

# NSGEV Computing Details

Yves Deville

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# 1 The TVGEV block maxima model

The model discussed here is for a timeseries  $Y_b$  of block maxima with GEV margins  $\boldsymbol{\theta}_b = [\mu_b, \sigma_b, \xi_b]^\top$ , that is  $Y_b \sim \text{GEV}\{\boldsymbol{\theta}_b\}$ . The GEV location parameter  $\mu_b$  depends on the time through a vector of  $p^\mu$  covariates  $\mathbf{x}_b^\mu(t)$  according to

$$\mu_b = \mathbf{x}_b^{\mu\top} \boldsymbol{\psi}^\mu$$

where  $\boldsymbol{\psi}^\mu$  is a vector of  $p^\mu$  fixed yet unknown parameters. Similar relations are used for the scale and shape parameters  $\sigma_b$  and  $\xi_b$ . A typical example uses a linear trend on the location parameter:  $\mu_b = \psi_0^\mu + \psi_1^\mu b$ , so the model uses  $p^\mu = 2$  parameters  $\boldsymbol{\psi}^\mu = [\psi_0^\mu, \psi_1^\mu]^\top$ . The relation between the vector  $\boldsymbol{\theta}_b$  of GEV parameters and the vector  $\boldsymbol{\psi}$  of model parameters is

$$\boldsymbol{\theta}_b = \begin{bmatrix} \mu_b \\ \sigma_b \\ \xi_b \end{bmatrix} = \begin{bmatrix} \mathbf{x}_b^{\mu\top} \boldsymbol{\psi}^\mu \\ \mathbf{x}_b^{\sigma\top} \boldsymbol{\psi}^\sigma \\ \mathbf{x}_b^{\xi\top} \boldsymbol{\psi}^\xi \end{bmatrix} = \begin{bmatrix} \mathbf{x}_b^{\mu\top} \mathbf{i}^\mu \\ \mathbf{x}_b^{\sigma\top} \mathbf{i}^\sigma \\ \mathbf{x}_b^{\xi\top} \mathbf{i}^\xi \end{bmatrix} \boldsymbol{\psi}$$

$3 \times p \quad p \times 1$

where for instance  $\mathbf{i}^\mu := [1_{p^\mu}^\top, \mathbf{0}^\top]$  is the vector of  $p$  one-or-zero elements which picks the “location part” in the whole vector of model parameters.

*Remark 1.* In practice the same covariates can be used for several parameters and the shape  $\xi$  is quite often maintained constant, so that  $\mathbf{x}_b^\xi \equiv 1$  and  $\boldsymbol{\psi}^\xi = \xi$ .

*Remark 2.* For numerical reasons, the scaling of the covariates can matter. For instance it is bad idea to take  $x_b$  as a year number such as  $x_b = 2000$ . A common practice is to scale the time.

*Remark 3.* One could allow a same parameter  $\psi_k$  to be used in several GEV parameters, typically both  $\mu$  and  $\sigma$ . The three  $B^* \times p$  matrices  $\mathbf{X}^\mu$ ,  $\mathbf{X}^\sigma$  and  $\mathbf{X}^\xi$  would be stored as a three-dimensional array say  $\tilde{\mathbf{X}}$  with dimension  $3 \times B^* \times p$ . For the  $i$ -th GEV parameter  $\theta^{[i]}$  ( $i = 1$  to  $3$ ), the slice  $\tilde{\mathbf{X}}[i, , ]$  would be a  $B^* \times p$  matrix such that the vector  $\boldsymbol{\theta}^{[i]}$  with length  $B^*$  is given by  $\boldsymbol{\theta}^{[i]} = \tilde{\mathbf{X}}[i, , ] \boldsymbol{\psi}$ . So the  $B^* \times 3$  matrix  $\boldsymbol{\Theta}$  would result from a product of arrays.

