Choosing the threshold in extreme value analysis

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Motivation: peaks over threshold

In the simplest applications:

1. we choose a high threshold u
   - equivalently, choose the number of upper order statistics $k \equiv n_u$ with threshold $u = X_{n-k}$.
2. we fit the limiting generalized Pareto distribution with scale σ_u and shape ξ to exceedances $X - u$ over threshold u.
   - if the shape $\xi > 0$, we can use rather Hill's estimator
3. we use the resulting model for extrapolation beyond u.

Threshold selection

Bias and variance trade-off:

- taking u too high will mean that the number of exceedances n_u is small (increase uncertainty)
- taking u too low will increase n_u, at the risk of a biased extrapolation.

Since the limit holds as u increases to the upper support point of X, we must use a so-called intermediate sequence $n_u/n \to 0$ as $n_u \to \infty$ for consistency.

Limiting distribution and threshold stability

- Limiting distribution of threshold exceedances is generalized Pareto.
- If the limit was exact and $X - u \sim \mathsf{GP}(\sigma_u, \xi)$ and $v > u$, then the conditional distribution of $X - v$ given that $X > v$ is also GPD, with the same shape parameter and scale parameter $\sigma_v = \sigma_u + \xi(v - u)$.

When $\xi > -1$, we have

$$\mathsf{E}(X - u) = \sigma_u/(1 + \xi).$$

Point process formulation

The GPD can be derived from a limiting Poisson process $\mathcal{P}$ under which rare events occur in the (t, y)-plane with measure

$$\Lambda[(t', t) \times [u, \infty)] = (t_2 - t_1)\{1 + \xi(u - \eta)/\sigma\}_+^{-1/\xi}, \qquad \eta \in \mathbb{R}, \sigma > 0.$$

The vertical coordinates of $\mathcal{P}$ can be generated as

$$\eta + \frac{\sigma}{\xi}\left\{\left(\sum_{j=1}^{r} E_j\right)^{-\xi} - 1\right\}, \quad r = 1, 2, \ldots;$$

where the E_j are independent exponential random variables.

Fit the Poisson process model and transform the data to a unit-rate Poisson process.

The choice of threshold then amounts to choosing the highest value for which the transformed observations are consistent with a unit-rate Poisson process.

Martingale residuals

Threshold-stability and the Markov nature of order statistics $X_{(1)} \leq \cdots \leq X_{(n)}$ of a simple random sample drawn from $\mathsf{GP}(\sigma, \xi)$ imply that the joint density of the order statistics is

$$\prod_{j=2}^{n} f(x_{(j)} \mid x_{(j-1)}) f(x_{(1)}) = \prod_{j=1}^{n} \frac{1}{\sigma_j} \left\{ 1 + \frac{\xi}{n+1-j} \frac{(x_{(j)} - x_{(j-1)})}{\sigma_j} \right\}_{+}^{-(n+1-j)/\xi - 1},$$

where $\sigma_j = (\sigma + \xi x_{j-1})/(n+1-j)$ and $x_{(0)} = 0$.

This extends the Rényi representation for exponential data and provides a likelihood if the parameters are allowed to change at order statistics, provided that the parameters for the increment $X_{(j)} - X_{(j-1)}$ depend on the order statistics up to $X_{(j-1)}$.

Stein (2023) explores this idea to replace the threshold by a weighting scheme of the observations.

Some problems with (most methods)

Consider the problem of selecting a threshold amongst candidates $u_1 < \cdots < u_k$.

- Sample overlap: Data above different thresholds are overlapping (so dependence between estimates or test statistics and P-values)
- Non-nested models: peaks-over-threshold methods only consider are conditional models (so most models are not nested).
- Multiple testing
- Potential for automation
- Non-stationarity

Literature review

There are earlier reviews of the topic, but the literature keeps increasing.

- The most comprehensive reviews are Scarrott and MacDonald (2012), Caeiro and Gomes (2016) and Langousis et al. (2016).
- Select numerical comparisons in Gomes and Oliveira (2001), Murphy, Tawn, and Varty (2025) and Schneider, Krajina, and Krivobokova (2021), among others.

