Machine learning methods for extremes

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Jointly with
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Prediction of extreme conditional quantiles
Generalized Pareto distribution

\[ \mathbb{P}(Y > y) \]
Generalized Pareto distribution

\[
\mathbb{P}(Y > y) = \mathbb{P}(Y > u) \times \mathbb{P}(Y > y \mid Y > u)
\]
Generalized Pareto distribution

\[
P(Y > y) = P(Y > u) \times P(Y > y \mid Y > u)
\approx P(Y > u) \times (1 - H_{\sigma, \gamma}(y - u))
\]

where \( H_{\sigma, \gamma} \) is the cdf of the GPD with scale and shape \( \sigma > 0 \) and \( \gamma \in \mathbb{R} \).
Generalized Pareto distribution

\[ P(Y > y) = P(Y > u) \times P(Y > y \mid Y > u) \]
\[ \approx P(Y > u) \times \left(1 - H_{\sigma,\gamma}(y - u)\right) \]
\[ = P(Y > u) \times \left(1 + \gamma \frac{y - u}{\sigma}\right)^{-1/\gamma} \]

where \( H_{\sigma,\gamma} \) is the cdf of the GPD with scale and shape \( \sigma > 0 \) and \( \gamma \in \mathbb{R} \).
Consider i.i.d. data $Y_1, \ldots, Y_n$ and estimate empirically the quantile $u = \hat{Q}(\tau_0)$ for an intermediate quantile level $\tau_0 < 1$.

Define the exceedances above the threshold as

$$Z_i = \left( Y_i - \hat{Q}(\tau_0) \right)_+.$$
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The likelihood of the GPD model with parameters \( \theta = (\sigma, \gamma) \) is

\[
\ell_{Z_i}(\theta) = - \left[ (1 + 1/\gamma) \log \left( 1 + \gamma \frac{Z_i}{\sigma} \right) + \log \sigma \right] I_{Z_i > 0}.
\]

Estimate the parameters by maximum likelihood

\[
\hat{\theta} = \arg\max_{\theta} \sum_{i=1}^{n} \ell_{Z_i}(\theta).
\]
Inverting the cdf $H_{\hat{\sigma}, \hat{\gamma}}$ of the GPD provides an approximation of the quantile for probability level $\tau > \tau_0$ by

$$\hat{Q}(\tau) = \hat{Q}(\tau_0) + \hat{\sigma} \left( \frac{1-\tau}{1-\tau_0} \right)^{-\hat{\gamma}} - 1.$$
Extreme quantile regression

Scale shift example with Student’s $t$-distribution (dof=4) for $Y$; $n = 2000$. 
Extreme quantile regression

- For i.i.d. data \((X_1, Y_1), \ldots, (X_n, Y_n)\) where \(X_i \in \mathbb{R}^d\) and \(Y_i \in \mathbb{R}\), the goal is to predict the conditional quantile at level \(\tau \in (0, 1)\)

\[Q_x(\tau) = F_Y^{-1}(\tau \mid X = x).\]
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- There are different scenarios depending on the quantile level \(\tau = \tau_n\):
  - \(\tau_n \equiv \tau_0 < 1\) (classical case)
  - \(\tau_n \to 1\), and \(n(1 - \tau_n) \to \infty\) (intermediate case)
  - \(\tau_n \to 1\), and \(n(1 - \tau_n) \to 0\) (extreme case)

Classical methods for quantile regression only work well in the case of fixed \(\tau_n \equiv \tau_0 < 1\).

Methods from extreme value theory are not flexible enough (Chernozhukov [2005], Chavez-Demoulin & Davison [2005]) or do not generalize well into higher dimensions (Daouia, Gardes & Girard [2013]).

Goal: Develop a new method for extreme quantile regression that works well with high-dimensional and complex data.
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Quantile regression

- Consider independent data \((X_1, Y_1), \ldots, (X_n, Y_n)\) where \(X_i \in \mathbb{R}^d\), \(Y_i \in \mathbb{R}\).
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- The goal is to predict the conditional quantile at level \(\tau \in (0, 1)\)
  \[ Q_x(\tau) = F_Y^{-1}(\tau | X = x). \]
- Most approaches for quantile estimation rely on the property
  \[ Q_x(\tau) = \arg\min_q \mathbb{E} [\rho_\tau(Y - q) | X = x] , \]
  where \(\rho_\tau(u) = (\tau - \mathbb{1}\{u < 0\})u\) is the quantile check function.
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\]

where \(\rho_\tau(u) = (\tau - \mathbb{I}\{u < 0\})u\) is the quantile check function.

