

# Learning extremal graphical models in high dimensions

Sebastian Engelke<sup>1</sup>   **Michaël Lalancette**<sup>2</sup>   Stanislav Volgushev<sup>2</sup>

<sup>1</sup>Research Center for Statistics, University of Geneva

<sup>2</sup>Department of Statistical Sciences, University of Toronto

SSC annual meeting, June 3, 2022

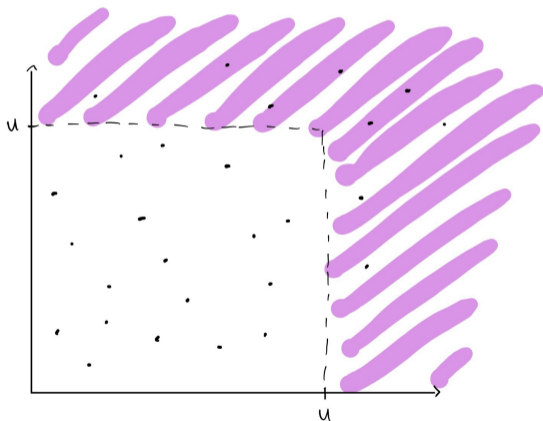


# Tail (or extremal) dependence

- Random vector  $\mathbf{X} \in \mathbb{R}^d$
- Tail dependence can be defined as the dependence structure of  $\mathbf{X}$  in extreme regions/conditional on an extreme event
- Extreme events:

$$\{X_1 > u\} \quad \text{or} \quad \{\max X_i > u\} \quad \text{or} \quad \{\min X_i > u\}$$

# Tail dependence: illustration



# Multivariate Pareto distributions

- Suppose that

$$\mathbb{P}(F(\mathbf{X}) \leq 1 - q/x \mid \max_i F_i(X_i) > 1 - q) \longrightarrow \mathbb{P}(\mathbf{Y} \leq \mathbf{x}), \quad q \downarrow 0,$$

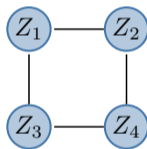
where  $F(\mathbf{X}) := (F_1(X_1), \dots, F_d(X_d))$

- “Given that at least one component of  $\mathbf{X}$  exceeds its  $(1 - q)$ th quantile,  $q/(1 - F(\mathbf{X})) \approx \mathbf{Y}$  in distribution”
- Then the random vector  $\mathbf{Y} \in \mathbb{R}^d$  satisfies
  1.  $\mathbf{Y} \in \mathcal{L} := \{\mathbf{y} \geq 0 : \|\mathbf{y}\|_\infty > 1\}$
  2.  $\mathbb{P}(Y_1 > 1) = \dots = \mathbb{P}(Y_d > 1)$
  3. For  $A \subset \mathcal{L}$  and  $t \geq 1$ ,  $\mathbb{P}(\mathbf{Y} \in tA) = t^{-1}\mathbb{P}(\mathbf{Y} \in A)$
- $\mathbf{Y}$  is *multivariate Pareto* (MP)
- $\mathbf{X}$  is in the *domain of attraction* of  $\mathbf{Y}$

# Graphical models

- $\mathbf{Z} = (Z_1, \dots, Z_d) \in \mathbb{R}^d$  a random vector indexed by  $V := \{1, \dots, d\}$

- $G := (V, E)$  an undirected graph
- $\mathbf{Z}$  is a graphical model on  $G$  if for each pair  $(i, j)$ ,



$$Z_i \perp Z_j \mid \mathbf{Z}_{\setminus\{i,j\}} \iff (i, j) \notin E$$

- Why this is important: if  $\mathbf{Z}$  has a positive density/mass on a product space, its density/mass can be factorized over the *cliques* of  $G$
- Requires knowledge of the graph  $\implies$  Learning graphical models

# Gaussian graphical models

- If  $\mathbf{Z} \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ ,  $\Theta := \boldsymbol{\Sigma}^{-1}$ ,

$$Z_i \perp Z_j \mid \mathbf{Z}_{\setminus\{i,j\}} \iff \Theta_{ij} = 0$$

- Graph structure is entirely encoded into the zero pattern of  $\Theta$
- Sparse estimation of  $\Theta \implies$  Estimation of  $G$