## 2 Distribution and quantile of the maximum $M$

### 2.1 Motivation

As a typical use of the model above, one may consider a period  $\mathcal{B}^*$ , most often a future period, that is: a set of future blocks  $b^*$ . This period is sometimes called the *design life period* Rootzén and Katz (2013). Due to the independence of the block maxima, the random maximum on the period, namely

$$M := \max_{b^* \in \mathcal{B}^*} \{Y_{b^*}\} \tag{1}$$

has its distribution function given by the product

$$F_M(m; \boldsymbol{\psi}) = \prod_{b^*} F_{\text{GEV}}(m; \boldsymbol{\theta}_{b^*}) \tag{2}$$

where the vector  $\boldsymbol{\theta}_{b^*} = \boldsymbol{\theta}_{b^*}(\boldsymbol{\psi})$  contains the GEV parameters for the block  $b^*$ . This GEV parameter vector depends linearly on  $\boldsymbol{\psi}$  and on the vector  $\mathbf{x}_b$  of covariates. Of course,  $M$  does not in general follow a GEV distribution.

A typical quantity of interest is the quantile  $q_M(p)$  corresponding to a probability  $p$  close to 1. For instance the period  $\mathcal{B}^*$  may correspond to the design life of a dike. Using observed

block maxima of the river level, one can fit a TVGEV model and the quantile corresponding to  $p = 0.99$  can be used to find the height of the dike corresponding to a 1% risk of being exceeded during the period.

The quantile  $q_M(p)$  is the solution  $m$  of the equation  $F_M(m) = p$  which allows its determination by a zero-finding numerical method where  $F_M(m)$  is evaluated by using (2). It helps much in the zero-finding to provide an interval  $[m_L, m_U]$  in which the quantile is granted to lie. This is actually required to use the R function `uniroot`. Fortunately, one can simply use here

$$m_U := q_{\text{GEV}}(p, \mu_U, \sigma_U, \xi_U)$$

where a GEV paramater pseudo-indexed by  $U$  means the maximum of the coresponding GEV parameters as in  $\mu_U := \max_{b^*} \{\mu_{b^*}\}$ . A lower bound  $m_L$  can be obtained similarly as the GEV quantile corresponding to the the minima of the GEV parameters.

In order to infer on the quantile  $q_M(p)$  we need to compute its dervivatives w.r.t. the vector  $\psi$  of model parameters. Since the `nieve` package provides the derivatives of the GEV probability functions w.r.t. the vector  $\theta$  of GEV parameters, one can actually get the wanted derivatives by using the chain rule and the implicit function theorem. We first have to compute the derivatives of the distribution function  $F_M(m; \psi)$  w.r.t. the vector  $\psi$  of model parameters, and then to use the implicit function theorem. This will be detailed below.

In the computation we will use matrices and arrays to store the GEV parameters and the derivatives. We will denote by  $\Theta^*$  the  $B^* \times 3$  matrix containing the GEV parameter vectors  $\theta_{b^*}$  as its rows. Then

$$\Theta^* = \left[ \begin{array}{c|c|c} \mathbf{X}^{*\mu} \psi^\mu & \mathbf{X}^{*\sigma} \psi^\sigma & \mathbf{X}^{*\xi} \psi^\xi \end{array} \right]_{B^* \times 3}$$

where each of the three blocks at r.h.s. is  $B^* \times 1$  and is the product of a “design matrix” with  $B^*$  rows by a subvector of the model parameter vector  $\psi$ .

## 2.2 Distribution function

### First-order

From (2)

$$\frac{\partial_{\psi_k} F_M(m; \psi)}{F_M(m; \psi)} = \sum_{b^*} \frac{\partial_{\psi_k} F_{\text{GEV}}(m; \theta_{b^*})}{F_{\text{GEV}}(m; \theta_{b^*})}. \quad (3)$$

### Second order

The second-order log-derivative w.r.t. the parameters  $\psi_\ell$  and  $\psi_k$  is

$$\begin{aligned} \frac{\partial_{\psi_\ell \psi_k}^2 F_M(m; \psi)}{F_M(m; \psi)} &= \left\{ \sum_{a^*} \frac{\partial_{\psi_\ell} F_{\text{GEV}, a^*}}{F_{\text{GEV}, a^*}} \right\} \left\{ \sum_{b^*} \frac{\partial_{\psi_k} F_{\text{GEV}, b^*}}{F_{\text{GEV}, b^*}} \right\} \\ &+ \left\{ \sum_{b^*} \frac{\partial_{\psi_\ell \psi_k}^2 F_{\text{GEV}, b^*}}{F_{\text{GEV}, b^*}} - \sum_{b^*} \frac{\partial_{\psi_\ell} F_{\text{GEV}, b^*} \partial_{\psi_k} F_{\text{GEV}, b^*}}{F_{\text{GEV}, b^*}^2} \right\} \end{aligned} \quad (4)$$

where  $F_{\text{GEV}, b^*}$  is used as a shortcut for  $F_{\text{GEV}}(m; \theta_{b^*})$ .