Without parametric assumption, a pointwise estimator is

\[
\hat{Q}_x(\tau) = \arg\min_q \sum_{i=1}^n w_i(x) \rho_\tau(Y_i - q).
\]

where \(w_1, \ldots, w_n\) is a sequence of localizing weight functions.
Extreme quantile regression

- Assume the GPD model

\[(Y - u \mid Y > u) \sim H_{\sigma, \gamma}\]
Extreme quantile regression

- Assume the conditional GPD model

\[(Y - u(x) \mid Y > u(x), X = x) \sim H_{\sigma(x), \gamma(x)}\]
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\[(Y - u(x) \mid Y > u(x), X = x) \sim H_{\sigma(x), \gamma(x)}\]

• Let \(\tau_0\) be an intermediate quantile level, and \(u(x) = \hat{Q}_x(\tau_0)\) be an estimate of the conditional \(\tau_0\) quantile of \(Y \mid X = x\); it can be estimated with classical methods, e.g., a quantile random forest.
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- For a possibly extreme level \(\tau > \tau_0\) we can estimate

\[
\hat{Q}_x(\tau) = \hat{Q}_x(\tau_0) + \hat{\sigma}(x) \left( \frac{1 - \tau}{1 - \tau_0} \right)^{-\hat{\gamma}(x)} - 1,
\]

where \(\hat{\theta}(x) = (\hat{\sigma}(x), \hat{\gamma}(x))\) is an estimate of the conditional GPD parameters.
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• For a possibly extreme level \(\tau > \tau_0\) we can estimate

\[
\hat{Q}_x(\tau) = \hat{Q}_x(\tau_0) + \hat{\sigma}(x) \frac{1 - \tau}{1 - \tau_0} \frac{1}{\hat{\gamma}(x)} - 1
\]

where \(\hat{\theta}(x) = (\hat{\sigma}(x), \hat{\gamma}(x))\) is an estimate of the conditional GPD parameters.

• The triple \((\hat{Q}_x(\tau_0), \hat{\sigma}(x), \hat{\gamma}(x))\) provides a model for the tail of \(Y \mid X = x\).
Scale shift example with Student’s $t$-distribution (dof=4) for $Y$; $n = 2000$. 
Extreme quantile regression

Scale shift example with Student’s $t$-distribution (dof=4) for $Y$; $n = 2000$. 
Extreme quantile regression

Two methods to estimate the GPD parameters $\hat{\theta}(x) = (\hat{\sigma}(x), \hat{\gamma}(x))$, both maximize a localized likelihood:

$$\hat{\theta}(x) = \arg\max_{\theta} \sum_{i=1}^{n} w_i(x) \ell_{Z_i}(\theta),$$

where $Z_i$ are the conditional exceedances.

– Extremal gradient boosting (GBEX): The weights $w_i(x)$ are obtained through gradient boosting.


– Extremal random forest (ERF): The weights $w_i(x)$ are obtained through a generalized random forest Athey, Tibshirani & Wager [2019].

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  https://arxiv.org/abs/2103.00808
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Simulation setup

Setup from [Athey, Tibshirani & Wager, 2019]:

- Different dimensions $d$ and sample size $n = 2000$.
- $X = (X_1, \ldots, X_d)$ uniform distributed on $[-1, 1]^d$.
- $Y$ follows a Student’s $t$-distribution with $\text{dof} = 4$ and scale
  \[ \text{scale}(x) = 1 + \mathbb{I}(x_1 > 0), \]
  that is $\gamma(x) \equiv 1/4$ and $\sigma(x) = \sigma(\tau_0)(1 + \mathbb{I}(x_1 > 0))$. 


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- Intermediate threshold $\tau_0 = 0.8$ and extreme probability levels of interest $\tau = 0.99, 0.995, 0.999$ and $0.9995$. 