Objective

We provide an extensive review of threshold selection mechanisms for peak over threshold analysis, including

- semiparametric methods based on Hill's estimator,
- visual diagnostics,
- goodness-of-fit tests,
- extended generalized Pareto models.

How to benchmark methods?

In practice, we care about

- the extrapolation, often a high quantile (return level), or
- a probability of exceedance.

Benchmarking the method based on proximity with the asymptotic shape parameter is not a good point of reference.

Scale and shape parameters are negatively correlated.

Penultimate effects

Smith (1987) show that a better approximation is obtained by letting the shape vary with u, with

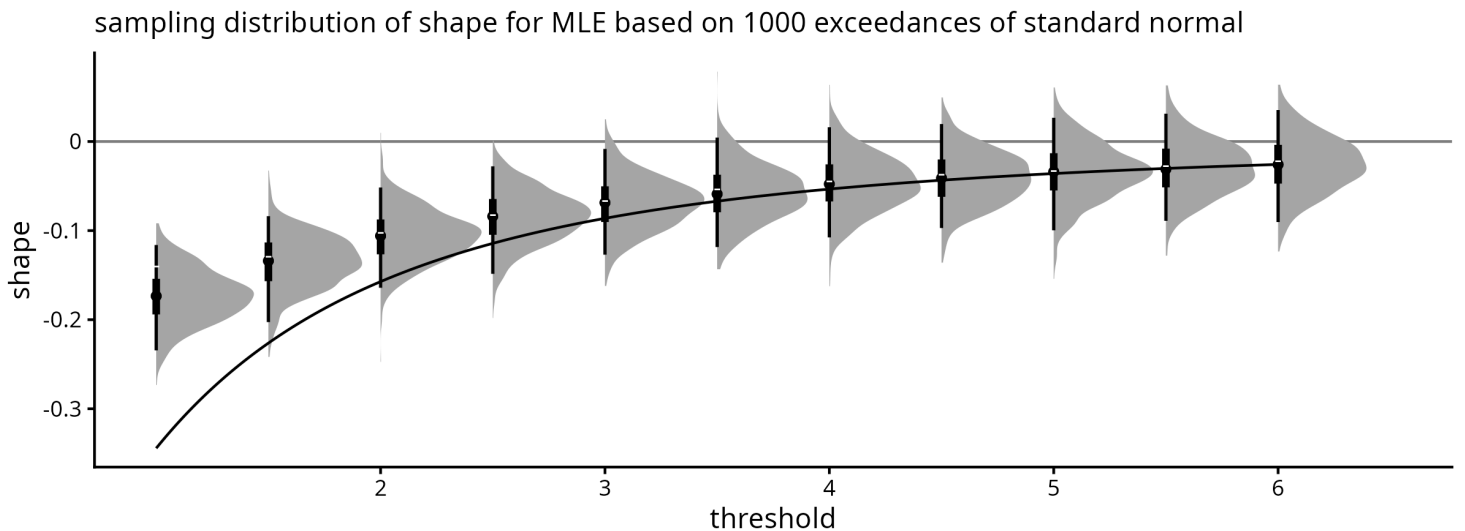
$$\xi_t = r'(u),$$

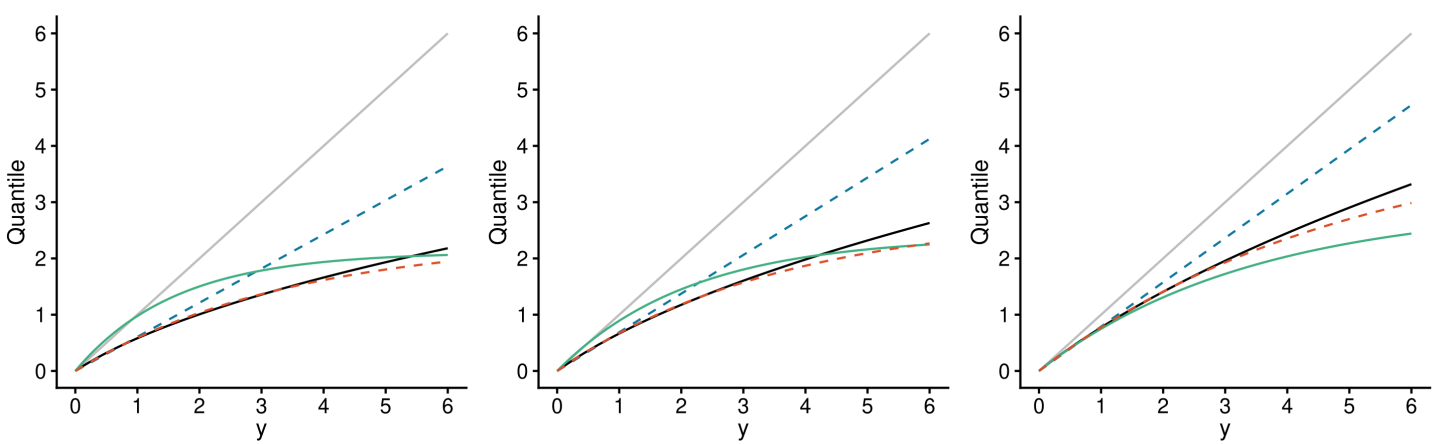
where

$$r(t) = \{1 - F(t)\}/f(t)$$

is the reciprocal hazard function.

