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EXTREMES OF SPHEROID SHAPE FACTOR BASED ON TWO DIMENSIONAL PROFILES

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The extremal shape factor of spheroidal particles is studied. Three dimensional particles are considered to be observed via their two dimensional profiles and the problem is to predict the extremal shape factor in a given size class. We proof the stability of the domain of attraction of the spheroid's and its profile shape factor under a tail equivalence condition. We show namely that the Farlie–Gumbel–Morgenstern bivariate distributions gives the tail uniformity. We provide a way how to find normalising constants for the shape factor extremes. The theory is illustrated on examples of distributions belonging to Gumbel and Fréchet domain of attraction. We discuss the ML estimator based on the largest observations and hence the possible statistical applications at the end.

Keywords: sample extremes, domain of attraction, normalising constants, FGM system of distributions

AMS Subject Classification: 60G70, 62G32, 62P30

1. INTRODUCTION

It is a common problem of material science to predict behaviour of three dimensional objects based on lower dimensional observations – profiles, projections etc. There is a specific problem to estimate tail behaviour of some particle characteristic as the damage of the material is claimed to be related rather to the extremes than to the mean values of the microstructure characteristics. A specific problem is to predict the extremes of size (radius) of sphere in Wicksell's corpuscle problem. There are several solutions of the problem, see [13, 14, 15] or [4] all based on the extreme value theory, see e. g. [5, 6, 11]. We generalise the problem of predicting extremal characteristics based on observed sections to spheroids, and we focus on the shape factor in the present paper. The shape factor is beside the size another characteristic of spheroid which is closely related to a further crack propagation, namely extremely flat particles are in focus, see e. g. [9] or [2]. For a stereological treatment of spheroids see [3], the extremes of spheroid size are studied in [8]. In [7] the extremal shape of spheroid was studied at the first time. The spheroid size was, however, assumed to be known in order to obtain a reasonable estimation of the extremal shape factor. In the present paper, we use the distribution family satisfying the uniformity condition of Theorem 2 in [7]. Then we can find the prediction of extremal shape factor based on known profile characteristics only. A simulation study illustrating the present approach can be found in [1].

Let us suppose that the joint probability density of the spheroid size X and shape factor T, defined in Section 2, is given by $g(x,t)$. The standard probabilistic notation is used throughout the paper, namely the upper case letters denote the random variable and the lower case letters its actual value. The joint density $f(y,z)$ of the observed profile size Y and shape factor Z is given in Section 2 as an integral transformation of $g(x,t)$. The unfolding of the density g based on estimator of f is an ill-posed problem. Therefore by studying extremes we propose an alternative way to this stereological unfolding problem based on the extreme value theory. The domains of attractions are also discussed in Section 2. We shall restrict to univariate extremes as we are looking for a prediction of extremal shape factor in a given size class.

In Section 3 we briefly discuss the uniformity condition of [7]. The theory is further illustrated on a family of distributions satisfying the uniformity, namely the Farlie–Gumbel–Morgenstern bivariate family. Then we can derive normalising constants for our model in Section 4. Further, in Section 5 we give examples using approximate exponential and polynomial tails of the shape factor distribution. These results go beyond the part 3.2 and Example 1 of [7] which are not very promising for applications as we need to consider the original size of the particle to be known. The results presented here can be considered as a useful basis for the statistical estimation. The statistical inference is briefly outlined in Section 6 using maximum likelihood estimator of normalising constants based on the k largest observations.

2. SPHEROIDS AND EXTREMES

2.1. Probability distribution of spheroid characteristics

Oblate spheroidal non-overlapping particles only are considered in our study. Oblate spheroids have *two equal major semi-axes* and *one minor semi-axis*. The restriction to this family rather than considering general spheroids is explained in [3]. We consider random spheroids, in particular the spheroid semi-axes lengths are random. Let us recall that the spheroids can be fully characterised by their *size* X and their *shape factor* T. The size is the length of the major semi-axes, and the shape factor is defined by $T = X^2/W^2 - 1$, W being the minor semi-axis length. Moreover, we assume that the particle arrangement in space is isotropic uniform random (without overlapping).

The profiles of spheroids generated by a random planar section of the material are ellipses. These ellipses are again fully characterised by their size Y and shape factor Z defined in a similar way as X and T again. Whereas the profiles can be observed and their characteristics Y and Z measured, the spheroid characteristics X and T are unknown in what follows.

Let us denote by $g(x,t)$ the joint probability density function of the size and the shape factor (X,T) of an oblate spheroid. We shall denote by ω and η the upper endpoints of the distributions of the size and the shape factor, respectively. In particular it holds $0 \le W \le X \le \omega$ and $0 \le T \le \eta$. The both ω and η may be infinite. Clearly $T = 0$ for balls. It follows from [3] that $0 \le Y \le X$ and $0 \le Z \le T$. These inequalities formalise the intuition that the size and shape factor of a profile cannot exceed the size and shape factor of a sectioned particle, respectively.

We shall use the notation $g(x,t)$, $G(x,t)$ for the joint probability density and distribution function of the size and shape factor of the spheroid, respectively. The joint density and the joint distribution function of the profile characteristics are $f(y,z)$ and $F(y,z)$, respectively. Further we shall denote by $g_x(t)$, $G_x(t)$, $f_y(t)$ and $F_y(t)$ the conditional densities and the conditional distribution functions of the shape factors given the size. The marginal distribution of the size will be denoted by $g_X(x)$, $G_X(x)$, $f_Y(y)$ and $F_Y(y)$. Hence the densities and distribution functions can be easily identified in what follows.

