# Uncertainties in return values from extreme value analysis of peaks over threshold using the generalised Pareto distribution

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# Abstract

We consider the estimation of return values in the presence of uncertain extreme value model parameters, using maximum likelihood and other estimation schemes. Estimators for return value, which yield identical values when parameter uncertainty is ignored, give different values when uncertainty is taken into account. Given uncertain shape  $\xi$  and scale parameters of a generalised Pareto (GP) distribution, four sample estimators q for the N-year return value  $q_0$ , popular in the engineering community, are considered. These are:  $q_1$ , the quantile of the distribution of the annual maximum event with non-exceedance probability 1 - 1/N, estimated using mean model parameters;  $q_2$ , the mean of different quantile estimates of the annual maximum event with non-exceedance probability 1 - 1/N;  $q_3$ , the quantile of the predictive distribution of the annual maximum event with non-exceedance probability 1 - 1/N; and  $q_4$ , the quantile of the predictive distribution of the N-year maximum event with non-exceedance probability  $\exp[-1]$ . Using theoretical arguments, and simulation of samples of GP-distributed peaks over threshold (with  $\xi \in [-0.4, 0.1]$ ) and different GP parameter estimation schemes, we show that the rank order of estimators q and true value  $q_0$  can be predicted, and that differences between estimators q and  $q_0$  can be large. Judgements concerning the relative performance of estimators depend on the choice of utility function adopted to assess them. We consider bias in return value, bias in exceedance probability and bias in log exceedance probability. None of the four estimators performs well with respect to all three utilities under maximum likelihood estimation, but the posterior mean  $q_2$  is probably the best overall. The estimation scheme of Zhang (2010) provides low bias for  $q_1$ .

Keywords: return value; extreme; significant wave height; predictive distribution;

# 1. Introduction

Current engineering guidelines (e.g. ISO19901-1 2015, NORSOK N-003 2017, DNVGL-RP-C205 2017) require that extreme ocean environments are characterised marginally and conditionally in terms of return values, often with respect to covariates such as direction. Sometimes the metocean engineer's task is to identify combinations of return values for dominant variables in combination with associated values for other variables to represent extreme conditions for a given environment; these can also be summarised in terms of environmental design contours.

Recent years have seen marked improvements in quality and availability of field measurements, better numerical models for storm environments, and computationally feasible approaches to statistical inference. These allow for realistic quantification of uncertainty in estimation of the tails of distributions of quantities such as significant wave height. Specifically, we can quantify the uncertainty with which the parameters of the distribution of peaks over high threshold, or of block maxima, are estimated from a sample of data. Since return values are defined as functions of tail parameters, we can then quantify the effect of parameter uncertainty on estimates for return values.

When the uncertainty in model parameters is ignored (e.g. when points estimates are used), return values can be estimated using a number of different approaches popular in the ocean engineering literature, yielding identical results. For example, the *N*-year return value is typically defined as the quantile of the distribution of the annual maximum of a random quantity with non-exceedance probability 1-1/N. However, some authors use a definition of return value in terms of the quantile of the distribution of the *N*-year maximum with non-exceedance probability  $\exp[-1]$ . For large *N* and given model parameters, these two definitions yield effectively identical results as discussed below. However, once parameter uncertainty is incorporated, different approaches (including the two just mentioned) to return value estimation yield different results. These differences are of fundamental concern to the practising ocean engineer, and have been noted at least anecdotally for some time.

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Estimation of the *N*-year return value often relies on an extreme value model fitted to a sample of data, from which an estimate for the distribution of the annual maximum event is made. The characteristics of fitted model parameter estimates depend on (a) the nature of the sample (e.g. block maxima or peaks over threshold, sample size; complications due to lack of independence of observations, covariates, etc.) and (b) the choice of estimation strategy (e.g. generalised extreme value (GEV) distribution for block maxima or generalised Pareto (GP) distribution for threshold exceedances; estimation method including e.g. maximum likelihood or probability weighted moments; accommodations for dependence and covariates, etc.). The characteristics of the fitted parameter estimates in turn influence those of the estimated *N*-year return value.

Peaks over threshold analysis is often preferred over direct analysis of annual maxima since in typical applications there are multiple occurrences of threshold exceedences per annum. This might be the case for analysis of storm peak significant wave height from extra-tropical storms and typical threshold levels. In this sense, the peaks over threshold analysis can be more efficient since the same period of observation provides more observations for model building and tail. Madsen et al. (1997) provides expressions for the asymptotic variance of return value estimates from GEV and GP estimation. They conclude that for all practical purposes, GP provides the most efficient return value estimator in the case of maximum likelihood estimation. Dombry and Ferreira (2019) further show that peaks over threshold is preferable under maximum likelihood estimation in terms of (a) lower asymptotic bias and (b) lower asymptotic mean square error of the GP shape parameter estimate; however, the block maximum (GEV) approach is preferred in terms of asymptotic variance. Similar findings are given by Ferreira and de Haan (2015) when parameter estimation is performed using the method of probability weighted moments.

From a Bayesian perspective, an optimal value (such as return value) for some random quantity can only be provided with respect to an appropriate loss or utility structure. Christensen and Huffman (1985), building on the work of Geisser (1971), discuss Bayesian point estimation when no loss function is specified, and argue in favour of the posterior mean estimator (analogous to  $q_2$  in the notation of the abstract). Smith (2003) discusses issues related to incorporation of parameter uncertainty in estimates for return values. Serinaldi (2015) emphasises that the preferred approach to estimate environmental risk subject to uncertainty should involve direct estimation of probabilities of exceedance, or of structural failure over a given design life, incorporating all sources of epistemic and aleatory uncertainty in play. Fawcett and Green (2018) assess the performance of (posterior) predictive return levels relative to their estimative counterparts, such as the mean and mode of the posterior distribution of return value. They conclude that, for the cases considered in a simulation study, the predictive return value (analogous to  $q_3$  in the notation of abstract) yields estimates of exceedance probabilities with much higher precision than the corresponding exceedance probabilities obtained from estimative summaries.

Design standards such as DNVGL-RP-C205 (2017) also support the estimation of return values using so-called 'all sea state' or 'global' models. In this situation, the full distribution of e.g. sea-state significant wave height is estimated from a sample of (typically dependent) values of sea-state significant wave height using some parametric form e.g. related to a Weibull distribution (see Haselsteiner and Thoben 2020). This approach is not addressed in the current work, which focusses on return value estimation using peaks over threshold analysis.

The purpose of this article is to describe some of the more common estimators of return values used in ocean engineering, and to consider how uncertainties in parameters of extreme value models influence estimation of the bias of (a) return value, (b) probability of exceedance and (c) logarithm of the exceedance probability associated with a return value.

The article is arranged as follows. In Section 2 we provide an outline of different definitions of the *N*-year return value used by ocean engineers. For a given application, when parameter uncertainty is ignored, all these approaches yield the same estimate of return value. In Section 3, we extend the definition of return value to incorporate parameter uncertainty, suggesting six different estimators; Section 4 presents the corresponding estimators for samples of peaks over threshold following a GP distribution. Section 5 then illustrates the characteristics of the different estimators in a simulation study, assuming that maximum likelihood is used to estimate GP parameters. Section 6 provides simple theoretical arguments to help understand why estimators from Section 4 yield different values. Section 7 provides discussion and recommendations.

# 2. Return value estimators in the absence of tail parameter uncertainty

Suppose that a random variable A represents the maximum value of some physical quantity X (such as storm peak significant wave height) per annum. The N-year return value q of X is then conventionally defined by the equation

$$F_A(q) = \Pr(A \le q) = 1 - \frac{1}{N} \tag{1}$$

where  $F_A$  is the cumulative distribution function of the annual maximum A. We might also say that q is the quantile of the distribution of A with non-exceedance probability 1 - 1/N and write

$$q = Q_A (1 - 1/N)$$
(2)

where  $Q_A$  is the inverse of  $F_A$ , i.e.  $Q_A = F_A^{-1}$ . To estimate q, we need knowledge of  $F_A$ . We might estimate  $F_A$  using extreme value analysis on a sample of independent observations of A. For ocean engineering applications however, it is typically more efficient to estimate the distribution  $F_{X|X>\psi}$  of threshold exceedances of X above some high threshold  $\psi$  using a sample of independent observations of X, and use this in turn to estimate  $F_A$  as outlined in the Appendix and discussed in Section 3.

Applying the expression in Equation 1 to a time period of N years, we can also write

$$F_{A_N}(q) = F_A^N(q) = \left(1 - \frac{1}{N}\right)^N$$

where  $A_N$  is the N-year maximum event,  $F_{A_N}$  its cumulative distribution function, and  $Q_{A_N}$  its quantile function. Motivated by the fact that  $(1 - 1/N)^N$  converges to  $\exp[-1]$  with increasing N (with percentage error of  $\approx 1\%$  for N = 50 and  $\approx 0.1\%$  for N = 500), we can write

$$F_{A_N}(q') = \exp[-1], \text{ or}$$
(3)

$$q' = Q_{A_N}(\exp[-1]) \tag{4}$$

and solve for q', the quantile of the distribution of the N-year maximum with non-exceedance probability  $\exp[-1]$ . In the absence of uncertainty, it is clear that with increasing N the estimators q and q' of return value from Equations 1 and 3 are asymptotically equivalent by definition.