Illustration of penultimate effects: normal example



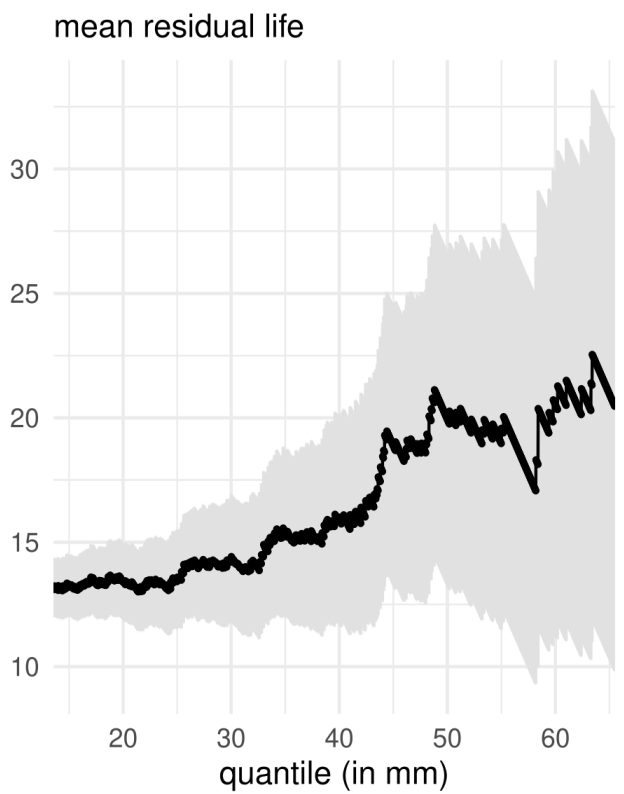


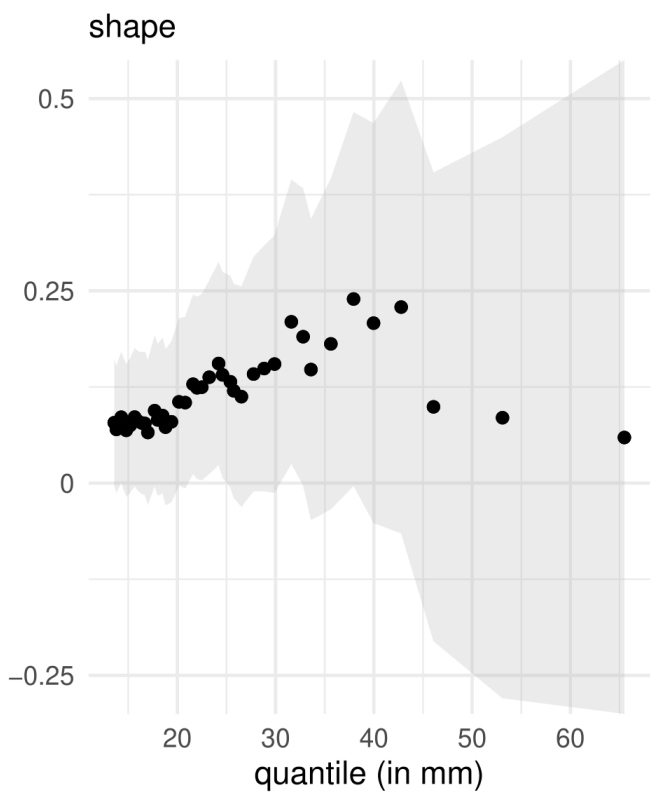
Graphical procedures

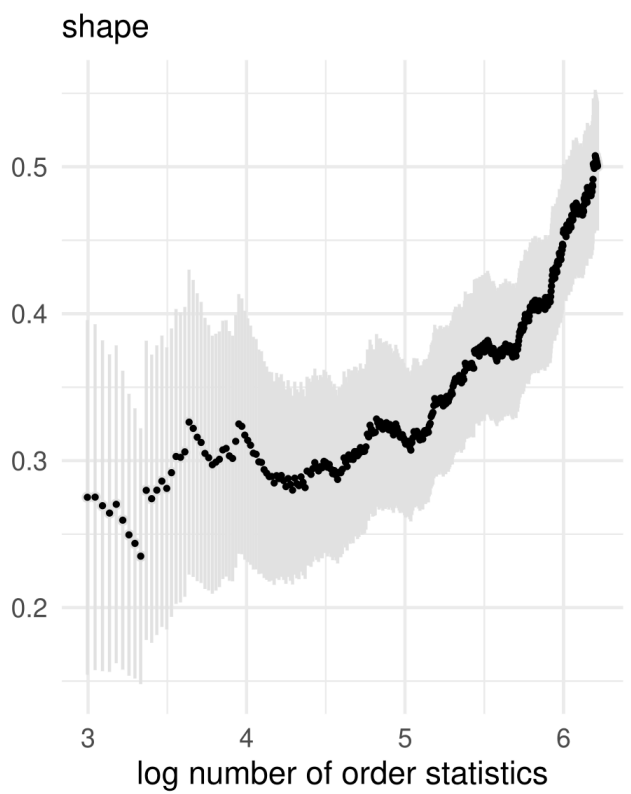
Generalized Pareto distribution is threshold stable (shape is constant).

- Mean residual life plots (Davison and Smith 1990)
- Threshold stability plots
- Hill plots; see, e.g., Resnick (2007)