Following [3], the distribution of the profile size and the profile shape factor (Y,Z) has the joint density

$$f(y,z) = \frac{y\sqrt{1+z}}{2M} \int_y^\eta \int_z^\omega \frac{g(x,t)\,\mathrm{d}t\mathrm{d}x}{\sqrt{t}\sqrt{1+t}\sqrt{t-z}\sqrt{x^2-y^2}}, \tag{1}$$

where M is the population mean size of particles (half of the mean calliper diameter). The conditional density of Z given $Y = y$ is given by

$$f_y(z) = \frac{y\sqrt{1+z}}{2Mf(y)} \int_y^\eta \int_z^\omega \frac{g_x(t)g_X(x)\,\mathrm{d}t\mathrm{d}x}{\sqrt{t}\sqrt{1+t}\sqrt{t-z}\sqrt{x^2-y^2}}, \tag{2}$$

where $g_x(t) = g(t|x) = g(x,t)/g_X(x)$ if $g_X(x) > 0$ and $g_x(t) = 0$ otherwise is the conditional density of the shape factor given the size. The density $g_X(x)$ is the marginal density of the spheroid size. The marginal density of the profile shape factor Z is given by

$$f(z) = \sqrt{1+z} \int_0^\eta \int_z^\omega \frac{g_x(t)g_X(x)\,\mathrm{d}t\mathrm{d}x}{M_x\sqrt{t}\sqrt{1+t}\sqrt{t-z}}, \tag{3}$$

where

$$M_x = \int_0^\omega \left[(t+1)^{-1/2} + \sqrt{\frac{t+1}{t}} \arctan\sqrt{t} \right] g_x(t)\,\mathrm{d}t. \tag{4}$$

Note that independence of size and shape factor results in a much simpler subsystem of cases which is not studied further.

2.2. Domain of attraction

Let us recall the very basic facts from the extreme value theory. There are three possible limit distribution of the univariate sample extreme under an affine transformation. These distributions are

$$L_{i,\alpha}(y) = \begin{cases} \exp(-y^{-\alpha}), & y \ge 0, \quad i = 1, \text{ “Fréchet”} \\ \exp(-(-y)^{\alpha}), & y \le 0, \quad i = 2, \text{ “Weibull”} \\ \exp(-\mathrm{e}^{-y}), & y \in \mathbb{R}, \quad i = 3, \text{ “Gumbel”} \end{cases} \tag{5}$$

where $\alpha > 0$. Let K be a distribution function. We shall write $K \in \mathcal{D}(L)$ if K is in the domain of attraction of L.

Let $\omega = \sup\{y : K(y) < 1\}$ denotes the upper endpoint of K. Then there are the following sufficient conditions for the distribution function K to be in $\mathcal{D}(L)$ under the condition that there exists a density k of K:

$$(C_{1,\alpha}): \quad \forall u > 0, \quad \omega = +\infty, \quad \lim_{s\to\infty} \frac{k(us)}{k(s)} = u^{-(\alpha+1)},$$

$$(C_{2,\alpha}): \quad \forall u > 0, \quad \omega < +\infty, \quad \lim_{s\searrow 0} \frac{k(\omega - us)}{k(\omega - s)} = u^{\alpha-1},$$

$$(C_3): \quad \forall u \in \mathbb{R}, \quad \lim_{s\nearrow\omega} \frac{k(s + ub(s))}{k(s)} = \mathrm{e}^{-u},$$

where $b(\cdot)$ is some auxiliary function. $b(\cdot)$ can be chosen in such a way that it is differentiable for $s < \omega$, $\lim_{s\to\omega} b'(s) = 0$, and $\lim_{s\to\infty} b(s)/s = 0$ if $\omega = \infty$, or $\lim_{s\to\omega} b(s)/(\omega - s) = 0$ if $\omega < \infty$. For further details concerning domains of attraction and for the choice of $b(\cdot)$ consult [6] or [5].

We will now recall a stability result for the domain of attraction of the object and profile characteristics. Theorems 2 and 3 of [7] read as follows

Theorem 1. Suppose that the conditional density $g_x(t)$ satisfies condition $(C_{i,\alpha})$ uniformly in x for some i and α. Assume, moreover, that the upper endpoint ω is constant for all x. Then

1. the conditional distribution function $F_y(z) \in \mathcal{D}(L_{i,\beta})$ for all y,
2. the marginal distribution function $F_Z(z) \in \mathcal{D}(L_{i,\beta})$ for all y,

where $\beta = \alpha$ if $i = 1$, and $\beta = \alpha + 1/2$ if $i = 2$.

Note that the uniformity condition follows naturally from the fact that the profile shape factor does not exceed the spheroid shape factor. It means that any particles with $T \geq z$ may contribute to the observations with the shape factor $Z = z$. Also when conditioning by the size $Y = y$ one should note that any spheroid of size $X \geq y$ may contribute to these observations. The uniformity can be also understood as a *tail equivalence* of the shape factors conditioned by the size.

The uniformity also means that there is an auxiliary function b (introduced in (C_3)) which can be used for all possible values of x.

On the other hand we don't know how much this uniformity condition can be relaxed or replaced by a weaker and simple one.

3. UNIFORMITY CONDITION AND FARLIE–GUMBEL–MORGENSTERN DISTRIBUTIONS

The tail uniformity assumption suggests to look for a bivariate model in the form

$$g(x,t) = g_X(x)g_x(t),$$

such that for $g_x(t)$ the tail uniformity holds. Roughly speaking the tail behaviour of $g_x(t)$ for large t should be "controlled" for all values of x "uniformly". The bivariate normal distribution, for example, is not a good candidate for such a model.

Remark. Suppose that (V,W) obey bivariate normal distribution

$$(V,W) \sim \mathrm{N}\big(\boldsymbol{\mu},\boldsymbol{\Sigma}\big), \quad \text{where } \boldsymbol{\mu} = \begin{pmatrix}\mu_1\\ \mu_2\end{pmatrix}, \ \boldsymbol{\Sigma} = \begin{pmatrix}\sigma_1^2 & \rho\sigma_1\sigma_2\\ \rho\sigma_1\sigma_2 & \sigma_2^2\end{pmatrix}.$$

Then the conditional density of W given $V=v$ is

$$f_v(w) = \frac{1}{\sqrt{2\pi}\sqrt{\sigma_1^2(1-\rho^2)}}\exp\left\{-\frac{1}{2\sigma_1^2(1-\rho^2)}\Big(v-\mu_1-\rho\frac{\sigma_1}{\sigma_2}(w-\mu_2)\Big)^2\right\}.$$

Without loosing generality we can set $\mu_1=\mu_2=0$, choose fixed $v\neq s$, $u\neq 0$ and find that

$$\lim_{w\to+\infty}\frac{f_s(w+ub(w))}{f_s(w)}\,\frac{f_v(w)}{f_v(w+ub(w))} = 1 \Leftrightarrow \lim_{w\to+\infty} 2\rho\frac{\sigma_1}{\sigma_2}ub(w)(v-s) = 0.$$

Since the latter limit can be zero iff $b(t)\to 0$ (which does not hold), or $\rho=0$, we can see that for a bivariate normal distribution the uniformity condition is satisfied if and only if it is a distribution of two independent normally distributed random variables.