The discussion above illustrates how return values might be estimated from the distribution of the annual maximum (Equation 1) or the N-year maximum (Equation 3), when we are certain (or have perfect knowledge) about the tail of the distribution of annual maxima. In reality, this is never the case, because we estimate the tail and its parameters from a sample of data. It is natural therefore to seek to understand how this epistemic uncertainty affects estimation for return values, in particular to consider if systematic bias occurs.

#### 3. Return value estimators accommodating uncertain tail parameters

We now assume that the distribution of annual maximum A is known conditional on uncertain extreme value model parameters Z, so that (given Z) we can use any of the approaches in Section 2 to estimate return values. We seek to propagate uncertainty about Z through to estimates of return values. There are a number of plausible ways to achieve this based on extensions of Equations 1 and 3. These different estimators perform differently given uncertain knowledge of model parameters.

The basic mathematical tools used to incorporate uncertainty are now explained, for some random variable Y (e.g. A or  $A_N$ ) whose distribution is known conditional on random variables Z (e.g. uncertain model parameters). If the conditional cumulative distribution function  $F_{Y|Z}$  and the joint density  $f_Z$  of Z are known, the unconditional predictive distribution  $\tilde{F}_Y$  can be evaluated using

$$\tilde{F}_{Y}(y) = \int_{\boldsymbol{\zeta}} F_{Y|\boldsymbol{Z}}(y|\boldsymbol{\zeta}) f_{\boldsymbol{Z}}(\boldsymbol{\zeta}) \ d\boldsymbol{\zeta}$$

where  $\zeta \in \mathcal{D}_Z$  for range of integration  $\mathcal{D}_Z$  is understood throughout. When the joint density  $f_Z$  is estimated using Bayesian inference (as joint density  $f_{Z|D}$  from sample D) the unconditional distribution is known as a posterior predictive distribution for Y; alternatively,  $f_Z$  might be estimated using a bootstrapping scheme, or some other procedure to generate empirical estimates of the relative probabilities of different values of Z from data. Analogously, the expected value E[g(Z)] of deterministic function g of uncertain parameters Z given  $f_Z$  is given by

$$E[g(\boldsymbol{Z})] = \int_{\boldsymbol{\zeta}} g(\boldsymbol{\zeta}) f_{\boldsymbol{Z}}(\boldsymbol{\zeta}) \ d\boldsymbol{\zeta}.$$

We might consider  $g(\mathbf{Z})$  to be the N-year return value as estimated from Equation 1 or Equation 3, a function of uncertain parameters. This motivates considering the following estimators for return values.

# 3.1. Return value estimators using expected values of parameters: $q_1, q'_1$

The first estimator is motivated by the widespread approach of ignoring uncertainty in parameters Z for estimation of return values. A suitable estimator in this case (see Equation 2) would be the return value estimated using the expected values of parameters

$$q_1 = Q_{A|Z}(1 - 1/N|E[Z])$$
(5)

where  $E[\mathbf{Z}] = \int_{\boldsymbol{\zeta}} \boldsymbol{\zeta} f_{\mathbf{Z}}(\boldsymbol{\zeta}) \, d\boldsymbol{\zeta}$ , and  $Q_{A|Z}(p|\mathbf{Z})$  is the conditional quantile function for the annual maximum evaluated at non-exceedance probability p given model parameters  $\mathbf{Z}$ . A related estimator  $q'_1$  is defined using the distribution of the N-year maximum  $A_N$ 

$$q_1' = Q_{A_N|\boldsymbol{Z}}(\exp[-1]|E[\boldsymbol{Z}])$$

By analogy with Equations 1 and 3,  $q'_1$  is asymptotically equivalent to  $q_1$  and will be considered no further.

# 3.2. Expected quantiles of distribution of A and $A_N$ : $q_2$ , $q'_2$

The second estimator  $q_2$  is the expected quantile of distribution of A with non-exceedance probability 1 - 1/N given by

$$q_2 = E[Q_{A|\boldsymbol{Z}}(1-1/N|\boldsymbol{Z}])] = \int_{\boldsymbol{\zeta}} Q_{A|\boldsymbol{Z}}(1-1/N|\boldsymbol{\zeta}) f_{\boldsymbol{Z}}(\boldsymbol{\zeta}) \ d\boldsymbol{\zeta}.$$
 (6)

Estimator  $q_2$  involves first solving for the quantile of the distribution of the annual maximum with non-exceedance probability 1 - 1/N for each a large number of parameter choices  $\zeta$ , and then averaging. A related estimator  $q'_2$  is the expected quantile of distribution of  $A_N$  with non-exceedance probability  $\exp[-1]$ ,

$$q_2' = \int_{\boldsymbol{\zeta}} Q_{A_N|Z}(\exp[-1]|\boldsymbol{\zeta}) f_{\boldsymbol{Z}}(\boldsymbol{\zeta}) \ d\boldsymbol{\zeta}.$$

That is,  $q'_2$  involves first solving for the quantile of the distribution of the N-year maximum with non-exceedance probability  $\exp[-1]$  for a large number of parameter choices  $\boldsymbol{\zeta}$ , and then averaging. Since  $Q_{A_N|\boldsymbol{Z}}(\exp[-1]|\boldsymbol{\zeta})$  is asymptotically equivalent to  $Q_{A|\boldsymbol{Z}}(1-1/N|\boldsymbol{\zeta})$ , by construction estimator  $q'_2$  is asymptotically equivalent to  $q_2$ . Hence,  $q'_2$  is no longer considered.

# 3.3. Quantiles of predictive distributions of A and $A_N$ : $q_3$ , $q_4$

The third estimator is the quantile of predictive distribution of A with non-exceedance probability 1 - 1/N defined by

$$q_3 = \tilde{Q}_A (1 - 1/N) \tag{7}$$

where  $Q_A$  is the predictive quantile function for A, defined as the inverse of the predictive cumulative distribution function  $\tilde{F}_A$  given by

$$\tilde{F}_A(x) = \int_{\boldsymbol{\zeta}} F_{A|\boldsymbol{Z}}(x|\boldsymbol{\zeta}) f_{\boldsymbol{Z}}(\boldsymbol{\zeta}) \, d\boldsymbol{\zeta}.$$

Estimating  $q_3$  involves first estimating  $F_A$ , then solving for its 1 - 1/N quantile. The related fourth estimator is the quantile of predictive distribution of  $A_N$  with non-exceedance probability  $\exp[-1]$ 

$$q_4 = \tilde{Q}_{A_N}(\exp[-1]) \tag{8}$$

where  $Q_{A_N}$  is the predictive quantile function for  $A_N$ , defined as the inverse of the predictive cumulative distribution function  $F_{A_N}$  given by

$$\tilde{F}_{A_N}(x) = \int_{\boldsymbol{\zeta}} F_{A_N | \boldsymbol{Z}}(x | \boldsymbol{\zeta}) f_{\boldsymbol{Z}}(\boldsymbol{\zeta}) \ d\boldsymbol{\zeta}.$$

Estimating using  $q_4$  involves first estimating  $\tilde{F}_{A_N}$ , then solving for its exp[-1] quantile.

In the absence of parameter uncertainty,  $q_1$ ,  $q_2$  and  $q_3$  are equal to q. Further  $q'_1$ ,  $q'_2$  and  $q_4$  are equal to q', which converges to q with increasing N, as discussed in Section 2. That is, when there is no uncertainty in the parameters

Z, or when that uncertainty is ignored, all estimators will yield the same return value estimate. In the presence of uncertainty, however, there is no reason to expect equality between estimates using the four estimators  $q_1$ ,  $q_2$ ,  $q_3$  and  $q_4$  because they incorporate the effects of parameter uncertainty in different ways.

Numerous questions therefore arise: which estimator is most appropriate to use in metocean design? Is there a universally best choice, or is the choice problem-specific? For typical samples of metocean data, how different are the estimates obtained? How reasonable is it to calculate and quote return values using different estimators in the presence of uncertainty? How should we quantify and communicate the characteristics of extreme environments for metocean design, subject to uncertainty? How should good design decisions be made? Are there approaches to specification of design conditions that are inherently better than return values?

#### 4. Sample estimators for peaks over threshold

Suppose we observe samples of independent threshold exceedances which follow a GP distribution. We now define four sample estimators for return value corresponding to those introduced in Section 3, based on sample estimates of the GP shape and scale parameters.

#### 4.1. Generalised Pareto data

Independent observations X of threshold exceedance are assumed to be GP-distributed with shape parameter  $\xi$  and scale parameter  $\sigma$ 

$$F_{X|X>\psi,\boldsymbol{Z}}(x|\boldsymbol{\zeta}) = 1 - \left(1 + \frac{\xi}{\sigma} \left(x - \psi\right)\right)_{+}^{-1/\xi}, \quad \xi \neq 0$$
(9)

for  $x > \psi$ ,  $\psi \in (-\infty, \infty)$ ,  $\xi \in (-\infty, \infty)$ ,  $\sigma \in (0, \infty)$ ,  $\zeta = (\xi, \sigma)$  and  $(y)_+ = y$  for y > 0 and = 0 otherwise. When  $\xi = 0$ , the conditional distribution takes the form  $1 - \exp[-(x - \psi)/\sigma)]$ . In the absence of parameter uncertainty, the Appendix shows that the value of the N-year return value q solving Equation 1 or 3 for large N is given by

$$q = \frac{\sigma}{\xi} \left( N_*^{\xi} - 1 \right) + \psi, \quad \xi \neq 0 \tag{10}$$

where  $N_*$  is the expected number of threshold exceedances in N years, and  $q = \sigma \log[N_*] + \psi$  when  $\xi = 0$ .