Visual diagnostics on Padova data





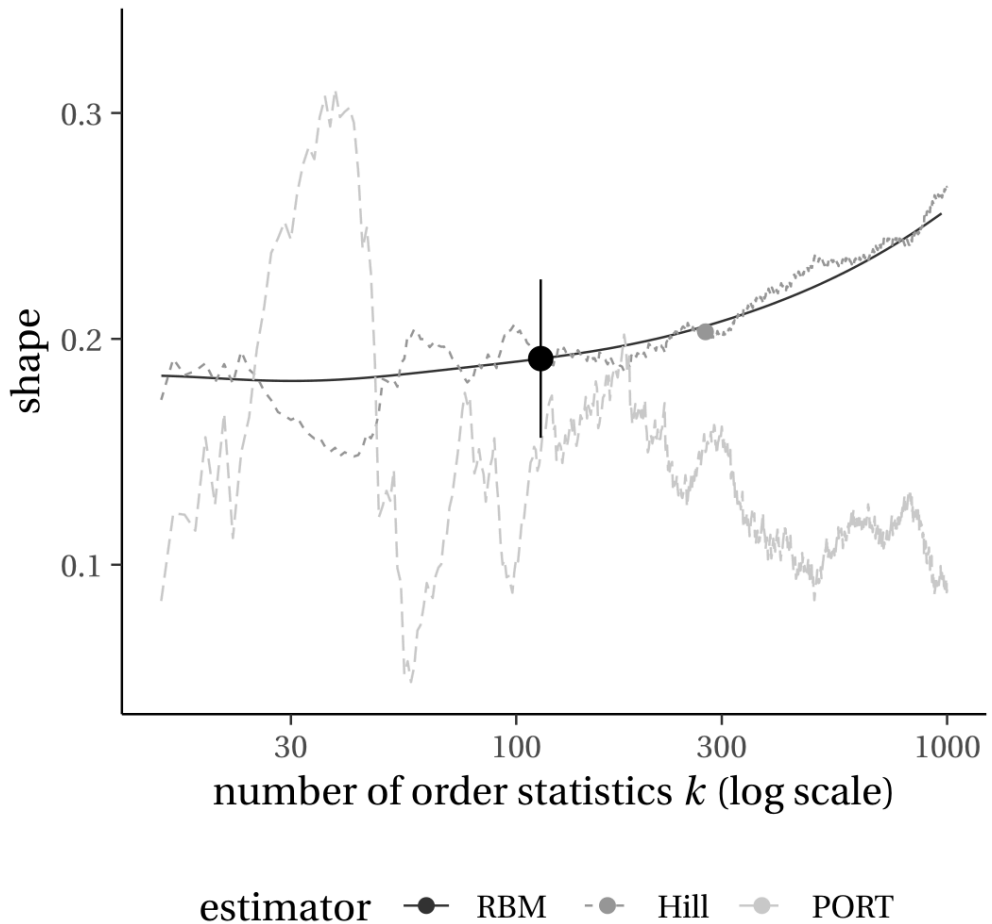


Which threshold would you choose?

Caveats

- Difficulty in automating selection (need visual inspection); proposals in Langousis et al. (2016) or Danielsson et al. (2019), but both fall short.
- sample overlap leads to dependence between estimates (pointwise confidence intervals) + multiple testing
- affected by penultimate effects (shape varies with u in practice)
- plots say nothing about goodness-of-fit!

Stability?



Hill, PORT and random block maxima (Wager 2014) estimates as a function of k (sample paths of RBM are $\mathcal{C}^\infty$).

Generalized Pareto model extensions

Build extended models with additional parameters (with continuity constraints) and test for equality of shape

Northrop and Coleman (2014): piecewise generalized Pareto model, score tests for equality.

- tests are dependent because the data are re-used; no control of overall error rate.
- the power of the test depends on the choice of thresholds and especially on u_K.

Extended generalized Pareto models

Embed generalized Pareto $F(x; \sigma, \xi)$ in a more flexible model with the same tail properties using a continuous distribution function G_κ on $[0, 1]$ (Naveau 2025).

The EGP(σ, ξ, G_κ) distribution function is then

$$\Pr(X \leq x) = G_\kappa\{F(x; \sigma, \xi)\}.$$

- Papastathopoulos and Tawn (2013): models imply the density at the origin is zero.
- Gamet and Jalbert (2022) (propose two models, but non-regular asymptotics).

Extended generalized Pareto models

Test for restriction to generalized Pareto sub-model using likelihood ratio tests (profile).

- Could allow for a bit more data to be included, at the expense of additional parameters to estimate.
- Same problems as parameter stability plots (sequential tests, overlapping data).

Splicing models

Glue a distribution for the bulk with one for the tail using a mixture of disjoint components below u (bulk) and above u (generalized Pareto). See Scarrott and MacDonald (2012) and Hu and Scarrott (2018).

- Leads to sample contamination, fit may be driven by bulk.
- profile likelihood for threshold u is non-monotone.
- Bayesian version (random threshold) leads to threshold selection uncertainty.

Goodness-of-fit measures

Some proposals

- Idea dates back to Pickands (1975).
- Choulakian and Stephens (2001), Bader, Yan, and Zhang (2018) (using ForwardStop)
- Recent proposals using L-moment estimators including Kiran and Srinivas (2021), Solari et al. (2017), Silva Lomba and Fraga Alves (2020).

Testing using maximum likelihood distribution

Thompson et al. (2009) propose using constant values

$$\tau_j = \widehat{\sigma}_j - \hat{\xi}_j u_j$$

and performing Pearson's test of normality for the differences $\tau_{j+1} - \tau_j$ ($j = 1, \ldots, k-1$), stopping whenever the hypothesis is rejected at level $\alpha = 0.2$.

Sequential analysis

Wadsworth (2016) obtains asymptotic joint distribution of MLE from a superposition of Poisson processes.

Build independent increments of shape to form a white noise sequence $\xi_i^* = (\hat{\xi}_{u_{i+1}} - \hat{\xi}_{u_i})/\{(I_{u_{i+1}}^{-1} - I_{u_i}^{-1})_{\xi,\xi}^{1/2}\}$.