Consequently, the tail uniformity strictly requires the independence of variables in the bivariate normal distribution. On the other hand there is another example.

Remark. Consider the joint density $h(x,w)$ of the spheroid major and minor semi-axes in the form

$$h(x,w) = g_X(x)h_x(w), \text{ where } h_x(w) = \frac{1}{x}.$$

Let us note that replacing the uniform distribution by the beta distribution on $[0,x]$ with parameters $a>0, b>0$ for example leads to the same conclusion.

Now we will make the transformation $(X,W)\mapsto(X,T)$, and since

$$(X,W) = (X, X/\sqrt{1+T}) \Rightarrow g(x,t) = g_X(x)\frac{1}{2(t+1)^{3/2}}, \ t\in[0,\infty).$$

Hence the size and the shape factor are independent and the tail uniformity is trivial.

We will use a general family of bivariate distributions based on two marginals for the illustration of the proposed procedure. The considered Farlie–Gumbel–Morgenstern (FGM) family is useful for random vectors with a modest correlation up to 1/3. This assumption is not very restrictive as we have seen in the last remark.

Let

$$g(x,t) = g_X(x)g_T(t)\,[1+\lambda\{2G_X(x)-1\}\{2G_T(t)-1\}] \tag{6}$$

holds for a large t and any x in what follows, where $|\lambda|<1$ is the FGM dependence parameter. Densities g_X and g_T are the marginal densities of g, and G_X, G_T are the corresponding marginal distribution functions. Note that the bivariate normal distribution does not belong to FGM class unless the correlation $\rho = 0$ and hence the two coordinates are independent.

First of all we prove the tail uniformity for the asymptotic FGM family.

Theorem 2. Consider that for all x and for large values of t the joint density $g(x,t)$ of the spheroid size and shape factor is of the form of FGM class. Assume that the conditional distribution $g_{x_0}(t)$ satisfies the condition $C_{i,\alpha}$ for some i and x_0. Then the condition $C_{i,\alpha}$ is fulfilled by the densities $g_x(t)$ uniformly in x.

Proof. We shall prove the theorem for the Gumbel and Fréchet distributions, assuming $\omega=\infty$ for the Gumbel. The other cases are quite similar. Let the distribution $g_{x_0}(t)$ does satisfy condition C_3 for some x_0 and $\omega=+\infty$. Than we shall prove that for any x

$$\lim_{t\to+\infty}\frac{g_x(t+ub(t))}{g_x(t)}\cdot\frac{g_{x_0}(t)}{g_{x_0}(t+ub(t))}=1, \tag{7}$$

from which the uniformity follows.

Note that (7) can be rewritten as

$$\begin{aligned}\lim_{t\to+\infty}&\frac{1+\lambda\{2G_T(t+ub(t))-1\}\{2G_X(x)-1\}}{1+\lambda\{2G_T(t)-1\}\{2G_X(x)-1\}}\times\\ &\times\frac{1+\lambda\{2G_T(t)-1\}\{2G_X(x_0)-1\}}{1+\lambda\{2G_T(t+ub(t))-1\}\{2G_X(x_0)-1\}}=1.\end{aligned} \tag{8}$$

Let us denote

$$\begin{aligned} a_0 &= \lambda\{2G_X(x_0)-1\}, & a &= \lambda\{2G_X(x)-1\},\\ c_t(0) &= 2G_T(t)-1, & c_t(u) &= 2G_T(t+ub(t))-1.\end{aligned}$$

Note that $|a|\le\lambda$ and $|a_0|\le\lambda$. We can write

$$\begin{aligned}&\left|\frac{(1+ac_t(u))(1+a_0c_t(0))}{(1+ac_t(0))(1+a_0c_t(u))}-1\right|\\ &\quad=\left|\frac{(c_t(u)-c_t(0))(a-a_0)}{(1+ac_t(0))(1+a_0c_t(u))}\right|\le\frac{|(c_t(u)-c_t(0))|(|a|+|a_0|)}{|(1+ac_t(0))(1+a_0c_t(u))|}\\ &\quad\le\frac{2|(c_t(u)-c_t(0))|}{|(1+ac_t(0))(1+a_0c_t(u))|}\le\frac{2|(c_t(u)-c_t(0))|}{(1-|\lambda|)^2}.\end{aligned} \tag{9}$$

Note that the last term does not depend on x. Since for any $\varepsilon > 0$ there exists t_ε such that for $s > t_\varepsilon$ the inequality $G_T(s) > 1 - \varepsilon/2$ holds then $c_t(u) - c_t(0) < \varepsilon$ for t large enough.

For an arbitrary x and t large enough we can conclude that

$$\begin{aligned}\left|\frac{g_x(t+ub(t))}{g_x(t)} - \mathrm{e}^{-u}\right| &= \left|\frac{g_x(t+ub(t))}{g_x(t)} - \frac{g_{x_0}(t+ub(t))}{g_{x_0}(t)} + \frac{g_{x_0}(t+ub(t))}{g_{x_0}(t)} - \mathrm{e}^{-u}\right| \\ &\le \left|\frac{g_x(t+ub(t))}{g_x(t)} - \frac{g_{x_0}(t+ub(t))}{g_{x_0}(t)}\right| + \left|\frac{g_{x_0}(t+ub(t))}{g_{x_0}(t)} - \mathrm{e}^{-u}\right| \\ &\le \varepsilon(1+\varepsilon)\mathrm{e}^{-u} + \varepsilon\mathrm{e}^{-u} < 3\varepsilon\mathrm{e}^{-u}. \qquad (10)\end{aligned}$$