# Sparse estimation of precision matrices

- Easy to estimate the covariance matrix  $\Sigma$  by the sample covariance  $\hat{\Sigma}$
- But if  $n < d$ ,  $\hat{\Sigma}^{-1}$  does not exist (certainly not sparse)
- Many algorithms turn an estimate of  $\Sigma$  into an estimate of the zero pattern of  $\Sigma^{-1}$ :

$$\mathcal{A}(\hat{\Sigma}) = \hat{\mathbb{1}}\{\Theta \neq 0\}$$

- Call  $\mathcal{A}$  a *base learner*
- Examples:
  - Neighborhood selection (Meinshausen & Bühlmann, 2006, Ann. Stat.)
  - Graphical lasso (Yuan & Lin, 2007, Biometrika)

# This talk

1. Do graphical models make sense for MP distributions?

Yes, but need a different notion of conditional independence

2. Given data from  $\mathbf{X}$  in the domain of attraction  $\mathbf{Y}$ , can we learn the graph structure of  $\mathbf{Y}$ ?

Yes, for a certain parametric model



# Extremal graphical models

- $\mathbf{Y} = (Y_1, \dots, Y_d)$  a MP indexed by  $V := \{1, \dots, d\}$  with positive density
- Support  $\neq$  product space
- We say that  $Y_i \perp_e Y_j \mid \mathbf{Y}_{\setminus\{i,j\}}$  if for some  $m \notin \{i,j\}$ ,

$$Y_i \perp Y_j \mid \{\mathbf{Y}_{\setminus\{i,j\}}, Y_m > 1\}$$

- $G := (V, E)$  an undirected graph
- $\mathbf{Y}$  is an *extremal graphical model* on  $G$  if for each pair  $(i, j)$ ,

$$Y_i \perp_e Y_j \mid \mathbf{Y}_{\setminus\{i,j\}} \iff (i, j) \notin E$$

- Engelke & Hitz (2020, JRSSB) show that this definition leads to density factorization

# Hüsler–Reiss distributions

- A family of MP distributions, parametrized by an extremal variogram matrix  $\Gamma \in \mathbb{R}^{d \times d}$

- If  $\mathbf{Y} \sim \text{HR}(\Gamma)$ ,

$$\Gamma_{ij} = \mathbb{V}\text{ar}(\log Y_i - \log Y_j \mid Y_m > 1)$$

- Density: complicated function of  $\Gamma$

# Estimating Hüsler–Reiss distributions: the empirical variogram

- $\mathbf{X}$  in the domain of attraction of  $\mathbf{Y} \sim \text{HR}(\Gamma)$ , iid data  $\mathbf{X}_1, \dots, \mathbf{X}_n \sim \mathbf{X}$
- For  $m \in V$ , estimate  $\Gamma_{ij}$  by

$$\widehat{\Gamma}_{ij}^{(m)} := \widehat{\text{Var}}\left(\log(1 - \widetilde{F}_i(X_{ti})) - \log(1 - \widetilde{F}_j(X_{tj})) \mid \widetilde{F}_m(X_{tm}) > 1 - k/n\right),$$

where  $k$  large,  $k/n$  small,  $\widetilde{F}_i$  are empirical df

- $\widehat{\Gamma} := d^{-1} \sum_{m=1}^d \widehat{\Gamma}^{(m)}$

## Theorem (Engelke, L. & Volgushev, 2021)

*Under (mild) assumptions, with probability at least  $1 - \delta$ ,*

$$\|\widehat{\Gamma} - \Gamma\|_{\infty} \lesssim \left(\frac{k}{n}\right)^{\xi} (\log(n/k))^2 + \sqrt{\frac{\log d + \log \frac{1}{\delta}}{k}}.$$

# HR graphical models

- If  $\mathbf{Y} \sim \text{HR}(\Gamma)$ , Engelke & Hitz (2020, JRSSB) find that for  $m \notin \{i, j\}$ ,

$$Y_i \perp_e Y_j \mid \mathbf{Y}_{\setminus\{i,j\}} \iff \Theta_{ij}^{(m)} = 0,$$

where  $\Theta^{(m)}$  is the (pseudo)inverse of

$$\Sigma^{(m)} := (\Gamma_{im} + \Gamma_{jm} - \Gamma_{ij})_{i,j \in V}, \quad m \in V$$