Evaluation metric is the integrated squared error (ISE) for level $\tau$

\[
\text{ISE} = \int_{-1}^{1} (\hat{Q}_x(\tau) - Q_x(\tau))^2 \, dx.
\]

Repeat experiment many times and compute the average of the ISE:

\[
\text{MISE} = \mathbb{E}(\text{ISE}).
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Results

\[ p = 10 \]

\[ \tau \]

\[ \text{RMISE} \]

Methods:
- ERF
- GRF
- Meinshausen
- Unconditional GPD
- Extreme GAM
- Taillardat QRF
- GBEX
Results

\[ \tau = 0.9995 \]

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RMISE

\[ \tau = 0.9995 \]

10 20 30

p

RMISE

\[ \tau = 0.9995 \]

10 20 30

p
GBEX: variable importance
Data

- Consider ensembles of numerical weather predictions for precipitation forecasts from the European Centre for Medium-Range Weather Forecasts.
- We have $M = 51$ ensembles and consider a lead time of 36 hours.
- Statistical post-processing is a second step to correct these forecasts for systematic biases and over- or underdispersion.
Precipitation forecasts and statistical post-processing

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- We have 9 years of daily data at 7 locations in the Netherlands.
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- We have 9 years of daily data at 7 locations in the Netherlands.
- We apply our gbex at each location with predictors from all locations:

  \[
  X_1, \ldots, X_7 = \text{ensemble mean from all locations} \\
  X_8, \ldots, X_{14} = \text{ensemble st. dev. from all locations} \\
  X_{15}, \ldots, X_{21} = \text{ensemble upper order statistics} \\
  X_{22} = \sin\left(\frac{2\pi \text{day}}{365}\right) \\
  X_{23} = \cos\left(\frac{2\pi \text{day}}{365}\right)
  \]
Partial dependence plots

Station name
- De Bilt
- De Kooy
- Eelde
- Maastricht
- Schiphol
- Twenthe
- Vlissingen

Day of the year

Ensemble standard deviation
evtGAN: combining EVT and GANs
Climate model data

- We use 2000 years of large ensemble simulations with the EC-Earth global climate model (v2.3, Hazeleger et al., 2012).
- Present-day climate conditions, stationary in time; see van der Wiel et al. (2019) for details.
- Data at $d = 18 \times 22$ grid points over western Europe.
- We consider annual maxima of precipitation and temperature, giving us $n = 2000$ observations of a random vector $Z = (Z_1, \ldots, Z_d)$. 

Goal: Realistic simulations of $Z$ for stress testing and extreme event simulation. Here we use $n_{\text{train}} = 50$ years for training, and $n_{\text{test}} = 1950$ for evaluation.
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Figure 1: GEV parameters for temperature (a-c) and precipitation (d-f): mean parameter $\mu$ (left), scale parameter $\sigma$ (center) and shape parameter $\xi$ (right).
Two approaches

Classical EVT approach

- Spatial extreme value theory provides statistical models for $Z$, e.g., a spatial max-stable model [Davison and Gholamrezaee, 2012].
- If the region is very large and heterogeneous, such models may not be flexible enough, because of:
  - spatial non-stationarities;
  - asymptotic independence between some stations;
  - etc.
Two approaches

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Our ML approach

- Generative Adversarial Networks (GANs) [Goodfellow et al., 2014] are a flexible way of learning and sampling from a multivariate distribution $Z$.
- They are usually used to sample from image data using convolutional neural networks.
- We can treat our spatial climatological data $Z$ as an image.
GAN architecture: generator and discriminator

Gaussian Noise $z$ \(100 \times 1\) → Output $G(z)$

**Generator:**
- 100 × 1 Gaussian Noise $z$
- Fully Connected (FC) layer
- Reshape + leaky ReLU (lrelu) + drop + Batch Normalization (BN)
- Deconvolution layers (Deconv1, Deconv2, Deconv3) with:
  - $F = 3 \times 3$ $S = 1 \times 1$
  - $F = 3 \times 4$ $S = 1 \times 1$
  - $F = 4 \times 6$ $S = 2 \times 2$
- Output

**Discriminator:**
- Input
- Fully Connected (FC) layer
- Convolution layers (Conv1, Conv2) with:
  - $F = 3 \times 3$ $S = 1 \times 1$
- Output $D(x)$
GAN architecture: generator and discriminator

Gaussian Noise $z_{100 \times 1}$

Output $G(z)$

FC

Reshape + lrelu(0.2) + drop(0.5) + BN

$7 \times 7 \times 512$

$F = 3 \times 3$

$S = 1 \times 1$

Deconv2 + lrelu(0.2) + drop(0.5) + BN

$256$

$10$

$9$

Deconv3

Output $G(z)$

Reshape

$25600$

$256$

$1024$

Deconv1 + lrelu(0.2) + drop(0.5) + BN

$1024$

$5$

$5$

Deconv1

Input

$5$

$5$

Conv1 + lrelu(0.2) + drop(0.5)