Now we shall consider the condition $C_{1,\alpha}$ to be fulfilled by $g_{x_0}(t)$ for some x_0. The proof is quite similar. We want to show that

$$\lim_{t\to\infty} \frac{g_x(ut)}{g_x(t)} \cdot \frac{g_{x_0}(t)}{g_{x_0}(ut)} = 1. \qquad (11)$$

It is possible to proceed as before denoting

$$\begin{aligned} a_0 = \lambda\{2G_X(x_0) - 1\},\ \ a = \lambda\{2G_X(x) - 1\}, \\ d_t(1) = 2G_T(t) - 1,\ \ d_t(u) = 2G_T(ut) - 1. \end{aligned}$$

□

4. NORMALISING CONSTANTS

We have already mentioned that the sample extreme $M_{n:n}$ (may) converge in distribution to one of the three limit distributions under an *affine transformation*. This limit behaviour means

$$\mathsf{P}\left[\frac{M_{n:n} - b_n}{a_n} \le v\right] \xrightarrow{w} L_{i,\alpha}(v),$$

here the couple (a_n, b_n) are the normalising constants. The normalising constants can be calculated from the tail behaviour of the distribution function. They are not uniquely defined since any sequence (a'_n, b'_n) such that

$$\lim_{n\to\infty} \frac{a_n}{a'_n} = 1,\ \ \lim_{n\to\infty} \frac{b_n - b'_n}{a_n} = 0$$

may be also considered as a sequence of normalising constants. Let us recall a way how to evaluate normalising constants for two tail behaviours, namely for the Gumbel and the Fréchet domains of attraction.

4.1. Normalising constants based on the tail behaviour of the distribution function

Proposition 1 of [12] is used to calculate the normalising constants for the Gumbel domain of attraction. The lemma reads

Lemma 3. Consider a distribution $K \in \mathcal{D}(L_3)$ with $\omega = \infty$. If there are constants a, b, c, d such that

$$\lim_{v\to\infty} \frac{1-K(v)}{av^b \exp\{-cv^d\}} = 1$$

holds then the normalising constants a_n, b_n can be chosen as

$$a_n = \left(\frac{\log n}{c}\right)^{1/d-1} \frac{1}{cd}, \quad b_n = \left(\frac{\log n}{c}\right)^{1/d} + \frac{\frac{b}{d}(\log\log n - \log c) + \log a}{\left(\frac{\log n}{c}\right)^{1-1/d} cd}. \tag{12}$$

Similar result is provided by

Lemma 4. Assume that the distribution function $K \in \mathcal{D}(L_{1,\alpha})$. If there exists constants C, a and b such that

$$\lim_{v\to\infty} \frac{1-K(v)}{C(\log v)^b v^{-a}} = 1$$

then the normalising constants can be chosen

$$a_n = \left[n \left(\frac{\log n}{a}\right)^b C\right]^{1/a}, \quad b_n \equiv 0. \tag{13}$$

For an exposition of normalising constants and their relation to quantiles one may consult also [6] or [5].

We shall complete the reasoning now as follows. For a bivariate density $g(x,t)$ which acquires for large t and all x the FGM form and such that the distribution function $G_x(t)$ is in a given domain of attraction (Gumbel with $\omega = \infty$ or Fréchet) we use the uniformity result and one of the lemmas above. It is clear that we should consider some approximate parametric form for the tail of the density $g_T(t)$. As we want to calculate the normalising constants for different spheroid sizes we will need to consider some form of the marginal density $g_X(x)$ as well. But this density is arbitrary in general.

4.2. Normalising constants for the "Gumbel" tail

We will consider the joint density $g(x,t)$ in the FGM family. The tail of the marginal distribution function of the shape factor is approximately equal to the tail of the gamma distribution in a sense

$$1 - G_T(t) \approx \int_t^\infty au^b \mathrm{e}^{-cu^d} \mathrm{d}u \approx \frac{a}{cd} t^{b+1-d} \mathrm{e}^{-ct^d} \text{ for large } t, \tag{14}$$

where for distribution functions we further write $1 - H_1(u) \approx 1 - H_2(u)$ when

$$\lim_{u\to\infty} \frac{1-H_1(u)}{1-H_2(u)} = 1.$$

These assumptions lead to Gumbel limit distribution and hence we shall use Lemma 3 when evaluating the normalising constants. Let us find the general form of the normalising constants for the shape factors. We are using three tails, for spheroid shape factor given its size, for profile shape factor given its size and for profile shape factor marginally. First of all let us note that under the assumption (14)

$$g_T(t)\,[1 - G_T(t)] \ll g_T(t) \text{ for large } t$$

holds and hence we can consider a simplified version of the tails only. Under this simplification the tails in focus become

$$\begin{aligned}
1 - G_x(t) =& [1 - \lambda(1 - 2G_X(x))] \int_t^\infty a u^b \exp\{-c u^d\} \mathrm{d}u, \\
1 - F_y(z) =& \frac{y}{2M f_Y(y)} \int_y^\eta \frac{g_X(x)\,[1 - \lambda(1 - 2G_X(x))]\,\mathrm{d}x}{\sqrt{x^2 - y^2}} \times \\
& \times \int_z^\infty \left(\sqrt{\frac{(1+z)(t-z)}{(1+t)t}} + \sqrt{\frac{1+t}{t}} \arctan \sqrt{\frac{t-z}{1+z}} \right) a t^b \exp\{-c t^d\}\,\mathrm{d}t, \\
1 - F_Y(z) =& \int_0^\eta \frac{g_X(x)\,[1 - \lambda(1 - 2G_X(x))]\,\mathrm{d}x}{M_x} \times \\
& \times \int_z^\infty \left(\sqrt{\frac{(1+z)(t-z)}{(1+t)t}} + \sqrt{\frac{1+t}{t}} \arctan \sqrt{\frac{t-z}{1+z}} \right) a t^b \exp\{-c t^d\}\,\mathrm{d}t.
\end{aligned} \tag{15}$$

It follows namely that the condition (the size) has only partial influence on the tail behaviour of the shape factor.