Comments on Wadsworth (2016)

Fails 17% of the time in our simulations with equally spaced quantiles.

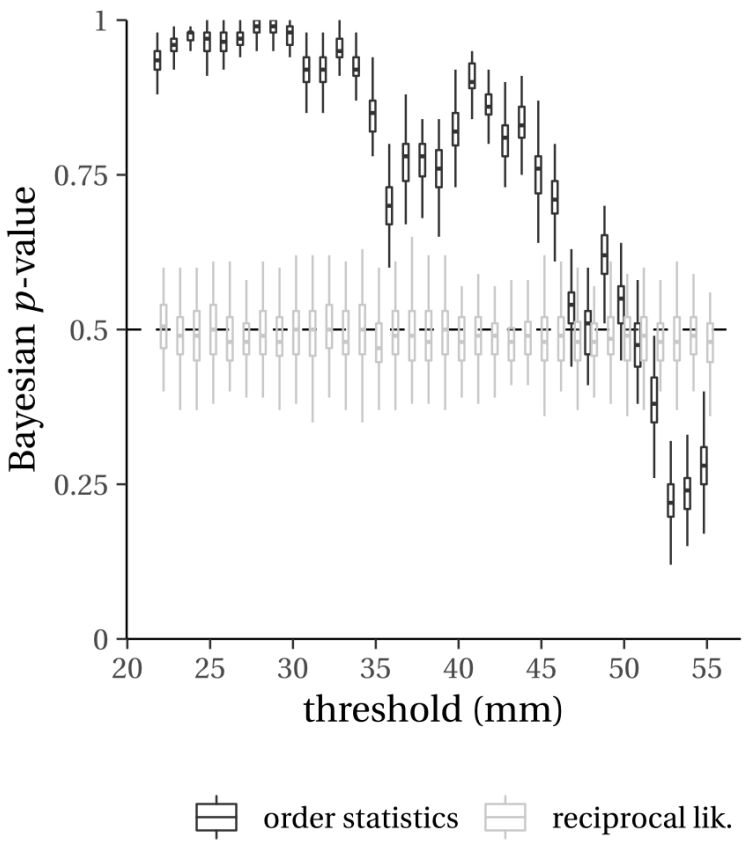
- Problems with positive definiteness of information matrices for shape increments.
- Method sensitive to rounding.
- Must choose the threshold sequence $u_1 \leq \cdots u_k$ carefully.

Bayesian measures of surprise

Lee, Fan, and Sisson (2015) propose constructing a threshold stability plot showing Bayesian p-value for a summary statistic against thresholds, capturing the agreement between sample and simulated data from the posterior distribution.

Under null hypothesis, p-values should be around 0.5.

- Need replications to assess null distribution (very computationally intensive).
- Choice of statistic matters!



Predictive distribution

Northrop, Attalides, and Jonathan (2017) propose a related Bayesian method based on leave-one-out cross validation with a binomial-generalized Pareto (BGP) model and a single validation threshold $v > u_k$ above which we assess the model performance.

The measure of goodness-of-fit proposed is an estimate of the negated Kullback–Leibler divergence,

$$\widehat{T}_v(u_i) = \sum_{i=1}^{n} \log\{\widehat{f}_v(x_r \mid \boldsymbol{x}_{-r}, u_i)\}.$$

The selected threshold is the one among the candidates maximizing this diagnostic.