Equation 10 illustrates that the relationship between q and  $\xi$  is non-linear, and that the cases  $\xi < 0$  and  $\xi \ge 0$  show different behaviours with increasing  $N_*$ : for  $\xi < 0$ , a finite upper limit for q as  $N_* \to \infty$  exists given by  $\psi + \sigma/(-\xi)$ , whereas for  $\xi \ge 0$  we see  $q \to \infty$  as  $N_* \to \infty$ . We might expect therefore that uncertain knowledge of  $\xi$  influences the value of q differently for different  $\xi$ , and that the approach we choose to take to estimate  $\xi$  (and  $\sigma$ ,  $\psi$  in general) and incorporate parameter uncertainty will influence our estimate of q. Section 4.2 below defines four estimators  $q_1, q_2, q_3$ and  $q_4$  of return value subject to uncertainty in  $\xi$  and  $\sigma$ , motivated by Section 3. Section 5 then explores differences between estimators q using numerical simulation. It is also possible to demonstrate some differences between return value estimators theoretically, as discussed in Section 6.

#### 4.2. Sample estimators of return values

We have a set  $\mathcal{Z} = \{\xi_i, \sigma_i\}_{i=1}^m$  of m independent estimates for the underlying (true known) parameters  $\xi_0, \sigma_0$  of a GP distribution  $F_{X|X>\psi,\mathbf{Z}}$  (see Equation 9), with fixed known extreme value threshold  $\psi$  corresponding to non-exceedance probability  $\tau$ . Without loss of generality, we assume that the pairs of elements of  $\mathcal{Z}$  are ordered in terms of decreasing  $\xi$ , so that  $\xi_1$  is the largest value of  $\xi$ .  $\mathcal{Z}$  might be output of a Markov chain Monte Carlo inference from some sample, a set of maximum likelihood parameter estimates from m different bootstrap resamples, or the judgements of m experts. We use  $\mathcal{Z}$  to construct return value estimators  $q_1, q_2, q_3$  and  $q_4$  as follows. First the Appendix provides expressions for  $F_A$  and  $F_{A_N}$  (from Section 2) and solves Equation 2, for  $F_{X|X>\psi,\mathbf{Z}}$  taking GP form; it also defines the expected number  $N_*$  of threshold exceedances in N years, and the expected number  $\lambda$  of events per annum. Then, replacing integration with respect to  $f_{\mathbf{Z}}(\boldsymbol{\zeta})d\boldsymbol{\zeta}$  with summation over the set  $\mathcal{Z}$ , Equations 5 and 10 yield

$$q_1 = \frac{\sum_i \sigma_i}{\sum_i \xi_i} \left( N_*^{\sum_i \xi_i/m} - 1 \right) + \psi \tag{11}$$

where summation is for i = 1, 2, ..., m. That is,  $q_1$  is formed using the mean values of uncertain GP parameter estimates in the standard equation for a return value. To estimate  $q_2$ , Equations 6 and 10 yield

$$q_2 = \frac{1}{m} \sum_{i} \frac{\sigma_i}{\xi_i} \left( N_*^{\xi_i} - 1 \right) + \psi.$$
 (12)

That is,  $q_2$  corresponds to the mean of m estimates, each corresponding to a different pair from  $\mathcal{Z}$ . To define  $q_3$ , we write Equation 7 as

$$\tilde{F}_A(x) = \frac{1}{m} \sum_i \exp\left[-\lambda \left(1-\tau\right) \left(1+\frac{\xi_i}{\sigma_i} \left(x-\psi\right)\right)^{-1/\xi_i}\right]$$
(13)

for  $\tilde{F}_A$ ; that is, we take the mean over *m* different estimates for the annual distribution (each corresponding to a different pair from  $\mathcal{Z}$ ) to form  $\tilde{F}_A(x)$  for each *x*. Then we set  $\tilde{F}_A(q_3) = 1 - 1/N$  such that

$$1 - \frac{1}{N} = \frac{1}{m} \sum_{i} \exp\left[-\lambda \left(1 - \tau\right) \left(1 + \frac{\xi_i}{\sigma_i} \left(q_3 - \psi\right)\right)^{-1/\xi_i}\right].$$
(14)

Finally, we estimate  $F_{A_N}$  as mean of *m* different estimates for the distribution of the *N*-year maximum using GP parameters taken from Z

$$\tilde{F}_{A_N}(q_4) = \frac{1}{m} \sum_i \exp\left[-N_* \left(1 + \frac{\xi_i}{\sigma_i} \left(q_4 - \psi\right)\right)^{-1/\xi_i}\right].$$

Equation 8 then gives  $q_4$  as quantile of the resulting distribution with non-exceedance probability  $\exp[-1]$ 

$$\exp[-1] = \frac{1}{m} \sum_{i} \exp\left[-N_* \left(1 + \frac{\xi_i}{\sigma_i} \left(q_4 - \psi\right)\right)^{-1/\xi_i}\right].$$
(15)

# 5. Differences between return value estimators explored by simulation and maximum likelihood estimation

We use simulation to explore the characteristics of the four return value estimators  $q_1$ ,  $q_2$ ,  $q_3$  and  $q_4$ . We assume that observations of threshold exceedances follow a GP distribution with shape  $\xi_0$ , scale  $\sigma_0 = 1$  and threshold  $\psi_0 = 0$  (and threshold non-exceedance probability  $\tau = 0$ ) for sample sizes are n = 100, 1,000 and 10,000. We estimate return values q using maximum likelihood estimates for  $\xi$  and  $\sigma$  from GP fits to  $m = 10^5$  realisations of samples, for true  $\xi_0$  values of -0.4, -0.35, ..., 0.1. This selection of values of  $\xi_0$  corresponds to those typically found in application to storm peak significant wave height from different ocean basins; for example, in the northern North Sea, values of  $\xi \in [-0.4, -0.1]$ have been reported (e.g. Elsinghorst et al. 1998, Ewans and Jonathan 2008, Randell et al. 2016); in the South China Sea, values of  $\xi \in [-0.1, +0.1]$  (e.g. Randell et al. 2015); and in the Gulf of Mexico,  $\xi \in [-0.1, +0.05]$  (e.g. Raghupathi et al. 2016).

Figure 1 gives scatter plots of the set  $\mathcal{Z} = \{\xi_i, \sigma_i\}$  of maximum likelihood parameter estimates  $\xi_i$ ,  $\sigma_i$  for the cases  $\xi_0 = -0.2$  and  $\xi_0 = 0.1$ . For larger sample sizes, the characteristics of the sample resemble those of the known Gaussian asymptotic form (e.g. Hosking and Wallis 1987), with  $\xi_i$  and  $\sigma_i$  approximately unbiased, but negatively correlated. For n = 100, the scatter plots appear non-Gaussian, with more occurrences of large negative values of  $\xi_i - \xi_0$  than of large positive ones. We might anticipate that the properties of return value estimators q relative to  $q_0$  depend on the characteristics of sample  $\mathcal{Z}$ , and hence on the method of parameter estimation.

# [Figure 1 about here.]

Differences between return value estimators and the known population return values are assessed as a function of  $\xi_0$ in Figures 2-5 below. For the purposes of return value calculations, we assume that the rate of occurrence  $\lambda = 100$  per annum. First we consider return period N = 100 years. Figure 2 illustrates the variation of true return value  $q_0$  as a function of  $\xi_0$ , for the three sample sizes under consideration, as a thick grey line. Differences in estimates  $\hat{q}$  for return values q are greatest for sample size n = 100; for larger sample sizes the differences between return value estimators is relatively small relative to the range of return values.

[Figure 2 about here.]

Figure 3 provides a better illustration of the differences between estimators q in terms of fractional bias

Fractional bias 
$$= \frac{q_j}{q_0} - 1$$
 for  $j = 1, 2, 3, 4$ .

Independent of sample size n, estimator  $q_2$  provides the smallest fractional bias. Recall, in the notation of Section 3, that  $q_2$  takes the form  $E[Q_{A|Z}(1-1/N|\mathbf{Z}])]$ ; that is,  $q_2$  is the average of m return value estimates, each corresponding to a pair of maximum likelihood parameter estimates. Return value estimator  $q_1$  provides consistent underestimation of return value. Recall that  $q_1$  is obtained by first estimating the mean of maximum likelihood parameters, then plugging these into the return value equation;  $q_1$  takes the form  $Q_{A|Z}(1-1/N|E[\mathbf{Z}])$  in the notation of Section 3.  $q_1$  can therefore be viewed as the return value estimated when we ignore variability in maximum likelihood parameter estimates, and simply use the average values of  $\xi$  and  $\sigma$  for return value calculation. Return value estimator  $q_4$  provides the largest negative bias, underestimating the return value. Referring to Section 3,  $q_4$  corresponds to the quantile of the predictive distribution for the N-year maximum  $A_N$  with non-exceedance probability  $\exp[-1]$ . Return value estimator  $q_3$  provides the largest positive bias, consistently overestimating the return value. Referring to Section 3,  $q_4$  corresponds to the quantile of the predictive distribution for the predictive distribution for the non-exceedance probability  $\exp[-1]$ . Return value estimator  $q_3$  provides the largest positive bias, consistently overestimating the return value. Referring to Section 3,  $q_4$  corresponds to the quantile of the predictive distribution for the predictive distribution for the annual maximum A with non-exceedance probability  $\exp[-1]$ . Return value estimator  $q_3$  provides the largest positive bias, consistently overestimating the return value. Referring to Section 3,  $q_3$  corresponds to the quantile of the predictive distribution for the annual maximum A with non-exceedance probability 1 - 1/N.