### Using matrices and arrays

Assume that  $\psi_k$  is a linear coefficient for the GEV location parameter  $\mu$  so that  $\psi_k = \psi_{i_k}^\mu$  for some  $i_k$  between 1 and  $p^\mu$ . Let  $\mathbf{u}^\mu$  be the vector with length  $B^*$  and with element

$$u_{b^*}^\mu := \partial_\mu \log F_{\text{GEV}}(m; \theta_{b^*}) \quad b^* = 1, \dots, B^*.$$

Then by chain rule the sum at the r.h.s. of (3) is the cross-product

$$\partial_{\psi_k} \log F_M(m; \boldsymbol{\psi}) = \mathbf{u}^{\mu^\top} \mathbf{X}^\mu[, i_k]. \quad (5)$$

The same computation holds for the other GEV parameter  $\sigma$  and  $\xi$ . Of course, if the GEV parameter is a constant  $\psi_k$  then the corresponding vector  $\mathbf{u}$  is a vector of ones and the cross-product in (5) is simply the sum of the elements of  $\mathbf{u}^\mu$ .

One can compute the derivatives of  $\log F_M$  for all the indices  $\psi_k$  corresponding to the same GEV parameter. For this aim, let us introduce some notations.

- Let  $i \in \{1, 2, 3\}$  be a “GEV parameter index” for the GEV parameter according to the rule  $\theta^{[1]} \equiv \mu$  for  $i = 1$ , to  $\theta^{[2]} \equiv \sigma$  for  $i = 2$  and to  $\theta^{[3]} \equiv \xi$  for  $i = 3$ . So  $\mathbf{X}^{\theta^{[i]}}$  is the design matrix with dimension  $B^* \times p_i$  for the GEV parameter number  $i$ . So for instance  $p_1 = p^\mu$ .
- For  $i \in \{1, 2, 3\}$  let  $\mathbf{k}_i$  the vector of indices in the vector  $\boldsymbol{\psi}$  corresponding to the GEV parameter  $\theta^{[i]}$ . So  $\mathbf{k}_i$  has length  $p_i$ .
- Let  $\mathbf{G}$  be the  $B^* \times 3$  Jacobian matrix of the vector-valued function with value  $[\log F_{\text{GEV}, b^*}]_{b^*}$ , the differentiation being w.r.t. the three GEV parameters  $\boldsymbol{\theta}^{[i]}$ . So

$$G[b^*, i] = \partial_{\theta^{[i]}} \log F_{\text{GEV}, b^*}, \quad 1 \leq b^* \leq B^*, \quad 1 \leq i \leq 3.$$

Then by chain rule we get as above in (5)

$$\partial_{\psi_{\mathbf{k}_i}} \log F_M = \mathbf{G}[, i]^\top \mathbf{X}^{\theta^{[i]}}, \quad i = 1, 2, 3.$$

If  $\theta^{[i]}$  is specified as being constant across blocks, then  $\mathbf{k}_i$  has length one and the matrix cross-product is simply the sum of the column  $i$  of  $\mathbf{G}$ . This will typically be the case for the GEV shape parameter  $\xi$ .

The second-order derivatives of  $\log F_{\text{GEV}}$  can be stored as a three-dimensional array  $\mathbf{H}$  with dimension  $B^* \times 3 \times 3$  and with element

$$H[b^*, i, j] = \partial_{\theta^{[i]} \theta^{[j]}}^2 \log F_{\text{GEV}, b^*}, \quad 1 \leq b^* \leq B^*, \quad 1 \leq i, j \leq 3.$$