Let us turn our attention to

$$\int_z^\infty \left(\sqrt{\frac{(1+z)(t-z)}{(1+t)t}} + \sqrt{\frac{1+t}{t}} \arctan \sqrt{\frac{t-z}{1+z}} \right) a t^b \exp\{-c t^d\}\,\mathrm{d}t.$$

It holds

$$\begin{aligned}
&\int_z^\infty \sqrt{\frac{(1+z)(t-z)}{(1+t)t}} a t^b \exp\{-c t^d\}\,\mathrm{d}t \\
&\qquad = \int_0^\infty \sqrt{\frac{(1+z)(w)}{(1+w+z)(w+z)}} + a(w+z)^b \exp\{-c(w+z)^d\}\,\mathrm{d}w \\
&\qquad = a z^{b-1/2} \int_0^\infty \sqrt{\frac{(1+z)(w)}{(1+w+z)}} + \left(1 + \frac{w}{z}\right)^{b-1/2} \exp\{-c(w+z)^d\}\,\mathrm{d}w \\
&\approx a z^{b-1/2} \int_0^\infty \sqrt{w} \exp\left\{-c z^d \left(1 + \frac{w}{z}\right)^d\right\} \mathrm{d}w \approx a z^{b-1/2} \mathrm{e}^{-c z^d} \int_0^\infty \sqrt{w} \mathrm{e}^{-c d z^{d-1} w}\,\mathrm{d}w \\
&\qquad = \frac{\sqrt{\pi}}{2} a (cd)^{-3/2} z^{b+1-3d/2} \mathrm{e}^{-c z^d},
\end{aligned} \tag{16}$$

and

$$\begin{aligned}
&\int_z^\infty \sqrt{\frac{1+t}{t}} \arctan\left(\sqrt{\frac{t-z}{1+z}}\right) at^b \exp\{-ct^d\}\,\mathrm{d}t \\
&\quad= \int_0^\infty \sqrt{\frac{1+w+z}{w+z}} \arctan\left(\sqrt{\frac{w}{1+z}}\right) a(w+z)^b \exp\{-c(w+z)^d\}\,\mathrm{d}w \\
&= az^{b-1/2} \int_0^\infty \sqrt{1+w+z} \arctan\left(\sqrt{\frac{w}{1+z}}\right) \left(1+\frac{w}{z}\right)^{b-1/2} \exp\{-c(w+z)^d\}\,\mathrm{d}w \\
&\qquad\approx az^{b-1/2}\mathrm{e}^{-cz^d} \int_0^\infty \sqrt{w}\mathrm{e}^{-cdz^{d-1}w}\,\mathrm{d}w \\
&\qquad\qquad= \frac{\sqrt{\pi}}{2} a(cd)^{-3/2} z^{b+1-3d/2}\mathrm{e}^{-cz^d}. \qquad (17)
\end{aligned}$$

Now it is possible to employ Lemma 3. The calculation of the normalising constants can be based on the following theorem.

Theorem 5. Let us assume a density $g(x,t)$ such that it is of FGM form for large values of t and $1 - G_x(t) \approx \int_t^\infty au^b\mathrm{e}^{-cu^d}\mathrm{d}u$ for large t. Consider the density $f(y,z)$ given by the transformation (1). Then it holds

$$\begin{aligned}
\lim_{t\to\infty} \frac{1-G_x(t)}{a(cd)^{-1}t^{b+1-d}\mathrm{e}^{-ct^d}} &= k_1(x), \\
\lim_{z\to\infty} \frac{1-F_y(z)}{\sqrt{\pi}a(cd)^{-3/2}z^{b+1-3d/2}\mathrm{e}^{-ct^d}} &= k_2(y), \qquad (18) \\
\lim_{z\to\infty} \frac{1-F(z)}{\sqrt{\pi}a(cd)^{-3/2}z^{b+1-3d/2}\mathrm{e}^{-ct^d}} &= k_3,
\end{aligned}$$

where k_1, k_2 and k_3 are constants with respect to t which can be calculated from (15)

$$\begin{aligned}
k_1(x) &= 1 - \lambda[1 - 2G_X(x)], \\
k_2(y) &= \frac{y}{2Mf_Y(y)} \int_y^\eta \frac{g_X(x)\,[1-\lambda(1-2G_X(x))]\,\mathrm{d}x}{\sqrt{x^2-y^2}} \\
&= \frac{\int_y^\eta \frac{g_X(x)[1-\lambda(1-2G_X(x))]}{\sqrt{x^2-y^2}}\mathrm{d}x}{\int_y^\eta \frac{g_X(x)M_x}{\sqrt{x^2-y^2}}\mathrm{d}x}, \qquad (19) \\
k_3 &= \int_0^\eta \frac{g_X(x)\,[1-\lambda(1-2G_X(x))]\,\mathrm{d}x}{M_x}.
\end{aligned}$$

We postpone the discussion of constants k_i and turn our attention to the Fréchet limit distribution.

4.3. Normalising constants for the "Fréchet" tail

Let us still assume the FGM form of the joint density $g(x,t)$ for large t while we change the form of the tail of the marginal distribution of the shape factor to

$$1 - G_T(t) \approx \int_t^\infty c(\log u)^b u^{-a-1} \approx \frac{c}{a}(\log t)^b t^{-a} \text{ for large t.}$$

Again it holds

$$g_T(t)\,[1 - G_T(t)] \ll g_T(t)$$

and hence we can use the same simplification as before in (15) with the appropriate density $g_T(t)$. We need to study

$$\int_z^\infty \left(\sqrt{\frac{(1+z)(t-z)}{(1+t)t}} + \sqrt{\frac{1+t}{t}} \arctan \sqrt{\frac{t-z}{1+z}}\right) c(\log t)^b t^{-a-1} \mathrm{d}t.$$