$64$

$10$

Conv2 + lrelu(0.2) + drop(0.5)

$128$

$7$

Conv2

$7$

Conv2 + lrelu(0.2) + drop(0.5) + BN

$256$

$5$

$5$

Conv2

Conv2 + lrelu(0.2) + drop(0.5) + BN

$6400$

Reshape

Output $D(x)$

FC + sigmoid
GANs for extremes

- GANs are trained on the bulk of the distribution.
- There are two main challenges concerning extremes:
  - accurate extrapolation of the marginal distributions;
  - accurate modeling of the extremal dependence structure.

"If the input noise is bounded/light-tailed, then the generator output is bounded/light-tailed" [Wiese et al., 2019].

Huster et al. (2021) and Allouche et al. (2021) develop GANs that can generate heavy-tailed output.

Bhatia et al. (2020) propose a conditional GAN for importance sampling of extreme events.

Our evtGAN is a copula approach where marginals use EVT approximations and the dependence structure is generated by the GAN.
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The evtGAN algorithm

**Input:** Annual maxima \( Z_i = (Z_{i1}, \ldots, Z_{id}), \ i = 1, \ldots, n. \)
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1. Fit a GEV distribution \( \hat{G}_j \) to the jth marginal with parameters \( (\hat{\mu}_j, \hat{\sigma}_j, \hat{\xi}_j). \)
The evtGAN algorithm

**Input:** Annual maxima $Z_i = (Z_{i1}, \ldots, Z_{id})$, $i = 1, \ldots, n$.

1. Fit a GEV distribution $\hat{G}_j$ to the $j$th marginal with parameters $(\hat{\mu}_j, \hat{\sigma}_j, \hat{\xi}_j)$.
2. Normalize empirically to a std uniform distribution to obtain *pseudo* observations
   
   $$U_i = (\hat{F}_1(Z_{i1}), \ldots, \hat{F}_d(Z_{id})), \quad i = 1, \ldots, n,$$

   where $\hat{F}_j$ is the empirical distribution function of the $Z_{1j}, \ldots, Z_{nj}$.
3. Train a GAN $G$ on the normalized data $U_1, \ldots, U_n$.

**Output:** Set of new generated observations $Z^*_i = (Z^*_{i1}, \ldots, Z^*_{id})$, $i = 1, \ldots, n^*$. 
The evtGAN algorithm

**Input:** Annual maxima $Z_i = (Z_{i1}, \ldots, Z_{id})$, $i = 1, \ldots, n$.

1. Fit a GEV distribution $\hat{G}_j$ to the $j$th marginal with parameters $(\hat{\mu}_j, \hat{\sigma}_j, \hat{\xi}_j)$.
2. Normalize empirically to a std uniform distribution to obtain pseudo observations

$$U_i = (\hat{F}_1(Z_{i1}), \ldots, \hat{F}_d(Z_{id})), \quad i = 1, \ldots, n,$$

where $\hat{F}_j$ is the empirical distribution function of the $Z_{1j}, \ldots, Z_{nj}$.

3. **Train a GAN** $G$ on the normalized data $U_1, \ldots, U_n$.
4. Generate $n^*$ new data points $U_{1*}, \ldots, U_{n*}$ from $G$ with uniform margins.
5. Normalize back to the scale of the original observations

$$Z^*_i = (\hat{G}_1^{-1}(U^*_{i1}), \ldots, \hat{G}_d^{-1}(U^*_{id})), \quad i = 1, \ldots, n^*.$$

**Output:** Set of new generated observations $Z^*_i = (Z^*_{i1}, \ldots, Z^*_{id})$, $i = 1, \ldots, n^*$.
Figure 2: GEV parameters for temperature (a-c) and precipitation (d-f): mean parameter $\mu$ (left), scale parameter $\sigma$ (center) and shape parameter $\xi$ (right).
Bivariate samples of temperature

Train set

Test set

evtGAN

DCGAN

Brown-Resnick

Temperature (°C)

a) b) c) d) e) f) g) h) i) j) k) l) m) n) o)
Bivariate samples of precipitation

![Bivariate samples of precipitation](image_url)
Extremal correlation plots

Train set  evtGAN  Brown–Resnick

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Model extremal correlation

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Test extremal correlation
Thank You!


References III