Then for the two GEV parameter vectors  $\theta^{[i]}$  and  $\theta^{[j]}$  the  $p_i \times p_j$  matrix of 2-nd order derivatives of  $\log F_{\text{GEV}, b^*}$  w.r.t.  $\psi_{\mathbf{k}_i}$  and  $\psi_{\mathbf{k}_j}$  is obtained by

$$\sum_{b^*} \partial_{\psi_{\mathbf{k}_i} \psi_{\mathbf{k}_j}}^2 \log F_{\text{GEV}, b^*} = \mathbf{X}^{\theta^{[i] \top}} \text{diag}(\mathbf{H}[, i, j]) \mathbf{X}^{\theta^{[j]}}$$

So, from (4), in the  $p \times p$  Hessian of  $\log F_M$ , the block corresponding to the indices  $\mathbf{k}_i$  and  $\mathbf{k}_j$  can be written in matrix form

$$\partial_{\psi_{\mathbf{k}_i} \psi_{\mathbf{k}_j}}^2 \log F_M = \mathbf{X}^{\theta^{[i] \top}} \left\{ \mathbf{G}[, i] \mathbf{G}[, j]^\top + \text{diag}(\mathbf{h}^{[ij]} - \mathbf{m}^{[ij]}) \right\} \mathbf{X}^{\theta^{[j]}} \quad (6)$$

where  $\mathbf{h}^{[ij]}$  and  $\mathbf{m}^{[ij]}$  are the two vectors with length  $B^*$  related to the Jacobian matrix  $\mathbf{G}$  and the Hessian array  $\mathbf{H}$  by

$$\mathbf{h}_{b^*}^{[ij]} := H[b^*, i, j], \quad \mathbf{m}_{b^*}^{[ij]} := G[b^*, i] G[b^*, j]. \quad (7)$$

## 2.3 Quantile

### First order

The partial derivative of the quantile  $q_M(p; \boldsymbol{\psi})$  with a given probability  $p$  comes by the implicit function theorem

$$\partial_{\psi_k} q_M(p; \boldsymbol{\psi}) = -\frac{\partial_{\psi_k} F_M(m_{\boldsymbol{\psi}}; \boldsymbol{\psi})}{f_M(m_{\boldsymbol{\psi}}; \boldsymbol{\psi})} \quad (8)$$

where  $q_M(p; \boldsymbol{\psi})$  is for simplicity denoted by  $m_{\boldsymbol{\psi}}$  at the r.h.s. The density at the denominator comes by evaluating the logarithmic derivative of the the product (2), that is

$$f_M(m; \boldsymbol{\psi}) = F_M(m; \boldsymbol{\psi}) \sum_{b^*} \frac{f_{\text{GEV}}(m; \boldsymbol{\theta}_{b^*})}{F_{\text{GEV}}(m; \boldsymbol{\theta}_{b^*})} \quad (9)$$

for  $m := m_{\boldsymbol{\psi}}$ .

### Second order

In order to differentiate (8) w.r.t. to a second parameter  $\psi_\ell$ , we need the partial derivative of the density at the denominator. For a *fixed* value  $m$  (not depending on  $\boldsymbol{\psi}$ ), by differentiating (9) w.r.t.  $\psi_\ell$  we get

$$\begin{aligned} \partial_{\psi_\ell} f_M(m; \boldsymbol{\psi}) &= \partial_{\psi_\ell} F_M(m; \boldsymbol{\psi}) \times \sum_{b^*} \frac{f_{\text{GEV}, b^*}}{F_{\text{GEV}, b^*}} \\ &+ F_M(m; \boldsymbol{\psi}) \times \sum_{b^*} \left\{ \frac{\partial_{\psi_\ell} f_{\text{GEV}, b^*}}{F_{\text{GEV}, b^*}} - \frac{f_{\text{GEV}, b^*} \partial_{\psi_\ell} F_{\text{GEV}, b^*}}{F_{\text{GEV}, b^*}^2} \right\} \end{aligned} \quad (10)$$

where as above  $f_{\text{GEV}, b^*} := f_{\text{GEV}}(m, \boldsymbol{\theta}_{b^*})$ . But since the density is to be evaluated at  $m_{\boldsymbol{\psi}} := q_M(p; \boldsymbol{\psi})$  which depends on  $\boldsymbol{\psi}$ , we get instead

$$\partial_{\psi_\ell} f_M(m_{\boldsymbol{\psi}}; \boldsymbol{\psi}) = \frac{\partial f_M}{\partial m} \frac{\partial m_{\boldsymbol{\psi}}}{\partial \psi_\ell} + \frac{\partial f_M}{\partial \psi_\ell} = -\partial_m f_M \frac{\partial_{\psi_\ell} F_M}{f_M} + \partial_{\psi_\ell} f_M \quad (11)$$

where all functions at the r.h.s are evaluated at  $m_{\boldsymbol{\psi}}$  and  $\boldsymbol{\psi}$ . The second equality was obtained by using (8) with  $k$  replaced by  $\ell$ .

