymbol{w}) \end{cases}$$







▶ Interested in when  $R \mid \{ \boldsymbol{W} = \boldsymbol{w} \}$  is large, or  $R > r_q(\boldsymbol{W})$ 



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Parametric approach: model fitting

Fit the model

 $R \mid \{\boldsymbol{W} = \boldsymbol{w}, R > r_q(\boldsymbol{W})\} \sim \mathsf{truncGamma}(\alpha, g(\boldsymbol{w}; \boldsymbol{\theta}))$ 

by maximizing

$$L(\alpha, \theta \mid r_{1:n}, \boldsymbol{w}_{1:n}) = \prod_{i:r_i > r_q(\boldsymbol{w}_i)} \frac{f_{\mathsf{Gamma}}(r_i; \alpha, g(\boldsymbol{w}_i; \theta))}{\bar{F}_{\mathsf{Gamma}}(r_q(\boldsymbol{w}_i); \alpha, g(\boldsymbol{w}_i; \theta))}$$

for different parametric choices of g.

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for different parametric choices of g.

Select best model using AIC.

Can estimate extremal probabilities via

 $\Pr(\boldsymbol{X} \in B) = \Pr(\boldsymbol{X} \in B | R > r_q(\boldsymbol{W})) \Pr(R > r_q(\boldsymbol{W}))$ 

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• Compute  $\Pr(R > r_q(W))$  empirically.

Can estimate extremal probabilities via

$$\Pr{(\boldsymbol{X} \in B)} = \Pr{(\boldsymbol{X} \in B | R > r_q(\boldsymbol{W}))} \Pr{(R > r_q(\boldsymbol{W}))}$$

- Compute  $\Pr(R > r_q(W))$  empirically.
- Compute  $\Pr(\mathbf{X} \in B | R > r_q(\mathbf{W}))$  via sampling:
  - 1. generate  $\boldsymbol{w}_1, \ldots, \boldsymbol{w}_N$
  - **2**. generate  $r_i$  from truncGamma $(\hat{\alpha}, g(\boldsymbol{w}_i; \hat{\boldsymbol{\theta}}))$  for  $i = 1, \dots, N$

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3. return  $x_i = r_i w_i$ , i = 1, ..., N



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The provided a set of the set of

- North Kensington site, London, UK
- carbon monoxide (CO, mg/m<sup>3</sup>), nitrogen dioxide (NO<sub>2</sub>, μg/m<sup>3</sup>), and particles with a diameter of 10 μm or less (PM10, mg/m<sup>3</sup>).
- n = 5,584 daily maximum measurements, October–April. 1996–2024.

The point of the pollution measurements (d = 3)

- North Kensington site, London, UK
- ► carbon monoxide (CO, mg/ $m^3$ ), nitrogen dioxide (NO<sub>2</sub>,  $\mu$ g/ $m^3$ ), and particles with a diameter of 10  $\mu$ m or less (PM10, mg/ $m^3$ ).
- n = 5,584 daily maximum measurements, October-April. 1996–2024.
- Evidence (Simpson et al., 2020) that PM10 is large when CO and NO<sub>2</sub> are small, and that all three grow large together.

## The provided a set of the pollution measurements (d = 3)

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# The product of the pollution measurements (d = 3)



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# The product of the pollution measurements (d = 3)



### Final Application to air pollution measurements (d = 3)

A commonly-used measure of extremal dependence is

$$\chi_{c}(u) = \left(\frac{1}{1-u}\right) \Pr\left[F_{E}\left(X_{j}\right) > u \,\forall j \in c \subseteq \{1,2,3\}\right]$$

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for u close to 1.

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for u close to 1.

• 
$$\chi_{12}(u) = \Pr(F_E(X_2) > u | F_E(X_1) > u)$$

• 
$$\chi_{13}(u) = \Pr(F_E(X_3) > u | F_E(X_1) > u)$$

• 
$$\chi_{23}(u) = \Pr(F_E(X_3) > u | F_E(X_2) > u)$$

•  $\chi_{123}(u) = \Pr(F_E(X_2) > u, F_E(X_3) > u | F_E(X_1) > u)$ 





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- A "rough sketch" on how to perform geometric multivariate extremal inference.
- Statistical inference for multivariate tails for any dependence structure.

- Comparable (and sometimes outperforms) conditional extremes.
- Simple inference.

### Parametric approach

Parametric models are too rigid for real-data examples, and mixing gauges is slow.

- Parameter estimation and sampling is slow when  $d \ge 3$ .
- Re-sampling exceedance angles with replacement is undesirable when d > 3, would like a model for
  W | {R > r<sub>q</sub>(W)}

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- Re-sampling exceedance angles with replacement is undesirable when d > 3, would like a model for W | {R > r<sub>q</sub>(W)}
- Current quantile regression approaches are only suitable for d = 2, 3.
- ▶ Ultimate goal is for a fast and accurate model when *d* = 4, 5, 6, ...