Figure 3 shows that the magnitude of fractional bias increases with  $\xi_0$  for all return value estimators except  $q_2$ , and for all sample sizes n, for the interval  $\xi_0 \in [-0.4, 0.1]$  (but see theoretical results in Section 6 which show that  $q_2 > q_3$ in the very unlikely case that  $\xi_0 > 1$ ). The figure also shows that, as n increases, fractional bias for all q reduces suggesting that all four approaches provide consistent estimation. However, for finite sample sizes, the bias in  $q_3$  in particular is very large, corresponding to around 20% for  $\xi_0 \approx -0.1$ . This is somewhat alarming given that  $q_3$  would be the default choice of many with a statistical background, defined in terms of the predictive distribution for the annual maximum.  $q_2$  clearly provides the least biased results, with fractional bias  $\leq 5\%$  for  $\xi_0 \in [-0.4, 0.05)$ , increasing for largest  $\xi_0$ .

#### [Figure 3 about here.]

Figure 4 assesses  $q_1, q_2, q_3$  and  $q_4$  in terms of the bias in their exceedance probabilities

Bias = 
$$\Pr(A > q_j) - \frac{1}{N} = 1 - F_A(q_j) - \frac{1}{N}$$
 for  $j = 1, 2, 3, 4$ .

Estimator  $q_3$  based on the annual predictive distribution provides the overall best performance for the smallest sample size n = 100, certainly for  $\xi_0 \in [-0.4, -0.1]$ . Unsurprisingly given the evidence of Figure 3,  $q_3$  nevertheless underestimates exceedance probability for all n. In fact, closer inspection of results shows that  $\Pr(A > q_3) = 0$  for n = 100 and  $\xi_0 < -0.2$ , as discussed further in relation to Figure 5 below. That is, estimator  $q_3$  lies beyond the upper end point of the distribution of the annual maximum A in these cases. Estimator  $q_4$  based on the predictive distribution for the N-year maximum provides the worst performance, and large overestimation of exceedance probability. For n = 1,000,  $q_2$  provides best performance for  $\xi_0 \ge -0.3$ . For n = 10,000,  $q_3$  provides best performance for  $\xi_0 \le -0.3$ , and  $q_2$  for  $\xi_0 \ge -0.2$ .

#### [Figure 4 about here.]

A third useful metric for comparison of return value estimators is bias in log exceedance probabilities

Bias = 
$$\log_{10}(\Pr(A > q_j)) - \log_{10}(\frac{1}{N}) = \log_{10}(1 - F_A(q_j)) + \log_{10}(N)$$
 for  $j = 1, 2, 3, 4$ .

This scale of comparison is useful since it is often more intuitive to assess errors in probabilities multiplicatively rather than additively. Results for N = 100 years are shown in Figure 5. The predictive estimator  $q_3$  performs poorly for sample size n = 100, with infinite bias in log exceedance probability for  $\xi_0 < -0.2$ . For  $n = 10,000, q_3$  performs better. Overall,  $q_2$  provides best performance.

#### [Figure 5 about here.]

Figure 6 considers return value estimator behaviour for return period N = 1,000 years. The general features of Figure 6 and Figure 3 (for N = 100) are very similar: the magnitude of fractional bias for N = 1,000 is greater than for N = 100 since we are extrapolating farther. Figure 7 considers the corresponding result for N = 10,000 years. We infer that return period (within the range considered) has little effect on the relative performance of return value estimators.

[Figure 6 about here.]

[Figure 7 about here.]

Figure 8 shows the bias in estimated exceedance probability for the case N = 10,000 years, for comparison with the results in Figure 4 (for N = 100).  $q_3$  provides the least biased estimate of exceedance probability for sample size n = 100. For larger n,  $\Pr(A > q_3) < 1/N$  for the interval of  $\xi_0$  considered. Conversely, all other estimators q produce overestimates of the exceedance probability. For  $n \ge 1,000$  and  $\xi_0 \ge -0.2$  there is little to choose between the estimators.

# [Figure 8 about here.]

In terms of bias in log exceedance probability, Figure 9 once again illustrates the relatively poor performance of the predictive estimator  $q_3$ , which yields infinite bias in a large proportion of the cases considered for return period N = 10,000 years since the estimate for  $q_3$  is beyond the upper end point of the distribution of the annual maximum A. Overall,  $q_2$  provides best performance.

#### [Figure 9 about here.]

Motivation for differences between return value estimators q and  $q_0$  is provided by Figure 10, which shows different annual maximum and N-year maximum cumulative distribution functions, and differences of cumulative distribution functions, for the case  $\xi_0 = -0.2$ , sample size n = 1,000 and return period N = 100 years.

# [Figure 10 about here.]

Comparison of the true N-year distribution  $F_{A_N}$  and its predictive estimate  $\tilde{F}_{A_N}$  in the left hand panel suggests that the latter is more spread; this is reasonable given evidence of parameter estimation variation in Figure 1. Consequently we expect predictive distributions  $\tilde{F}_A$  and  $\tilde{F}_{A_N}$  to have more mass in their tails compared to the true distributions  $F_A$ and  $F_{A_N}$ : this is shown to be the case in the top right hand panel. With increasing x, differences  $\tilde{F}_A(x) - F_A(x)$  and  $\tilde{F}_{A_N}(x) - F_{A_N}(x)$  start at zero, are then positive and then negative and ultimately zero again in both cases, except that the intervals corresponding to positive and negative differences is not the same. Clearly the locations of positive and negative differences are determined by the characteristics of set  $\mathcal{Z}$ . We are specifically interested in the value of the difference at the (true) N-year return value, indicated by a vertical line in the top right panel. Here,  $\tilde{F}_{A_N}$ overestimates the true distribution, and hence a return value estimator based on  $\tilde{F}_{A_N}$  will be biased low (and therefore  $q_4 < q_0$ ). The opposite is true for  $\tilde{F}_A$  (and therefore  $q_3 > q_0$ ).

Referring to Equation 15, taking the  $N^{\text{th}}$  root of each side, and applying the approximation  $\exp[-1/N] \approx 1 - 1/N$  for large N suggests that solving  $1 - 1/N = \tilde{F}_{A_N}^{1/N}(q_4)$  provides a good approximation to  $q_4$ . The top right panel illustrates that the difference  $\tilde{F}_{A_N}^{1/N} - \tilde{F}_A$  is never negative; this suggests that in particular  $q_3 \ge q_4$ . This ordering is clear from inspection of the bottom right panel, where the 1 - 1/N = 0.99 level is shown as a horizontal line.

#### 6. Differences between return value estimators demonstrated theoretically

We show theoretically that, in certain situations, there are systematic differences between different point estimators of return values. We first present a tabular summary of differences between return value estimators  $q_1, q_2, q_3$  and  $q_4$ and the true known value  $q_0$  given certain assumptions about the set  $\mathcal{Z} = \{\xi_i, \sigma_i\}$  of GP parameter estimates, and the true parameter values  $\xi_0, \sigma_0$ , with  $\psi_0=0$  assumed, and sufficiently large  $N_*$ . We then provide outline proofs of the inequalities. These inequalities are not specific to maximum likelihood estimates for GP parameter estimates.

[Table 1 about here.]

Inequality I1 occurs since  $x^N$  ( $x \ge 0, N = 1, 2, ...$ ) is a convex function. Jensen's inequality states that for m weights  $\{\omega_i\}_{i=1}^m$  such that  $\omega_i \ge 0$  and  $\Sigma_i \omega_i = 1$ , and a convex function  $\varphi(x)$  on some domain (such that  $\partial^2 \varphi / \partial x^2 \ge 0$ ), then  $\varphi(\Sigma_i \omega_i x_i) \le \Sigma_i \omega_i \varphi(x_i)$ . Setting  $\varphi(x) = x^N$ ,  $\omega_i = 1/m$  and  $x_i = \exp[-\lambda(1-\tau)(1+(\xi_i/\sigma_i)(x-\psi))^{-1/\xi_i}]$ , Jensen's inequality gives

$$\left(\frac{1}{m}\sum_{i} \exp[-\lambda(1-\tau)(1+(\xi_i/\sigma_i)(x-\psi))^{-1/\xi_i}]\right)^N \leqslant \frac{1}{m}\sum_{i} \exp[-N\lambda(1-\tau)(1+(\xi_i/\sigma_i)(x-\psi))^{-1/\xi_i}] \text{ or } \tilde{F}_A^N(x) \leqslant \tilde{F}_{A_N}(x)$$

for all x, referring to Equations 14 and 15. Therefore, with increasing x,  $\tilde{F}_{A_N}(x)$  will rise to a value of  $\exp[-1]$  (at  $q_4$ ) before  $\tilde{F}_A^N(x)$  does (at  $q_3$ ). For large N, the latter is equivalent to  $\tilde{F}_A(x)$  reaching a value of  $\exp[-1/N] \approx (1 - 1/N)$ . We deduce that  $q_3 \ge q_4$  for all choices of  $\mathcal{Z}$ . Inspection of the top right panel of Figure 10 illustrates this behaviour for specific conditions. Inspection of Figures 3, 5 and 6 shows that this inequality holds in our simulation study.