Similarly when differentiating the numerator of (8) w.r.t.  $\psi_\ell$  we get

$$\partial_{\psi_\ell} \left\{ \partial_{\psi_k} F_M(m_{\boldsymbol{\psi}}; \boldsymbol{\psi}) \right\} = -\partial_{m\psi_k}^2 F_M \frac{\partial_{\psi_\ell} F_M}{f_M} + \partial_{\psi_\ell \psi_k}^2 F_M = -\partial_{\psi_k} f_M \frac{\partial_{\psi_\ell} F_M}{f_M} + \partial_{\psi_\ell \psi_k}^2 F_M.$$

So by differentiating (8) w.r.t.  $\psi_\ell$

$$\partial_{\psi_\ell \psi_k}^2 q_M(p; \boldsymbol{\psi}) = -\frac{1}{f_M} \left\{ -\partial_{\psi_k} f_M \frac{\partial_{\psi_\ell} F_M}{f_M} + \partial_{\psi_\ell \psi_k}^2 F_M \right\} + \frac{\partial_{\psi_k} F_M}{f_M^2} \times \left\{ -\partial_m f_M \frac{\partial_{\psi_\ell} F_M}{f_M} + \partial_{\psi_\ell} f_M \right\}$$

where at the r.h.s. the quantity  $\partial_{\psi_\ell} f_M$  between the curly braces corresponds to (10) for  $m := m_{\boldsymbol{\psi}}$ . Similarly  $\partial_{\psi_k} f_M$  is given by (10) where  $\ell$  is replaced by  $k$ . By rearranging, we get the expression involving  $p \times p$  matrices

$$\begin{aligned} \partial_{\psi_\ell \psi_k}^2 q_M(p; \boldsymbol{\psi}) &= -\frac{1}{f_M} \partial_{\psi_\ell \psi_k}^2 F_M \\ &+ \frac{1}{f_M^2} \left[ \{ \partial_{\psi_k} f_M \} \{ \partial_{\psi_\ell} F_M \} + \{ \partial_{\psi_\ell} f_M \} \{ \partial_{\psi_k} F_M \} \right] \\ &- \frac{\partial_m f_M}{f_M^3} \{ \partial_{\psi_k} F_M \} \{ \partial_{\psi_\ell} F_M \}. \end{aligned} \quad (12)$$

Note that the expression for  $\partial_{\psi_\ell \psi_k}^2 q_M$  is symmetric in  $\ell$  and  $k$ , as expected.

The last formula can be used in matrix form

$$\partial_{\psi\psi}^2 q_M = -\frac{1}{f_M} \partial_{\psi\psi}^2 F_M + \frac{1}{f_M^2} \left[ \partial_\psi f_M \partial_\psi F_M^\top + \partial_\psi F_M \partial_\psi f_M^\top \right] - \frac{\partial_m f_M}{f_M^3} \partial_\psi F_M \partial_\psi F_M^\top. \quad (13)$$

Note that some care is needed in the evaluation because  $f_M^3$  can be very small. We now give details on the computation of  $\partial_m f_M(m)$ .

### Computing $\partial_m f_M(m)$

In the formula (11), we need the derivative of  $f_M(m)$  w.r.t.  $m$ . For the  $\text{GEV}(\mu, \sigma, \xi)$  distribution, the formula

$$\log f_{\text{GEV}}(m; \mu, \sigma, \xi) = -\log \sigma - \frac{\xi + 1}{\xi} \log \left\{ 1 + \xi [m - \mu] / \sigma \right\} + \log F_{\text{GEV}}(m; \mu, \sigma, \xi)$$

holds wherever  $\sigma + \xi [m - \mu] > 0$ . So by differentiating there w.r.t.  $m$

$$\frac{\partial}{\partial m} \log f_{\text{GEV}}(m) = -\frac{\xi + 1}{\sigma + \xi [m - \mu]} + \frac{f_{\text{GEV}}(m)}{F_{\text{GEV}}(m)} \quad (14)$$

where the dependence on the GEV parameters is omitted for simplicity. The condition  $\sigma + \xi [m - \mu] > 0$  defines the support of the GEV distribution and the derivative is zero when this condition does not hold.