It holds

$$\int_z^\infty \sqrt{\frac{(1+z)(t-z)}{(1+t)t}} c(\log t)^b t^{-a-1} \mathrm{d}t$$

$$\int_1^\infty \sqrt{\frac{(1+z)z(w-1)}{(1+wz)wz}} c(\log z + \log w)^b (zw)^{-a-1} z \mathrm{d}w$$

$$\approx c(\log z)^b z^{-a} \int_1^\infty \frac{\sqrt{w-1}}{w} w^{-a-1} \mathrm{d}w = c(\log z)^b z^{-a} \mathrm{B}\left(a + \frac{1}{2}, \frac{3}{2}\right), \quad (20)$$

where $\mathrm{B}(\cdot,\cdot)$ is the beta function and

$$\int_z^\infty \sqrt{\frac{1+t}{t}} \arctan \sqrt{\frac{t-z}{1+z}} c(\log t)^b t^{-a-1} \mathrm{d}t$$

$$= \int_1^\infty \sqrt{\frac{1+wz}{wz}} \arctan \sqrt{\frac{z(w-1)}{1+z}} c(\log z + \log w)^b (zw)^{-a-1} z \mathrm{d}w$$

$$\approx c(\log z)^b z^{-a} \int_1^\infty w^{-a-1} \arctan \sqrt{w-1} \mathrm{d}w = c(\log z)^b z^{-a} \frac{1}{2a} \mathrm{B}\left(a + \frac{1}{2}, \frac{1}{2}\right). \quad (21)$$

It is possible to use Lemma 4 now and derive the normalising constants from the next theorem.

Theorem 6. Let us assume a density $g(x,t)$ such that it is of FGM form for large values of t and $1 - G_x(t) \approx \int_u^\infty c(\log u)^b u^{-a-1} \mathrm{d}u$ for large t. Consider density $f(y,z)$ given by the transformation (1). Then it holds

$$\lim_{t\to\infty} \frac{1 - G_x(t)}{ca^{-1}(\log t)^b t^{-a}} = k_1(x),$$

$$\lim_{t\to\infty} \frac{1 - F_y(z)}{c(2 + a^{-1})\mathrm{B}(a + 1/2, 3/2)(\log z)^b z^{-a}} = k_2(y), \quad (22)$$

$$\lim_{t\to\infty} \frac{1 - F(z)}{c(2 + a^{-1})\mathrm{B}(a + 1/2, 3/2)(\log z)^b z^{-a}} = k_3,$$

where k_1, k_2, and k_3 are the same constants as in (19).

5. EXAMPLES

We shall provide examples of the sets of normalising constants in this section. We shall use the notation

1. a_n, b_n for the normalising constants of the spheroid shape factor T given the spheroid size $X = x$,
2. a_n^s, b_n^s for the normalising constants of the profile shape factor Z given the profile size $Y = y$,
3. a_n^m, b_n^m for the profile shape factor Z marginally.

Let us postpone the question of $k_1(x), k_2(y)$ and k_3 for a moment.

Example – Gamma tail. Let us consider that the tail of the shape factor density can be approximated by the gamma density, namely

$$1 - G_T(t) \approx \int_t^\infty \frac{\mu^\gamma u^{\gamma-1}}{\Gamma(\gamma)} \mathrm{e}^{-\mu u} \mathrm{d}u \quad \text{for large } t,$$

where $\mu > 0$ and $\gamma > 0$. The limit distribution of the sample extremes is the Gumbel distribution and it is not difficult to use Lemma 3 and to see that

$$\begin{aligned} a_n = a_n^s &= a_n^m = \frac{1}{\mu}, \\ b_n &= a_n \left[\log n + (\gamma - 1) \log \log n + \log \frac{k_1(x)}{\Gamma(\gamma)} \right], \\ b_n^s &= a_n \left[\log n + \left(\gamma - \frac{3}{2} \right) \log \log n + \log \frac{\sqrt{\pi} k_2(y)}{\Gamma(\gamma)} \right], \\ b_n^m &= a_n \left[\log n + \left(\gamma - \frac{3}{2} \right) \log \log n + \log \frac{\sqrt{\pi} k_3}{\Gamma(\gamma)} \right]. \end{aligned}$$

Example – Pareto tail. We shall now suppose that the density $g(t)$ is approximately of the Pareto form, namely

$$1 - G_T(t) \approx \int_t^\infty \frac{\gamma}{\sigma} \left(\frac{\sigma}{u} \right)^{\gamma+1} \mathrm{d}u \quad \text{for large } t,$$

where $\sigma > 0$ and $\gamma > 0$. The limit distribution is Fréchet and it is not difficult to evaluate

$$b_n = b_n^s = b_n^m = 0,$$
$$a_n = \sigma[nk_1(x)]^{1/\gamma},$$
$$a_n^s = \sigma\left[nk_2(y)(2\gamma+1)\mathrm{B}\left(\gamma+\frac{1}{2},\frac{3}{2}\right)\right]^{1/\gamma},$$
$$a_n^m = \sigma\left[nk_3(2\gamma+1)\mathrm{B}\left(\gamma+\frac{1}{2},\frac{3}{2}\right)\right]^{1/\gamma}.$$

Example – Weibull tail. Let us consider the density $g(t)$ such that

$$1 - G_T(t) \approx \int_t^\infty \mu\gamma u^{\gamma-1}\exp\{-\mu u^\gamma\}\mathrm{d}u \quad \text{for large } t,$$

where $\mu > 0$ and $\gamma > 0$. This distribution is in the domain of attraction of the Gumbel distribution again and one can easily check that

$$a_n = a_n^s = a_n^m = \left(\frac{\log n}{\mu}\right)^{1/\gamma-1}\frac{1}{\mu\gamma},$$
$$b_n = a_n[\gamma\log n + \log k_1(x)],$$
$$b_n^s = a_n\left[\gamma\log n - \frac{1}{2}\log\log n + \log\left(\sqrt{\frac{\pi}{\gamma}}k_2(y)\right)\right],$$
$$b_n^m = a_n\left[\gamma\log n - \frac{1}{2}\log\log n + \log\left(\sqrt{\frac{\pi}{\gamma}}k_3\right)\right].$$

Note that the Weibull and gamma cases agree for $\gamma = 1$ as the both cases result in the exponential distribution with parameter μ. The sets of normalising constants of the profile and the original shape factor are closely related and it should be noted that in all three examples one is either known (b_n for Pareto) or is the same for particles and their profiles (a_n for gamma and Weibull).