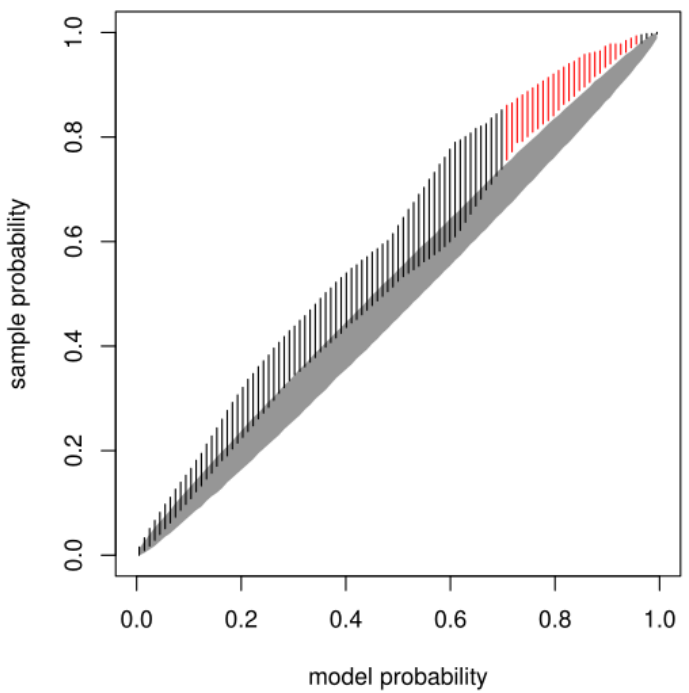
Further propose using Bayesian model averaging to account for the uncertainty originating from threshold selection.

Metric-based diagnostic

Build quantile-quantile (QQ-) plot, with pointwise confidence intervals can be obtained using a parametric bootstrap.

Each bootstrap sample $b = 1, \ldots, B$, estimate the empirical quantile function F_b, which is evaluated at the plotting position $p_i = i/(n+1)$ for $i = 1, \ldots, n$.