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For d = 2...

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For d = 2...

▶ Define a set of *N* reference angles  $w^{*1}, \ldots, w^{*N} \in [0, 1]$ .

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For d = 2...

- ▶ Define a set of *N* reference angles  $w^{\star 1}, \ldots, w^{\star N} \in [0, 1]$ .
- ▶ Results in N-1 regions:  $[w^{\star 1}, w^{\star 2}], \ldots, [w^{\star N-1}, w^{\star N}].$

For d = 2...

- ▶ Define a set of *N* reference angles  $w^{\star 1}, \ldots, w^{\star N} \in [0, 1]$ .
- ▶ Results in N-1 regions:  $[w^{\star 1}, w^{\star 2}], \ldots, [w^{\star N-1}, w^{\star N}].$
- At each w<sup>\*k</sup>, define a parameter θ<sub>k</sub> > 0 such that θ<sub>i</sub>(w<sup>\*k</sup>, 1 − w<sup>\*k</sup>)<sup>⊤</sup> lies on the boundary of the limit set.

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- Linear interpolation between neighbouring points points.
- At a point  $(x_1, x_2)^{\top}$ , the gauge function value is given by

$$g(x_1, x_2; \theta) = \sum_{k=1}^{N-1} \mathbf{1}_{(w^{\star k}, w^{\star k+1})} \left( \frac{x_1}{x_1 + x_2} \right) \\ \times \frac{\left[ \theta_k (1 - w^{\star k}) - \theta_{k+1} (1 - w^{\star k+1}) \right] x_1 - \left[ \theta_k w^{\star k} - \theta_{k+1} w^{\star k+1} \right] x_2}{\left[ \theta_k (1 - w^{\star k}) - \theta_{k+1} (1 - w^{\star k+1}) \right] \theta_k w^{\star k} - \left[ \theta_k w^{\star k} - \theta_{k+1} w^{\star k+1} \right] \theta_k (1 - w^{\star k})}$$



In *d*-dimensions...



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• Results in *M* regions:  $\triangle^{(1)}, \triangle^{(2)}, \dots, \triangle^{(M)}$ .

In d-dimensions...

- Define a set of N reference angles  $\boldsymbol{w}^{\star 1}, \ldots, \boldsymbol{w}^{\star N} \in \mathcal{S}_{d-1}$ .
- Results in *M* regions:  $\triangle^{(1)}, \triangle^{(2)}, \dots, \triangle^{(M)}$ .
- Region  $\triangle^{(k)}$  has d vertices:  $\theta_1^{(k)} \boldsymbol{w}^{\star(k),1}, \dots, \theta_d^{(k)} \boldsymbol{w}^{\star(k),d}$

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- Region  $\triangle^{(k)}$  has d vertices:  $\theta_1^{(k)} \boldsymbol{w}^{\star(k),1}, \dots, \theta_d^{(k)} \boldsymbol{w}^{\star(k),d}$
- At a point  $\boldsymbol{x}$ , the gauge function value is given by

$$g(\boldsymbol{x};\boldsymbol{\theta}) = \sum_{k=1}^{M} \mathbf{1}_{\triangle^{(k)}} \left( \boldsymbol{x} / \|\boldsymbol{x}\| \right) \frac{\boldsymbol{n}^{(k)\top} \boldsymbol{x}}{\boldsymbol{n}^{(k)\top} \theta_1^{(k)} \boldsymbol{w}^{\star(k),1}}$$

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**Problem:** *N* large leads to variability in MLEs  $\hat{\theta}$ .

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- **Problem:** *N* large leads to variability in MLEs  $\hat{\theta}$ .
- **Solution:** Penalise the gradients during model fitting:

$$\widehat{\boldsymbol{\theta}} = \underset{\boldsymbol{\theta} \in \mathbb{R}^{d}_{+}}{\operatorname{argmin}} - \log L(\boldsymbol{\theta} \mid \boldsymbol{r}_{1:n}, \boldsymbol{w}_{1:m}) + \lambda \sum_{(i,j) \in \mathcal{I}} \left\| \nabla g_{\boldsymbol{\theta}}^{(i)} - \nabla g_{\boldsymbol{\theta}}^{(j)} \right\|_{2}^{2}$$

 $\lambda \geq 0.$ 



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# Air pollution revisited





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- Lack of a unified approach for multivariate extremal inference.
- Geometric approach tackles problems with difficult dependence structures.
- Wadsworth and Campbell (2024) is first to use the geometric approach for statistical inference.
- ► The parametric approach works well in d = 2, 3, is okay when d = 4, hasn't been tested for d ≥ 5.
- Campbell and Wadsworth (???) can scale up to d = 5, 6, 7, ...

We also have improved modelling the angles and quantile estimation!

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