Let us turn our attention to the constants k_1, k_2 and k_3 now. We will assume that the marginal distribution of the size has some parametric form and hence we will be able to evaluate these constants.

Let us note first that from (4) it follows

$$2Mf(y) = y\int_y^\eta \frac{g_X(x)M_x}{\sqrt{x^2-y^2}}\mathrm{d}x$$
$$= y\int_y^\eta \frac{g_X(x)}{\sqrt{x^2-y^2}}\int_0^\omega\left((1+t)^{-1/2} + \sqrt{\frac{1+t}{t}}\arctan\sqrt{t}\right)g_x(t)\,\mathrm{d}t\mathrm{d}x.$$

As we assume the parametric form of $g_x(t)$ for the large values of t only, the evaluation of the above integral is not possible. We may only estimate the marginal density of the profile size $f(y)$ from the section and to treat the value M as an unknown nuisance parameter.

Some examples of calculating the constants k_i are presented for different distributions in what follows.

Exponential distribution of the size. Let us suppose that

$$g_X(x) = \nu \mathrm{e}^{-\nu x}, \; G_X(x) = 1 - \mathrm{e}^{-\nu x}, \; \nu, x > 0.$$

Then it holds

$$\begin{aligned} k_1(x) &= 1 - \lambda(2\mathrm{e}^{-\nu x} - 1), \\ k_2(y) &= \frac{y}{2Mf(y)}[(1+\lambda)K_B(0, \nu y) - \lambda K_B(0, 2\nu y)], \\ k_3 &= (1+\lambda)\int_0^\infty \frac{\nu \mathrm{e}^{-\nu x}}{M_x}\mathrm{d}x - \lambda \int_0^\infty \frac{2\nu \mathrm{e}^{-2\nu x}}{M_x}\mathrm{d}x, \end{aligned}$$

where $K_B(\cdot,\cdot)$ denotes the Bessel K function.

Uniformly distributed size. Consider the density and the distribution function of the spheroid size in the form

$$g_X(x) = \frac{1}{b}, \; G_X(x) = \frac{x}{b}, \; b > 0, 0 < x < b.$$

Then the constants are

$$\begin{aligned} k_1(x) &= 1 - \lambda\left(1 - \frac{2x}{b}\right), \\ k_2(y) &= \frac{y}{2Mf(y)}\left(\frac{1-\lambda}{b}\log\left\{\frac{b + \sqrt{b^2 - y^2}}{y}\right\} + \frac{2\lambda}{b^2}\sqrt{b^2 - y^2}\right), \\ k_3 &= \frac{1-\lambda}{b}\int_0^b \frac{\mathrm{d}x}{M_x} + \frac{2\lambda}{b^2}\int_0^b \frac{x\mathrm{d}x}{M_x}. \end{aligned}$$

Pareto distribution of the size. The last example is the Pareto distribution with

$$g(x) = \frac{\nu}{\beta}\left(\frac{\beta}{x}\right)^{\nu+1}, \; G(x) = 1 - \left(\frac{\beta}{x}\right)^{\nu}, \; \nu, \beta > 0, x > \beta.$$

It is not difficult to check that

$$\begin{aligned} k_1(x) &= 1 - \lambda\left[2\left(\frac{\beta}{x}\right)^{\nu} - 1\right], \\ k_2(y) &= \frac{y}{2Mf(y)}\left[\frac{(1+\lambda)\nu\beta^{\nu}}{y^{\nu+1}}\mathrm{B}\left(\frac{\nu+1}{2}, \frac{1}{2}\right) + \frac{2\lambda\nu\beta^{2\nu}}{y^{2\nu+1}}\mathrm{B}\left(\frac{2\nu+1}{2}, \frac{1}{2}\right)\right], \\ k_3 &= (1-\lambda)\int_0^\infty \frac{\nu}{\beta M_x}\left(\frac{\beta}{x}\right)^{\nu+1}\mathrm{d}x + 2\lambda\int_0^\infty \frac{\nu}{\beta M_x}\left(\frac{\beta}{x}\right)^{2\nu+1}\mathrm{d}x, \end{aligned}$$

where $\mathrm{B}(\cdot,\cdot)$ is the beta function again.

6. STATISTICAL APPLICATION

We are naturally interested in the prediction of extremes of the shape factor for spheroids of given size. Therefore we need to estimate the normalising constants a_n and b_n for fixed $X = x$ since for the normalised shape factor extreme $T_{n:n}$

$$\mathsf{P}\left[\frac{T_{n:n} - b_n}{a_n} < t | X = x\right] \xrightarrow{w} L_{i,\alpha}(t)$$

holds for the appropriate i and α. Note that the parameter α for the Fréchet limit distribution will be also estimated by the MLE method described below.

The distribution of the shape factor extreme is therefore approximated by the distribution function $L_{i,\alpha}\big((t - b_n)/a_n\big)$ and its quantiles are approximated by $q_p = b_n - a_n \log\log(1/p)$, while for the mean we have $\mathsf{E}T_{n:n} = b_n - a_n\mathfrak{e}$, $\mathfrak{e} = 0.577\ldots$ being the Euler constant. Hence confidence intervals, upper confidence limits and other characteristics of the extremal shape factor may be predicted.

The first task is to obtain the estimations of a_n^s and b_n^s or a_n^m and b_n^m from the observed profiles. Let be $Z_1, Z_2, \ldots, Z_n$ the observed shape factors of profiles (either in some size class or marginally) and $M_1 \geq M_2 \geq \cdots \geq M_k$ the k largest observations with the average of these observations $\overline{M_k}$. These $k + 1$ values form the basis of the maximum likelihood estimator proposed for this purpose. The reader may consult [17] or [10] for the derivation of the *ML estimators based on k largest observations.* Let us recall the estimators both for Gumbel and Fréchet limit distribution.