Inequalities I2 and I3 occur when the maximum value  $\xi_1$  of  $\xi$  from  $\mathcal{Z}$  is greater than the maximum of the true underlying value  $\xi_0$ , and zero. Recall we assume pairs of elements in  $\mathcal{Z}$  to be ordered in terms of decreasing  $\xi$ , so that  $\xi_1$  is the largest value of  $\xi$  in  $\mathcal{Z}$ .  $\xi_1 > \max(\xi_0, 0)$  is a relatively likely scenario in practice for a variable such as storm peak  $H_S$ . Fundamental physical understanding suggests a finite upper value to storm peak  $H_S$  (and hence  $\xi < 0$ ); there is considerable empirical evidence to support this also. Nevertheless, for a Bayesian inference we might specify a prior for  $\xi$  which includes 0 so as not to be too restrictive; estimates of  $\xi > 0$  would therefore be expected. For maximum likelihood inference with small samples, estimates for GP shape parameter exceeding zero are typical even for storm peak  $H_S$ . For other oceanographic variables such as wind speed,  $\xi > 0$  is typically expected.

To motivate I2, Equations 12 and 10 give

$$\frac{q_2}{q_0} = \frac{\frac{1}{m} \sum_i (\sigma_i / \xi_i) \left[ N_*^{\xi_i} - 1 \right]}{(\sigma_0 / \xi_0) \left[ N_*^{\xi_0} - 1 \right]}$$

for  $\xi \neq 0$  and the analogous expression when  $\xi = 0$ . For  $\xi_1 > \max(\xi_0, 0)$ , we can see that

$$\frac{q_2}{q_0} \approx \begin{cases} m^{-1} \left[ (\sigma_1 \xi_0) / (\sigma_0 \xi_1) \right] N_*^{\xi_1 - \xi_0}, & \xi_0 > 0 \\ m^{-1} \left[ \sigma_1 / (\sigma_0 \xi_1) \right] N_*^{\xi_1} / \log N_*, & \xi_0 = 0 \\ m^{-1} \left[ (-\sigma_1 \xi_0) / (\sigma_0 \xi_1) \right] N_*^{\xi_1}, & \xi_0 < 0, \end{cases}$$

all of which diverge to infinity with increasing  $N_*$ . That is,  $q_2$  always overestimates the true return value for large  $N_*$  when the largest value of  $\xi$  in  $\mathcal{Z}$  exceeds the maximum of the true value  $\xi_0$ , and 0. Inspection of Figures 3, 6 and 7 illustrates this for N = 1,000 and N = 10,000.

To demonstrate I3, we first approximate Equation 14 of Section 4.2 when  $q_3$  is large using the approximation  $\exp[x] \approx 1 + x$  for small x, so that

$$1 - \frac{1}{N} \approx \frac{1}{m} \sum_{i} \left( 1 - \lambda \left( 1 - \tau \right) \left( 1 + \frac{\xi_i}{\sigma_i} \left( q_3 - \psi \right) \right)^{-1/\xi_i} \right)$$
$$= 1 - \frac{1}{m} \sum_{i} \left( \lambda \left( 1 - \tau \right) \left( 1 + \frac{\xi_i}{\sigma_i} \left( q_3 - \psi \right) \right)^{-1/\xi_i} \right)$$

from which we obtain

$$\frac{1}{N_*} \approx \frac{1}{m} \sum_i \left( 1 + \frac{\xi_i}{\sigma_i} \left( q_3 - \psi \right) \right)^{-1/\xi_i}.$$

Substituting this expression for  $N_*$  into Equation 12 gives

$$q_{2} = \frac{1}{m} \sum_{i=1}^{m} \frac{\sigma_{i}}{\xi_{i}} \left[ \left\{ \frac{1}{m} \sum_{j=1}^{m} \left[ 1 + \frac{\xi_{j}}{\sigma_{j}} q_{3} \right]^{-1/\xi_{j}} \right\}^{-\xi_{i}} - 1 \right].$$

With  $\xi_1 > \max(\xi_0, 0)$ , the predictive distribution  $F_A$  has an infinite upper end point, and hence  $q_3 \to \infty$  as  $N_* \to \infty$ . Hence we can expand the above expression to give

$$\begin{split} q_2 &= \frac{1}{m} \left[ \frac{\sigma_1}{\xi_1} m^{\xi_1} \left[ 1 + \frac{\xi_1}{\sigma_1} q_3 \right] \left( 1 + \sum_{j=2}^m \left[ 1 + \frac{\xi_j}{\sigma_j} q_3 \right]^{-1/\xi_j} \left[ 1 + \frac{\xi_1}{\sigma_1} q_3 \right]^{1/\xi_1} \right)^{-\xi_1} \right. \\ &+ \left. \sum_{i=2}^m \frac{\sigma_i}{\xi_i} m^{\xi_i} \left[ 1 + \frac{\xi_1}{\sigma_1} q_3 \right]^{\xi_i/\xi_1} \left( 1 + \sum_{j=2}^m \left[ 1 + \frac{\xi_j}{\sigma_j} q_3 \right]^{-1/\xi_j} \left[ 1 + \frac{\xi_1}{\sigma_1} q_3 \right]^{1/\xi_1} \right)^{-\xi_i} \right] \\ &- \left. \frac{1}{m} \sum_{i=1}^m \frac{\sigma_i}{\xi_i} \right] \\ &\approx m^{\xi_1 - 1} q_3 \text{ for large } N_*. \end{split}$$

Hence as  $N_* \to \infty$ ,  $q_2, q_3 \to \infty$  and  $q_2/q_3 \to m^{\xi_1-1}$ . For  $\xi_1 < 1$ , highly likely for environmental variables like storm peak  $H_S$ , we conclude that  $q_3 > q_2$ . That is,  $q_3$  exceeds  $q_2$  for large  $N_*$  when  $1 > \xi_1 > \max(\xi_0, 0)$ . Combining this result with that from paragraph above, we deduce that  $q_3 > q_2 > q_0$  for large  $N_*$  when  $1 > \xi_1 > \max(\xi_0, 0)$ . Figures 3, 6 and 7 illustrate this ordering. For  $\xi_1 = 1$  and  $\xi_1 > \max(\xi_0, 0)$ , we observe that  $q_2$  and  $q_3$  are asymptotically equivalent. For  $\xi_1 > 1$ , we have  $q_2 > q_3$  for large  $N_*$  and  $\xi_1 > \max(\xi_0, 0)$ .

Unfortunately useful approximation of Equation 15 for large  $q_4$  and  $N_*$ , mimicking the approximation of Equation 14 for large  $q_3$  and large N here, is not possible, since the arguments of the exponent summands in Equation 15 do not become small with increasing  $q_4$  and  $N_*$ .

We can also demonstrate orderings of return value estimators when  $\xi_1 < \max(\xi_0, 0)$  to support the simulation study results. Inequalities I4, I5 and I6 occur when  $\xi_0 < 0$ , typically of relevance for extremes of storm peak  $H_S$ . In this situation, a true upper end point  $\psi + \sigma_0/(-\xi_0)$  exists. We can restrict discussion to  $\xi_1 < 0$ , since the case  $\xi_1 > 0$  has already been considered in I2 and I3. The relative ordering of  $q_0$ ,  $q_1$ ,  $q_2$  and  $q_3$  can be shown to be related to the relative sizes of different estimates for ratios of  $\sigma/\xi$  from  $\mathcal{Z}$  as outlined below, relative to  $q_0$ .

To motivate I4, we see from Equation 11 that the maximum value for  $q_1$  (at  $N_* = \infty$ ) is  $\psi + (1/m \sum_i \sigma_i)/(1/m \sum_i (-\xi_i))$ . Therefore, if  $(1/m \sum_i \sigma_i)/(1/m \sum_i (-\xi_i)) > \sigma_0/(-\xi_0)$ , the maximum value of  $q_1$  will exceed the true upper end point of the distribution  $F_A$ ;  $q_1$  must show positive bias in this case for sufficiently large  $N_*$ . More generally, the bias in  $q_1$  for large  $N_*$  is determined by the relative sizes of  $(1/m \sum_i \sigma_i)/(1/m \sum_i (-\xi_i))$  and  $\sigma_0/(-\xi_0)$ , and is not known prior to analysis. For I5, a similar argument, using Equation 12, shows that if  $(1/m) \sum_i (\sigma_i/(-\xi_i)) > \sigma_0/(-\xi_0)$ , the maximum value of  $q_2$  will exceed the true upper end point of the distribution  $F_A$ ;  $q_2$  must show positive bias in this case for sufficiently large  $N_*$ . More generally, the bias in  $q_2$  for large  $N_*$  is determined by the relative sizes of  $(1/m) \sum_i (\sigma_i/(-\xi_i))$  and  $\sigma_0/(-\xi_0)$ , and is not known prior to analysis. For I6, referring to Equation 13 for  $\xi_0 < 0$  and  $\xi_1 \in (\xi_0, 0)$ , suppose that the pair  $(\xi_{k^*}, \sigma_{k^*})$  provides the maximum value of  $\sigma/(-\xi)$  in  $\mathcal{Z}$ . Then  $\tilde{F}_A$  could have upper end point  $\psi + \sigma_{k^*}/(-\xi_{k^*}) > \psi + \sigma_0/(-\xi_0)$ . In this situation,  $q_3$  would exhibit positive bias for sufficiently large  $N_*$ . More generally, the bias in  $q_3$  for large  $N_*$  is determined by the relative sizes of known prior to analysis.