- Extremal graph structure is encoded into the zero pattern of the matrices  $\Theta^{(m)}$
- Estimate the sparsity pattern of the  $\Theta^{(m)}$  and combine them through majority voting

# EGlearn: learning HR graphical models

- For  $m \in V$ ,

1. Compute

$$\widehat{\Sigma}^{(m)} := (\widehat{\Gamma}_{im} + \widehat{\Gamma}_{jm} - \widehat{\Gamma}_{ij})_{i,j \in V}, \quad m \in V$$

2. Throw  $\widehat{\Sigma}^{(m)}$  into a base learner  $\mathcal{A}$  to obtain a sparse estimate  $\widehat{\mathbf{1}}\{\Theta^{(m)} \neq 0\}$

- For each pair  $(i, j)$ , add an edge to  $\widehat{E}$  if and only if

$$\frac{1}{d-2} \# \left\{ m \in V \setminus \{i, j\} : \widehat{\mathbf{1}}\{\Theta_{ij}^{(m)} \neq 0\} = 1 \right\} > \frac{1}{2}$$

- Graph estimate  $\widehat{G} := (V, \widehat{E})$

# EGlearn: illustration

$$\begin{pmatrix} \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 0 & 1 \\ \cdot & 0 & \cdot & 1 \\ \cdot & 1 & 1 & \cdot \end{pmatrix} \quad \begin{pmatrix} \cdot & \cdot & 1 & 1 \\ \cdot & \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot & 1 \\ 1 & \cdot & 1 & \cdot \end{pmatrix} \quad \begin{pmatrix} \cdot & 1 & \cdot & 0 \\ 1 & \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot & \cdot \\ 0 & 1 & \cdot & \cdot \end{pmatrix} \quad \begin{pmatrix} \cdot & 1 & 1 & \cdot \\ 1 & \cdot & 1 & \cdot \\ 1 & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{pmatrix}$$

Figure: Estimated sparsity pattern of  $\Theta^{(m)}$ ,  $m = 1, 2, 3, 4$

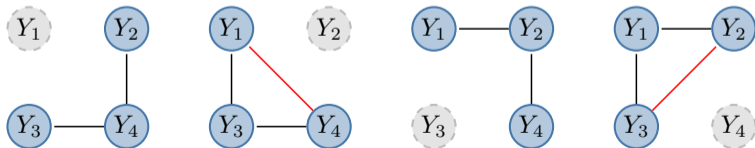


Figure: Corresponding votes

## Theorem (Engelke, L. & Volgushev, 2022+)

If  $\mathcal{A}$  is *neighborhood selection* or *graphical lasso*, under assumptions,

$$\mathbb{P}(\hat{G} = G) \longrightarrow 1$$

as long as  $\log d = o(k/(\log k)^8)$ .

# Selected references

## Extremal graphical models

Engelke, S. and A. S. Hitz (2020). Graphical models for extremes (with discussion). *J. R. Stat. Soc. Ser. B Stat. Methodol.* 82, 871–932.

Engelke, S. and S. Volgushev (2021). Structure learning for extremal tree models. *arXiv preprint arXiv:2012.06179*.

Engelke, S., M. Lalancette and S. Volgushev (2022+). Learning extremal graphical models in high dimensions. *In preparation*.

## Gaussian graphical models and sparse precision matrix estimation

Meinshausen, N. and P. Bühlmann (2006). High-dimensional graphs and variable selection with the lasso. *The Annals of Statistics* 34(3), 1436–1462.

Yuan, M. and Y. Lin (2007). Model selection and estimation in the Gaussian graphical model. *Biometrika* 94(1), 19–35.



# Summary

- Extremal graphical models allow lower dimensional representation of extremal dependence structure
- In the HR parametric family, they can be learned from data even in exponentially high dimension
- We do so using majority voting combined with Gaussian graphical modeling tools
- Preprint out very soon
  - Complete methodology + extensions
  - Theoretical justifications + proofs
  - Simulation studies
  - Application
- [mic-lalancette.github.io](https://mic-lalancette.github.io)

**Thank you for your attention!**