Gumbel limit distribution. As the joint density of $(M_1, M_2, \ldots, M_k)$ normalised by the affine transformation is

$$d(m_1, m_2, \ldots, m_k) = (a_n^s)^{-k} \exp\left\{-\mathrm{e}^{-(m_k - b_n^s)/a_n^s} - \sum_{i=1}^{k} \frac{x_i - b_n^s}{a_n^s}\right\}$$

one may easily derive the ML estimators

$$\widehat{a_n^s} = \overline{M_k} - M_k, \;\; \widehat{b_n^s} = \widehat{a_n^s} \log k + M_k. \tag{23}$$

Fréchet limit distribution. The joint density of $(M_1, M_2, \ldots, M_k)$ normalised by the affine transformation is

$$d(m_1, m_2, \ldots, m_k) = \exp\left\{\sum_{i=1}^{k}(\log\beta + \beta\log a_n^s + (1-\beta)\log m_i) + m_k^{-1} - \left(\frac{m_k}{a_n^s}\right)^{-\beta}\right\}$$

and we can derive the ML estimators

$$\widehat{a_n^s} = k^{1/\widehat{\beta}} M_k, \;\; \widehat{\beta} = k\left(\sum_{i=1}^{k}(\log M_i - \log M_k)\right)^{-1}. \tag{24}$$

Recalculation of the normalising constants. The normalising constants and the respective parameter of the limit distribution must be obtained from the observations of a fixed size. As the size distribution is considered to be continuous one must in fact make a compromise and use a size interval (as narrow as possible) instead of some exact size. It is also possible to use the a_n^m and b_n^m normalising constants avoiding the problem nevertheless usually we need to estimate more than just one set of the normalising constants. The reason follows from the examples of Section 5.

We will illustrate our approach on a specific example but the ideas may be used generally. Let us consider a bivariate FGM distribution where the size is exponentially distributed with parameter ν and the shape factor follows gamma distribution with parameters μ and γ. According to the above results we know that $a_n = a_n^s = \mu^{-1}$ and

$$\begin{aligned} b_n &= a_n \left[\log n + (\gamma - 1)\log\log n + \log \frac{k_1(x)}{\Gamma(\gamma)}\right], \\ b_n^s &= a_n \left[\log n + \left(\gamma - \frac{3}{2}\right)\log\log n + \log \frac{\sqrt{\pi} k_2(y)}{\Gamma(\gamma)}\right], \\ k_1(x) &= 1 - \lambda(2\mathrm{e}^{-\nu x} - 1), \\ k_2(y) &= \frac{y}{2Mf(y)}[(1+\lambda)K_B(0,\nu y) - \lambda K_B(0, 2\nu y)]. \end{aligned} \tag{25}$$

It is naturally quite easy to estimate $\widehat{a_n} = \widehat{a_n^s}$ (note that it is independent of the sample size n) and to estimate $\widehat{\mu} = \left(\widehat{a_n^s}\right)^{-1}$. Now, with the estimate $\widehat{b_n^s}$ known for n and y we would like to get $\widehat{b_m}$ for the chosen x and the expected number of particles m (estimating m is a classical stereological problem, see e. g. [9]).

Recall that we are able to estimate $\widehat{\mu}$ and the marginal density of profile size $\widehat{f(y)}$. Hence it may be a good idea to estimate more normalising constants for different sizes of appropriate sample sizes, namely $\widehat{b_n^s}(y_i)$, $i = 1, \dots, l$. We obtain

$$\frac{\widehat{b_n^s}(y_i) - \widehat{b_n^s}(y_j)}{\widehat{a_n^s}} = \log \frac{y_i \widehat{f(y_j)}}{\widehat{f(y_i)} y_j} + \log \frac{(1+\lambda)K_B(0,\nu y_i) - \lambda K_B(0,2\nu y_i)}{(1+\lambda)K_B(0,\nu y_j) - \lambda K_B(0,2\nu y_j)}. \tag{26}$$

The parameters λ and ν now may be estimated numerically from these equations.

The last parameter to be estimated is γ as we note that we need not M for $\widehat{b_m}$. We may proceed as before with the difference that size classes with different sample sizes are required to obtain

$$\begin{aligned} &\frac{\widehat{b_n^s}(y_i) - \widehat{b_n^s}(y_j)}{\widehat{a_n^s}} \\ &= \left(\gamma - \frac{3}{2}\right)\log\left(\frac{\log n_i}{\log n_j}\right) + \log \frac{n_i y_i \widehat{f(y_j)}}{n_j \widehat{f(y_i)} y_j} \cdot \frac{(1+\widehat{\lambda})K_B(0,\widehat{\nu} y_i) - \widehat{\lambda} K_B(0,2\widehat{\nu} y_i)}{(1+\widehat{\lambda})K_B(0,\widehat{\nu} y_j) - \widehat{\lambda} K_B(0,2\widehat{\nu} y_j)}. \end{aligned} \tag{27}$$

Note that we may use the last equation for the simultaneous estimation of λ, ν and γ instead of the two-stage procedure.

The estimates $\widehat{a_m}$ and $\widehat{b_m}$ of the normalising constants are now obvious.

Conclusion. There is quite a straightforward method, although numerically not a simple one how to obtain the normalising constants in such specific cases. Unfortunately, being restricted to parametric form of the tail behaviour one cannot expect general solution of our problem.

There is another way how to obtain the ML estimators. We may base our MLE on the *maximal observations in k disjoint regions*. The limit joint density of the *independent* normalised maximas is easy to calculate. Nevertheless the estimators are not explicitely given and we do prefer the MLE based on k largest observations here.

In the classical extreme value theory it is natural to avoid parametric models and approximate the distribution of the sample extremes by one of the limiting cases. Hence one needs to decide into which domain of attraction the distribution belongs and to estimate the normalising constants (n.c.). It is exactly what we can do also for the profile characteristics without any parametric model. There is, however, the problem that we need the normalising constants for the spheroid characteristics rather than for the profile characteristics. Unfortunately there is not known any general (distribution free) way of estimating n.c. of the spheroids based on the n.c. of the profiles. One of possible approaches (see e. g. [16]) is to consider parametric tails of the distribution, derive the explicit formula for the normalising constants both for spheroids and profiles, and proceed to the end. In our case we need also to consider a relation between the two characteristics (size and shape factor) of the spheroids as the tail uniformity of Theorem 1 is required. Hence the form of the bivariate distribution of (X, T) must be specified.

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