For illustration, in the simulation study in Section 5, the values of  $\sum_i \sigma_i / \sum_i (-\xi_i)$ ,  $\sum_i (\sigma_i / (-\xi_i)) / m$  and  $\sigma_{k^*} / (-\xi_{k^*})$  produce an increasing sequence for every choice of n and  $\xi_0$  considered, when  $\xi_1 = \max_{k \in (1,2,...,m)}(\xi_k) < 0$ ; that is, we expect  $q_1 < q_2 < q_3$ . Further, for small  $\xi_0$  the value of  $\sigma_0 / (-\xi_0)$  falls between the second and third terms in the sequence, indicating  $q_1 < q_2 < q_0 < q_3$  as observed in the simulation results. For large sample size n = 10,000 (for which  $\xi_1 < 0$ ) and  $\xi_0 \ge -0.15$ , the value of  $\sigma_0 / (-\xi_0)$  falls between the first and second terms so that  $q_1 < q_0 < q_2 < q_3$  for sufficiently large N. In fact, for simulations of the  $N = 10^8$  year return value, we observe that the function  $q_2 - q_0$  (of  $\xi_0$ ) crosses zero for n = 10,000 at approximately  $\xi_0 = -0.13$ .

## 7. Discussion and conclusions

This paper discusses the estimation of return values in the presence of uncertainty in extreme value model parameters. We show that different estimators for return value, which yield identical estimates when parameter uncertainty is ignored, yield different values when uncertainty is taken into account. Given uncertain shape and scale parameters Z of a GP distribution, four sample estimators for the *N*-year return value are considered:  $q_1 (= Q_{A|Z}(1 - 1/N|E|Z))$ , where  $Q_{A|Z}$  is the quantile of the annual maximum event *A* given parameters Z),  $q_2 (= E(Q_{A|Z}(1 - 1/N|Z)), q_3)$   $(= \tilde{Q}_A(1 - 1/N)$ , where  $\tilde{Q}$  is a predictive quantile) and  $q_4 (= \tilde{Q}_{A_N}(\exp[-1]))$ . We show by simulation and theory that, for given circumstances, the order of estimators q and true value  $q_0$  can be predicted, and that differences between estimators q and  $q_0$  can be very large. The ordering  $q_4 \leq q_1 \leq q_2 \leq q_3$  is observed in our simulation study, when Z corresponds to maximum likelihood estimates for a sample of peaks over threshold of sizes n = 100, 1,000 and 10,000 for true parameters  $\xi_0 \in [-0.4, 0.1]$  and  $\sigma_0 = 1$ . The true value  $q_0$  lies between  $q_1$  and  $q_3$ .

In general for maximum likelihood estimation and values of parameters typical for extreme value modelling of storm peak significant wave height, estimator  $q_2$  yields lowest bias, and the predictive estimator  $q_3$  is obviously the worst performer in terms of bias. In terms of exceedance probability Pr(A > q),  $q_3$  is in general a relatively good performer for  $\xi_0 < -0.2$ . In our simulations, this tends to be because  $q_3$  provides an estimate which is beyond the (known) upper end point of the distribution of annual maximum A. For larger  $\xi_0$ ,  $q_2$  and  $q_3$  are competitive. In terms of log exceedance probability,  $q_3$  performs spectacularly poorly for small sample size n;  $q_2$  is overall the best performer.

#### 7.1. The role of parameter estimation scheme

Many approaches exist to fit a GP distribution to a sample of independent threshold exceedances, e.g. as reviewed by Hosking and Wallis (1987); Madsen et al. (1997); Ashkar and Nwentsa Tatsambon (2007); de Zea Bermudez and Kotz (2010a,b); Mackay et al. (2011). Maximum likelihood estimation is the most popular approach (de Zea Bermudez and

Kotz 2010a), but the method of moments (MOM) and probability weighted moments (PWM) are also popular in the environmental and engineering literature. The procedures of Zhang and Stephens (2009) and Zhang (2010), referred to here as empirical Bayesian (EB), also also attractive due to their low parameter bias characteristics. The simulation study of Section 5 assumes that maximum likelihood estimation is used for model parameter inference and construction of set Z; the findings of the simulation study are therefore only directly relevant for this method of inference. Maximum likelihood estimation is a natural choice from the statistical perspectives of consistency, asymptotic Gaussianity and asymptotic efficiency (for  $\xi > -0.5$ , Davison and Smith 1990). However, other estimation schemes are known to perform particularly well e.g. for small samples. For large samples, it is also known (Hosking and Wallis 1987) that shape and scale parameters estimates for each of maximum likelihood, MOM and PWM inference are asymptotically Gaussian-distributed with variance-covariance matrix which converges to zero with increasing sample size n, and that shape and scale parameter estimates exhibit negative correlation. This suggests that the results of the maximumlikelihood-based simulation study are generally indicative of the influence of model parameter uncertainty on return value estimators for large sample size n.

Moreover, the theoretical arguments presented in Section 6 to explain the rank ordering of estimators q and truth  $q_0$  for given conditions are applicable using parameter estimates  $\mathcal{Z}$  from any estimation scheme of choice, including maximum likelihood, MOM, PWM and other approaches such as the method of Zhang (2010).

The values of estimates for  $q_1$ ,  $q_2$ ,  $q_3$  and  $q_4$  are deterministic functions of the set  $\mathcal{Z}$  of parameter estimates. Different parameter estimation schemes provide different sets  $\mathcal{Z}$ , as illustrated in Figure 11. Visual inspection of the figure suggests that, for given sample size n, differences between sets  $\mathcal{Z}$  are relatively small.

#### [Figure 11 about here.]

Nevertheless, for finite sample sizes n, it is interesting to estimate the relative characteristics of estimators q using this set of relatively popular estimation schemes. Figure 12 shows estimates  $\hat{q}_1$ ,  $\hat{q}_2$ ,  $\hat{q}_3$  and  $\hat{q}_4$  for sample size n = 100 from each of empirical Bayesian (EB), method of moments (MOM) and probability weighted moments (PWM) estimation schemes. Details of the methods used are given by e.g. Mackay et al. (2011), and software is available from Jonathan (2020).

# [Figure 12 about here.]

The general characteristics of Figure 12 are similar to those of Figure 3 for maximum likelihood, in particular regarding the ordering of estimators by bias. The EB estimation scheme of Zhang (2010) is designed to provide low bias in GP parameter estimates, and hence provides estimates for  $q_1$  with lowest bias. However, the performance of the EB scheme is qualitatively no better to that of the other estimation schemes for estimates of  $q_2$ ,  $q_3$  and  $q_4$ . Results for other sample sizes reflect those for n = 100, and are reported in Jonathan (2020), together with simulation code for estimation of bias in return value, exceedance probability and log exceedance probability for any combination of estimator and estimation scheme. For larger sample sizes, the EB again provides  $q_1$  estimates with low bias, and hence relatively low bias with respect to (log-) exceedance probability also.

More generally, characteristics of posterior Bayesian estimates for GP shape and scale can of course be strongly influenced by prior specification. Zhang (2007) proposes a likelihood moment estimator with high asymptotic efficiency. Further, non-parametric approaches including the moment (M) estimator of Dekkers et al. (1989) are available.

# 7.2. Wave loading

The wave loading on a structure, or its response to wave loading, might typically vary as a monotonically increasing function  $\mathcal{R}$  of variable X. In this situation, we might be interested in quantities such as  $\Pr(A^* > s)$ , where  $A^*$  is the annual maximum event for loading (or response)  $\mathcal{R}(X)$ , and s might represent structural strength (or critical response). Following the arguments of Section 2, in the absence of uncertainty, the *N*-year structural strength  $q^*$  for  $\mathcal{R}(X)$  (analogous to the *N*-year return value q for X in Equation 10) is given by  $q^* = \mathcal{R}(q)$  where  $q = \frac{\sigma}{\xi} \left( N_*^{\xi} - 1 \right) + \psi$ , for  $\xi \neq 0$  with the corresponding limiting expression when  $\xi = 0$ . Note that the \* superscript indicates a quantity related to a load or response variable. Sample estimators  $q_1^*$ ,  $q_2^*$ ,  $q_3^*$  and  $q_4^*$  for  $q^*$  are easily derived from those in Section 4. Figure 13 shows fractional bias for estimators of the 100-year structural strength using the simulation procedure described in Section 5, for the case  $\mathcal{R}(x) = x^2$ .

# [Figure 13 about here.]

Comparing Figures 13 and Figure 3, gross bias characteristics of q and  $q^*$  estimators are the same for this choice of  $\mathcal{R}$ , except that the extent of bias is greater for  $q^*$  that for q. By definition, the exceedance probabilities associated with  $q^*$  (in the distribution of the annual maximum  $A^*$  of  $\mathcal{R}(X)$ ) and q (in the distribution of the annual maximum A of

X) must be equal. Therefore Figures 4 and 5 provide the relevant assessment. The bias of estimators q relative to  $q_0$  will be influenced by the specification of  $\mathcal{R}$ .