Varty et al. (2021) and Murphy, Tawn, and Varty (2025) propose repeating this with simulated iid data from F_0 (tolerance intervals).



Metric-based adjustment

Build metric based on exponential (or generalized Pareto quantile $F_0^{-1}\{p_i\}$ against $F_b^{-1}(p_i)$ with mean absolute difference or mean squared difference.

Pick the threshold with the smallest average distance is chosen.

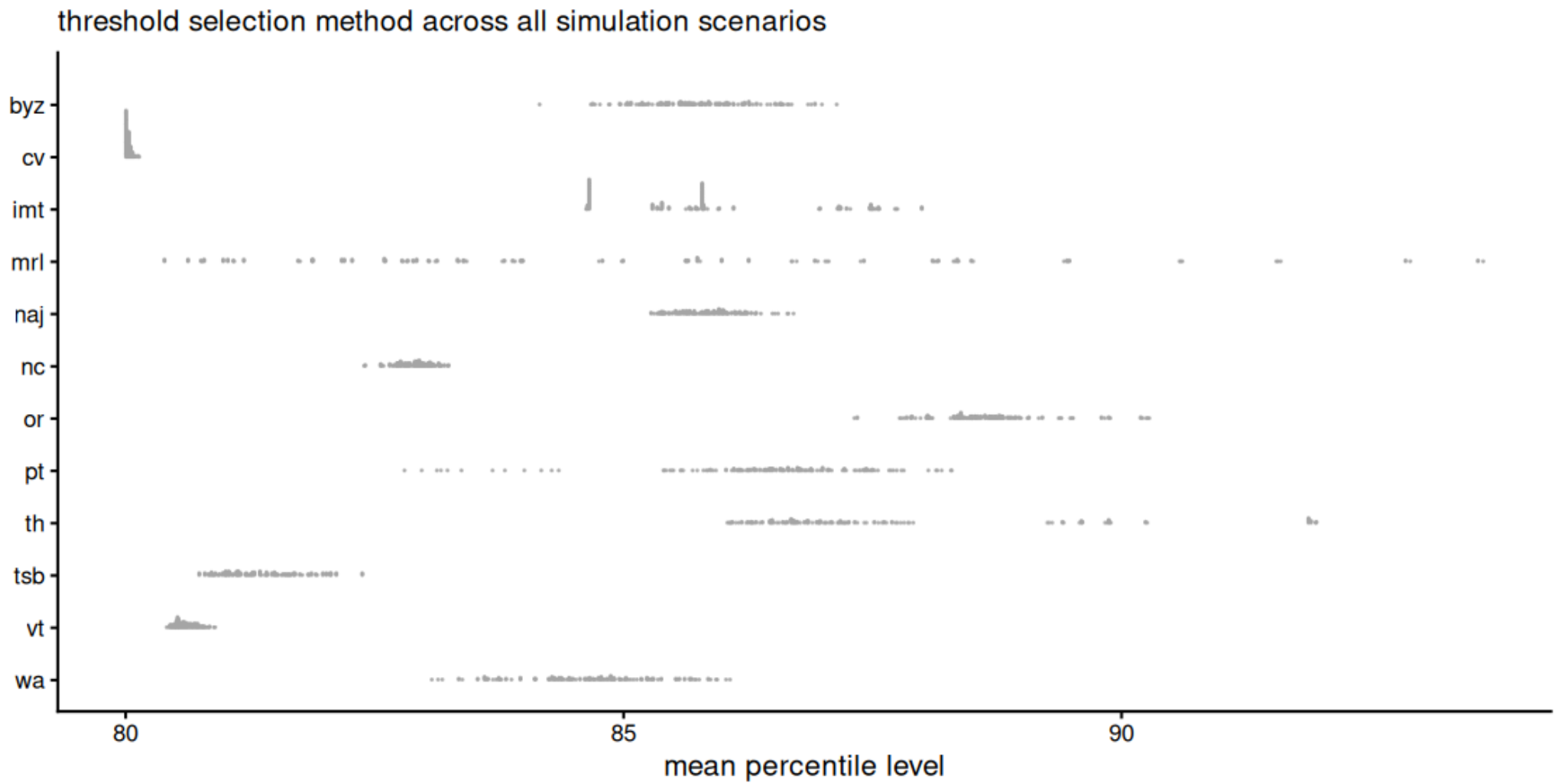
- amenable to different sampling schemes (censoring, non-identically distributed data, time-varying thresholds).
- computationally-intensive by design.