Now let us consider the expression for  $f_M(m)$

$$f_M(m) = F_M(m) \sum_{b^*} \frac{f_{\text{GEV}, b^*}(m)}{F_{\text{GEV}, b^*}(m)}.$$

By differentiating w.r.t.  $m$

$$\frac{\partial}{\partial m} f_M(m) = f_M(m) \sum_{b^*} \frac{f'_{\text{GEV}, b^*}(m)}{F_{\text{GEV}, b^*}(m)} + F_M(m) \sum_{b^*} \left\{ \frac{f'_{\text{GEV}, b^*}(m)}{F_{\text{GEV}, b^*}(m)} - \frac{f_{\text{GEV}, b^*}(m)^2}{F_{\text{GEV}, b^*}(m)^2} \right\}$$

where a prime stands for a differentiation w.r.t.  $m$ . But by (14)

$$\frac{f'_{\text{GEV}, b^*}(m)}{f_{\text{GEV}, b^*}(m)} = -\frac{\xi_{b^*} + 1}{\sigma_{b^*} + \xi_{b^*} [m - \mu_{b^*}]} + \frac{f_{\text{GEV}, b^*}(m)}{F_{\text{GEV}, b^*}(m)}$$

provided that  $\sigma_{b^*} + \xi_{b^*} [m - \mu_{b^*}] > 0$  which defines the set  $\mathcal{S}^*(m)$  of the block indices  $b^*$  such that  $m$  lies in the support of  $\text{GEV}(\mu_{b^*}, \sigma_{b^*}, \xi_{b^*})$ . Hence when  $b^* \in \mathcal{S}^*(m)$

$$\frac{f'_{\text{GEV}, b^*}(m)}{F_{\text{GEV}, b^*}(m)} = -\left\{ \frac{\xi_{b^*} + 1}{\sigma_{b^*} + \xi_{b^*} [m - \mu_{b^*}]} \right\} \times \frac{f_{\text{GEV}, b^*}(m)}{F_{\text{GEV}, b^*}(m)} + \frac{f_{\text{GEV}, b^*}(m)^2}{F_{\text{GEV}, b^*}(m)^2}.$$

So finally, since the sums are actually for  $b^* \in \mathcal{S}(m)$

$$\frac{\partial}{\partial m} f_M(m) = \frac{f_M(m)^2}{F_M(m)} - F_M(m) \sum_{b^* \in \mathcal{S}^*(m)} \left\{ \frac{\xi_{b^*} + 1}{\sigma_{b^*} + \xi_{b^*} [m - \mu_{b^*}]} \right\} \times \frac{f_{\text{GEV}, b^*}(m)}{F_{\text{GEV}, b^*}(m)}. \quad (15)$$

### Computing the crossed derivative $\partial_{p,\psi}^2 q_M(p; \psi)$

The crossed derivative  $\partial_{p,\psi}^2 q_M(p; \psi)$  can be useful e.g., when an Ordinary Differential Equation (ODE) method is to be used to get the confidence limits on the quantile  $q_M(p)$ .

For a given probability  $p$  let  $m_\psi$  denote as before the quantile defined by  $F_M(m_\psi; \psi) = p$ . By differentiating this relation w.r.t.  $p$  we get:  $\partial_p m_\psi = 1/f_M(m_\psi; \psi)$ , hence with a new differentiation

$$\partial_{p,\psi}^2 m_\psi = \frac{-\partial_\psi f_M(m_\psi; \psi)}{f_M(m_\psi; \psi)^2}$$

where the derivative at the numerator of the fraction is given by (11) above.

## References

Rootzén H, Katz RW (2013). “Design Life Level: Quantifying Risk in a Changing Climate.” *Water Resources Research*, **42**, 5964–5972. doi:10.1002/wrcr.20425.