More generally, loading R given environmental variable X will not be a deterministic function. However, the conditional distribution  $F_{R|X}$  for a single loading event is usually accessible using numerical modelling, wave tank experiments or Morison-type fluid loading approximations (e.g. Tromans and Vanderschuren 1995; Ross et al. 2019). The conditional distribution  $F_{R|Z}$  for load given uncertain extreme value parameters Z for X can be evaluated using

$$F_{R|\mathbf{Z}}(r|\boldsymbol{\zeta}) = \int_{x} F_{R|X}(r|x) f_{X|\mathbf{Z}}(x|\boldsymbol{\zeta}) \, dx$$

for  $x \in \mathcal{D}_X$  for domain  $\mathcal{D}_X$ , where  $f_{X|Z}$  is the conditional density of X given Z. Following the derivation  $F_{A_N|Z}$  in the Appendix, the conditional cumulative distribution function  $F_{A_N|Z}$  of the maximum N-year loading given Z is then

$$F_{A_N^*|\boldsymbol{Z}}(r|\boldsymbol{\zeta}) = \exp\left[-N\lambda\left(1 - F_{R|\boldsymbol{Z}}(x|\boldsymbol{\zeta})\right)\right].$$

The probability of structural failure  $p_F$  during a design life of N years given fixed structural strength s due to loading R can then be estimated using the predictive distribution  $\tilde{F}_{A_N^*}$  given by

$$\tilde{F}_{A_N^*}(r) = \int_{\boldsymbol{\zeta}} F_{A_N^*|\boldsymbol{Z}}(r|\boldsymbol{\zeta}) f_{\boldsymbol{Z}}(\boldsymbol{\zeta}) \ d\boldsymbol{\zeta}$$

and setting  $p_F = \Pr(A_N^* > s) = 1 - \tilde{F}_{A_N^*}(s)$ . This derivation is analogous to that underlying return value estimator  $q_4$ , except that the value of N would typically be smaller, and  $p_F$  would be considerably smaller than  $\exp[-1]$ . However, as the discussion around the characteristics of  $q_4$  and Figure 13 shows, this estimator will also typically suffer from bias.

#### 7.3. Conclusions

Theoretical results in Section 6 demonstrate that a systematic ordering of return value estimates q occurs for any parameter estimation scheme, including maximum likelihood. Theoretical results supported by simulations in Sections 5 suggest that none of the estimators q performs well with respect to all three performance measures considered here for maximum likelihood estimation; the predictive mean estimator  $q_2$  performs best overall.

The work of Zhang and Stephens (2009) and Zhang (2010) supported by simulation results in Section 7.1 suggests that their empirical Bayesian estimation scheme provides low bias in GP parameter estimates and hence good performance for estimation of  $q_1$ . In relatively simple applications, where the effects of other sources of random and systematic variability can be ignored, estimator  $q_1$  estimated using the method of Zhang (2010) offers lowest bias in return values over all estimators and estimation schemes.

As sample size n increases, biases in the four return value estimators q reduce in magnitude. Given a sufficiently large n, differences between estimators can be reduced to acceptable levels using any parameter estimation scheme; but the required n might well be very large. Moreover, a typical environmental extreme value analysis requires modelling of other sources of variation including extreme value threshold, rate of occurrence, potential extremal dependence and the effects of covariates. Even with a large n, the effective sample size for GP parameter estimation given specific covariate values might be < 100 in many applications. We might therefore anticipate large differences between estimators q. From a statistical modelling perspective, maximum likelihood estimation provides a flexible framework for incorporation of competing sources of variation; it also offers asymptotic efficiency.

From the perspective of predictive inference, estimators  $q_3$  and  $q_4$  might be considered preferable since they are estimated from predictive distributions which incorporate modelling uncertainty explicitly. In this case, inequality I1 shows that  $q_3 \ge q_4$  always. Simulation suggests further that  $q_3 \ge q_0 \ge q_4$  always for the situations considered. An estimator of the form  $\alpha q_3 + (1 - \alpha)q_4$  (for  $\alpha \in [0, 1]$ ) might provide a pragmatic compromise with better performance than either  $q_3$  and  $q_4$ . Preliminary evaluation of  $(q_3 + q_4)/2$  using maximum likelihood estimation suggests this is a promising candidate. In terms of bias, it is competitive with  $q_2$ . The bias of its exceedance probability is similar to that of  $q_3$  and generally better than that of  $q_2$ . The bias of its log probability is lower in magnitude than that of  $q_3$ , but not as low as that of  $q_2$ .

Summarising multivariate distributions for metocean variables in terms of return values has obvious advantages in terms of conciseness of description of an extreme ocean environment, for communication between different parties involved in offshore structural design. However, in reality, the accurate estimation of probability of structural failure should be the clear focus of analysis. From a predictive perspective, the effects of all sources of modelling uncertainty should be propagated carefully through the entire sequence of design calculations, expressed probabilistically, so that (a) the estimation of failure probability reflects these uncertainties as fully and fairly as possible, and (b) resources

can hence be devoted to reducing the largest sources of uncertainty on failure probability in a rational and systematic manner. In this light, the use of summary statistics such as metocean return values at intermediate design stages in place of full distributions of variables (when available) should be avoided.

Judgements regarding the performance of estimators depend on the choice of utility or loss function adopted to assess it. It is likely that many discussions of return value estimates by environmental and engineering practitioners occur with insufficient awareness of systematic differences between estimators and estimation schemes highlighted by the current work, and of the importance of appropriate utilities to assess return value estimator characteristics appropriately.

#### 8. Acknowledgements

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# Appendix : Estimating the distribution of annual maximum A, the N-year maximum $A_N$ and return values

According to asymptotic statistical theory, under the assumption that the random variable X belongs to the maximum domain of attraction of a non-degenerate distribution, the distribution of X exceeding threshold  $\psi$  converges (Pickands 1975) to the generalised Pareto (GP) distribution as the threshold increases. We therefore typically assume, for sufficiently large threshold  $\psi$  that the conditional distribution function  $F_{X|X>\psi,Z}$  for parameters Z follows GP form as defined in Section 3. Usually, the value of threshold is set prior to estimation of  $\xi$  and  $\sigma$  from the sample of values for X (e.g. by examining a mean residual life plot, Coles 2001), although this is not always the case (Scarrott and MacDonald 2012). Various approaches to estimation of  $\xi$  and  $\sigma$  as used, including maximum likelihood, the method of moments and probability weighted moments. We emphasise the conditioning of distributions with respect to Z explicitly, since different approaches to incorporating the uncertainty in Z lead to the differences between return value estimators discussed in this work.

# $F_{A|\mathbf{Z}}$ and $F_{A_N|\mathbf{Z}}$

Given  $F_{X|X>\psi,\mathbf{Z}}$ , the distribution  $F_{A|\mathbf{Z}}$  of annual maxima can be derived using

$$F_{A|\mathbf{Z}}(x|\boldsymbol{\zeta}) = \Pr(A \le x|\boldsymbol{\zeta}) = \sum_{k=0}^{\infty} f_C(k) F_{X|\mathbf{Z}}^k(x|\boldsymbol{\zeta})$$

where C is the number of occurrences of X per annum, with probability mass function  $f_C$  and

$$F_{X|\mathbf{Z}}(x|\boldsymbol{\zeta}) = \tau + (1-\tau)F_{X|X>\psi,\mathbf{Z}}(x|\boldsymbol{\zeta})$$

where  $\tau = \Pr(X < \psi)$ . In practice,  $f_C$  is unknown and must also be estimated from data. Density  $f_C$  is often described by a Poisson distribution such that  $f_C(k) = \exp[-\lambda]\lambda^k/k!$ , k = 0, 1, 2, ..., for annual rate  $\lambda > 0$  to be estimated. Assuming for simplicity that  $\lambda$  is known, the expression for  $F_{A|Z}$  simplifies (e.g. Ross et al. 2017) to

$$F_{A|\boldsymbol{Z}}(x|\boldsymbol{\zeta}) = \exp[-\lambda \left(1 - F_{X|\boldsymbol{Z}}(x|\boldsymbol{\zeta})\right)].$$

Applying the above expression to a time period of N years, we evaluate the distribution of the N-year maximum  $A_N$  to be

$$F_{A_N|\boldsymbol{Z}}(x|\boldsymbol{\zeta}) = F_{A|\boldsymbol{Z}}^N(x|\boldsymbol{\zeta}) = \exp[-N\lambda\left(1 - F_{X|\boldsymbol{Z}}(x|\boldsymbol{\zeta})\right)].$$