Simulation study: comparison of methods

We considered 13 different distributions from simulation studies in Choulakian and Stephens (2001) and Schneider, Krajina, and Krivobokova (2021).

- Consider 1000 replications of IID data, data with serial correlation in the tail, rounded observations.
- Data of size $n \in \{1000, 2000\}$ with candidate thresholds at the sample $\{0.8, 0.81, \ldots, 0.99\}$ quantiles, keeping a minimum of 20 exceedances.
- Evaluate bias, variance, RMSE of point estimator for 0.999 quantile.
- Compare to oracle (model with the closest quantile estimate among candidates).

Which quantile level on average?



Findings

- No universally better method.
- Goodness-of-fit tests null distributions require adjustment for rounded values (estimate null via Monte Carlo).
- Many of the automated procedures return the lowest possible threshold.
- Using Forward stop method to account for multiple testing leads to thresholds that are much lower.

More comments

- Mean residual life plots are uniformly scattered.
- Varty metric diagnostic also leads to very small thresholds (mean is near 80%).
- Northrop, Attalides, and Jonathan (2017) and Thompson et al. (2009) lead to much less agreement and a greater variability of selected quantile levels for the thresholds. For the cross-validation approach, this is in line with findings of Murphy, Tawn, and Varty (2025).
- The oracle method returns value that are on average between the 87% and the 90% quantile.
- Wadsworth's sequential testing performs best with heavy tailed distributions, but otherwise is one of the worst in terms of ranking.

Conclusions and future work

- Is the problem well-formulated? There is no “correct” threshold, so are we barking up the wrong tree?
- Weighting with different threshold choices to account for uncertainty.
- Should we be fitting sub-asymptotic models to much more data?

Semiparametric methods

The paper also compares 18 different semiparametric methods using Hill-type estimator for heavy-tailed data.

- Careful: many numerical implementations don't specify a minimum sample size!
- Primer: methods based on minimization of the asymptotic mean squared error of the Hill estimator (Caeiro and Gomes 2016), or the double nonparametric bootstrap scheme Gomes, Figueiredo, and Neves (2012), and random block maxima estimator of Wager (2014) with empirical risk minimization perform best.

Don’t use the following

- Methods based on minimization of the asymptotic mean squared error can break down catastrophically for particular data sets.
- Methods by Gomes et al. (2013) and Hall and Welsh (1985) behave erratically with small shape parameters: these procedures lead to strongly biased shape parameter estimates. This is due to them keeping more than 15% of the data for inference.
- Drees and Kaufmann (1998) bias-reduction method leads to small number of order statistics, with very large width of the confidence intervals (unwanted variability).
- Many other methods are extremely variable.

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