Writing  $\bar{F}_{X|X>\psi,\mathbf{Z}}$  for the conditional tail distribution  $1 - F_{X|X>\psi,\mathbf{Z}}$ , the expressions for  $F_{A|\mathbf{Z}}$  and  $F_{A_N|\mathbf{Z}}$  become

$$F_{A|\mathbf{Z}}(x|\boldsymbol{\zeta}) = \exp[-\lambda (1-\tau) \bar{F}_{X|X>\psi,\mathbf{Z}}(x|\boldsymbol{\zeta})] \text{ and } F_{A_N|\mathbf{Z}}(x|\boldsymbol{\zeta}) = \exp[-N\lambda (1-\tau) \bar{F}_{X|X>\psi,\mathbf{Z}}(x|\boldsymbol{\zeta})]$$

where for the GP distribution

$$\bar{F}_{X|X>\psi,\mathbf{Z}}(x|\boldsymbol{\zeta}) = \left(1 + \frac{\xi}{\sigma} \left(x - \psi\right)\right)_{+}^{-1/\xi}$$

and  $= \exp[-(x - \psi)/\sigma)]$  when  $\xi = 0$ . That is, the annual maximum A and N-year maximum  $A_N$  follow generalised extreme value distributions. An alternative approach to the derivation above (e.g. Smith 1987; Northrop et al. 2017) starts by assuming that the number  $\lambda$  of events X per annum is given (i.e. estimated independently), but that the number of events exceeding threshold  $\psi$  is random and follows a binomial distribution  $\operatorname{Bin}(\lambda, (1 - \tau))$ , which can be approximated by  $\operatorname{Poiss}(\lambda(1 - \tau))$  when  $\lambda$  is large and  $(1 - \tau)$  is near zero. Then for  $F_{X|Z} \approx 1$ ,  $\overline{F}_{X|Z} \ll 1$  and  $\log(1 - \overline{F}_{X|Z}) \approx -\overline{F}_{X|Z}$ . Hence  $F_{A|Z}(x)$  can be approximated using

$$F_{A|\mathbf{Z}}(x|\boldsymbol{\zeta}) = F_{X|\mathbf{Z}}(x|\boldsymbol{\zeta})^{\lambda} = \exp\left[\lambda\log\left(F_{X|\mathbf{Z}}(x|\boldsymbol{\zeta})\right)\right] = \exp\left[\lambda\log\left(1 - \bar{F}_{X|\mathbf{Z}}(x|\boldsymbol{\zeta})\right)\right]$$
  
$$\approx \exp\left[-\lambda\Pr(X > x|X > \psi, \mathbf{Z} = \boldsymbol{\zeta})(1 - \tau)\right] \text{ when } F_{X|\mathbf{Z}} \approx 1$$
  
$$= \exp\left[-\lambda\left(1 - \tau\right)\bar{F}_{X|X > \psi, \mathbf{Z}}(x|\boldsymbol{\zeta})\right]$$

as before.

# Return values

The expressions for  $F_{A|Z}$  however derived and  $F_{A_N|Z}$  facilitate estimation of different return value estimators given  $F_{X|X>\psi,Z}$  (with parameters  $\xi$  and  $\sigma$ ) for any return period N, as described in Section 4. For brevity, we write the expected number  $N_*$  of occurrences of threshold exceedances in N years as  $N_* = N\lambda (1 - \tau)$ .

Given  $\xi$  and  $\sigma$ , the N-year return value q (conditional on  $\mathbf{Z} = \boldsymbol{\zeta}$ ) can be found by solving Equation 1

$$1 - 1/N = \exp[-\lambda (1 - \tau) \bar{F}_{X|X > \psi, \mathbf{Z}}(q|\boldsymbol{\zeta})] \text{ so that}$$
$$\log\left[\frac{1}{1 - 1/N}\right] = \lambda (1 - \tau) \bar{F}_{X|X > \psi, \mathbf{Z}}(q|\boldsymbol{\zeta}).$$

With  $\log[1/(1-1/N)] = 1/N + 1/(2N^2) + 1/(3N^3) + ... \approx 1/N$  for large N, this yields

$$\frac{1}{N_*} = \bar{F}_{X|X>\psi, \mathbf{Z}}(q|\boldsymbol{\zeta}) = \left(1 + \frac{\xi}{\sigma} \left(q - \psi\right)\right)_+^{-1/\xi}$$

and hence, conditional on  $\mathbf{Z} = \boldsymbol{\zeta}$ , the return value is given by  $q = \frac{\sigma}{\xi} \left( N_*^{\xi} - 1 \right) + \psi$  as given in the main text. When  $\xi = 0$ , the last two equations read  $1/N_* = \exp[-(q - \psi)/\sigma]$  and  $q = \sigma \log[N_*] + \psi$ .

#### Dependence

When observations of X exhibit dependence, the equations for  $F_{A|Z}$  and  $F_{A_N|Z}$  can be adjusted by incorporating an extremal index  $\theta$  (e.g. Davison et al. 2012) such that

$$F_{A|\boldsymbol{Z}}(x) = \sum_{k=0}^{\infty} f_C(k) F_{X|\boldsymbol{Z}}^{k\theta}(x|\boldsymbol{\zeta})$$

where  $\theta$  must also be estimated. This approach might be advantageous when estimating e.g.  $F_{A|Z}$  from dependent sea-state  $H_S$  instead of independent storm peak  $H_S$ .

#### Covariates

Further, the equations above also assume that X does not exhibit systematic variation with covariates (such as storm direction or season in the case of significant wave height). In the presence of a single covariate  $\Phi$ , distributions above are conditional on  $\Phi$ , and parameters functions of  $\Phi$ . The inference becomes non-stationary and computationally more demanding, but we can still evaluate unconditional distributions e.g.  $F_{A|Z}$  by marginalisation using

$$F_{A|\mathbf{Z}}(x|\boldsymbol{\zeta}) = \int_{\phi} F_{A|\mathbf{Z},\Phi}(x|\boldsymbol{\zeta},\phi) f_{\Phi}(\phi) \ d\phi$$

where  $f_{\Phi}$  is the density of  $\Phi$  which must itself also be estimated.

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Figure 1: Scatter plots of  $10^5$  maximum likelihood GP parameter estimates  $\xi_i$  and  $\sigma_i$  for the cases  $\xi_0 = -0.2$  (top) and  $\xi_0 = 0.1$  (bottom). Columns from left to right correspond to sample sizes n of 100, 1,000 and 10,000.



Figure 2: Return value estimates  $\hat{q}_1$  (solid),  $\hat{q}_2$  (dashed),  $\hat{q}_3$  (dotted),  $\hat{q}_4$  (dot-dashed) for a return period of 100 years, assuming 100 events per annum drawn from a generalised Pareto distribution with shape  $\xi_0$ , scale  $\sigma_0 = 1$  and threshold  $\psi_0 = 0$ . Return values estimated using maximum likelihood parameter estimates from  $10^5$  realisations of samples of size 100 (left), 1,000 (centre) and 10,000 (right). Thick grey lines indicate true return value behaviour.



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Figure 4: Bias in exceedance probabilities corresponding to return value estimates  $\hat{q}_1$  (solid),  $\hat{q}_2$  (dashed),  $\hat{q}_3$  (dotted),  $\hat{q}_4$  (dot-dashed) for a return period of 100 years, assuming 100 events per annum drawn from a GP distribution with shape  $\xi_0$ , scale  $\sigma_0 = 1$  and threshold  $\psi_0 = 0$ . Bias estimated using maximum likelihood parameter estimates from  $10^5$  realisations of samples of size 100 (left), 1,000 (centre) and 10,000 (right).



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Figure 10: Motivation for differences between return value estimators for the case  $\xi_0 = -0.2$ , sample size n = 1,000 and return period N = 100 years. The left hand panel shows the following cumulative distribution functions (cdfs):  $F_A$ , the (true) distribution of the annual maximum;  $\tilde{F}_{A_N}$ , the (true) distribution of the *N*-year maximum;  $\tilde{F}_A$ , the predictive distribution for the annual maximum;  $\tilde{F}_{A_N}$ , the predictive distribution for the *N*-year maximum;  $\tilde{F}_{A_N}^{1/N}$ , the *N*-th predictive distribution for the *N*-year maximum. The top right panel gives differences between cdfs, with the vertical line indicating the true *N*-year return value. The bottom right panel illustrates annual maximum cdfs  $F_A$ ,  $\tilde{F}_A$  together with  $\tilde{F}_{A_N}^{1/N}$  for non-exceedance probabilities near to 1 - 1/N; the horizontal line is drawn at this level.



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Figure 12: Fractional bias for return value estimates  $\hat{q}_1$  (solid),  $\hat{q}_2$  (dashed),  $\hat{q}_3$  (dotted),  $\hat{q}_4$  (dot-dashed) for a return period of 100 years, assuming 100 events per annum drawn from a GP distribution with shape  $\xi_0$ , scale  $\sigma_0 = 1$  and threshold  $\psi_0 = 0$ . Parameter estimates estimated from  $10^5$  realisations of samples of size 100 using empirical Bayesian (EB), method of moments (MOM) and probability weighted moments (PWM) estimation schemes. Unbiased estimates would have fractional bias of zero. Corresponding results for maximum likelihood estimation given in Figure 3.



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|---|---|----|
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|    | Inequality    | Condition  |
|----|---------------|--|
| I1 | $q_3 \ge q_4$ | Always   |
| I2 | $q_2 > q_0$   | $\xi_1 > \max(\xi_0, 0)$   |
| I3 | $q_3 > q_2$   | $1 > \xi_1 > \max(\xi_0, 0)$   |
| I4 | $q_1 > q_0$   | $\xi_0, \xi_1 < 0, \ \sum_i \sigma_i / \sum_i (-\xi_i) > \sigma_0 / (-\xi_0)$              |
| I5 | $q_2 > q_0$   | $\xi_0, \xi_1 < 0, \ (1/m) \sum_i (\sigma_i / (-\xi_i)) > \sigma_0 / (-\xi_0)$             |
| I6 | $q_3 > q_0$   | $\xi_0, \xi_1 < 0, \max_{k \in (1,2,\dots,m)} (\sigma_k / (-\xi_k)) > \sigma_0 / (-\xi_0)$ |

Table 1: Inequalities involving sample estimators for N-year return values, and conditions necessary for their validity. Note that the condition  $N \rightarrow \infty$  applies to all these cases. Inequalities are not specific to maximum likelihood estimation of GP parameters.