Shape Theory via QR decomposition

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Abstract
This work sets the non isotropic noncentral elliptical shape distributions via QR decomposition in the context of zonal polynomials, avoiding the invariant polynomials and the open problems for their computation. The new shape distributions are easily computable and then the inference procedure can be studied under exact densities instead under the published approximations and asymptotic densities under isotropic models. An application in Biology is studied under the classical gaussian approach and a two non gaussian models.

1 Introduction and the main principle

Considering the non isotropy in the non central shape theory has been very problematic, even in the gaussian case, see for example [Goodall and Mardia (1993)] the corresponding shape densities involve expansions products of powers of traces of different matrices, which forces the apparition of invariant polynomials [Davis (1908)]. Then the resulting densities enlarge the list of uncountable densities in the noncentral multivariate statistics, which can not be computable, and remains as theoretical results, very far from the inference and the applications. So, the applications in shape theory have been force to avoid those polynomials, but at a very high cost, the assumption of isotropy. However, in this, the resulting densities were series of zonal polynomials, and they could not studied properly (before the works of [Koev and Edelman (2006)], and again they forced to the use of approximations and asymptotic distribution to perform inference. [Goodall and Mardia (1993), Dryden and Mardia (1998)], and the references therein.

The following principle solves the first and more important problem, avoiding the invariant polynomials, and setting the new shape distributions in terms of series of zonal

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From the point of view of applications, the isotropic assumption \( \Theta = I_K \) for an elliptical shape model of the form \( X \sim E_{N \times K}(\mu_x, \Sigma_x, \Theta, h) \), restricts substantially the correlations of the landmarks in the figure. So, we expect the non isotropic model, with any positive definite matrix \( \Theta \), as the best model for considering all the possible correlations among the anatomical (geometrical or mathematical) points. However, using the classical approach of the published literature of shape (see for example [Goodall and Mardia (1993)]) under the non isotropic model, we obtain immediately invariant polynomials, which can not be computed at this time for large degrees.

In order to avoid this problem consider the following procedure: Let

\[
X \sim E_{N \times K}(\mu_x, \Sigma_x, \Theta, h),
\]

if \( \Theta^{1/2} \) is the positive definite square root of the matrix \( \Theta \), i.e. \( \Theta = (\Theta^{1/2})^2 \), with \( \Theta^{1/2} : K \times K \) [2], and noting that

\[
X \Theta^{-1/2} X' = X (\Theta^{-1/2} \Theta^{-1/2})^{-1} X' = X \Theta^{-1/2} (X \Theta^{-1/2})' = ZZ',
\]

where

\[
Z = X \Theta^{-1/2},
\]

then

\[
Z \sim E_{N \times K}(\mu_z, \Sigma_z, I_K, h)
\]

with \( \mu_z = \mu_x \Theta^{-1/2} \), (see [Gupta and Varga (1993) p. 20]).

And we arrive at the classical starting point in shape theory where the original landmark matrix is replaced by \( Z = X \Theta^{-1/2} \). Then we can proceed as usual, removing from \( Z \), translation, scale, rotation and/or reflection in order to obtain the shape of \( Z \) (or \( X \)) via the QR decomposition, for example.

Namely, the QR shape coordinates \( u \) of \( X \) are constructed in several steps summarized in the expression

\[
LX \Theta^{-1/2} = LZ = Y = TH = rW H = rW (u) H,
\]

which we discuss next. Observe that \( \mu_z = \mu_x \Theta^{-1/2} \) and the QR shape coordinates of \( \mu_z \) are defined analogously. The matrix \( L : (N-1) \times N \) has orthonormal rows to \( I = (1, \ldots, 1)' \).

Let \( \Theta = L \mu_x \), then \( Y : (N-1) \times K \) is invariant to translations of the figure \( Z \), and

\[
Y \sim E_{N-1 \times K}(\mu \Theta^{-1/2}, \Sigma \otimes I_K, h),
\]

where \( \Sigma = L \Sigma_x L' \).

Now, let be \( n = \min(N-1, K) \) and \( p = \text{rank} \mu \). In [11], \( Y = TH \) is the QR decomposition, where \( T : (N-1) \times n \) is lower triangular with \( t_{ii} > 0, i = 1, \ldots, \min(n, K-1) \), and \( H : n \times K \), \( H \in V_{n,K} \), the Stiefel manifold. Note that \( T \) is invariant to translations and rotations of \( Z \). The matrix \( T \) is referred as the QR size-and-shape and their elements are the QR size-and-shape coordinates of the original landmark data \( Z \). Typically in shape analysis there are more landmarks than dimensions \( (N > K) \). \( H \) acts on the right to transform \( \mathbb{R}^K \) instead of acting on the left as in the multivariate analysis. In our case we see the landmarks as variables and the dimensions as observations, then the transposes of our matrices \( Z \) and \( Y \) can be seen as classical multivariate data matrices.

According to the nature of the base \( H \) and providing that \( N-1 \geq K \), we say that \( T \) contains the \( QR \) reflection size-and-shape coordinates if \( H \) includes reflection, i.e. \( H \in \mathbb{R}^K \).
\( O(K) \), \( |H| = \pm 1 \) and \( t_{KK} \geq 0 \); otherwise, if \( H \) excludes reflection, \( H \in SO(K) \), \( |H| = +1 \), \( t_{KK} \) is not restricted, we say that \( T \) contains the QR size-and-shape coordinates. These cases will denote by \( T^R \) and \( T^{NR} \), respectively. In the classical multivariate case, \( n < K \), we do not have such classifications for \( T \).

Now, if we divide \( T \) by its size, the centroid size of \( Z \),

\[ r = \|T\| = \sqrt{\text{tr}T'T} = \|Y\|. \]

we obtain the so called \( QR \) shape matrix \( W \) in (1). We define \( W^R = T^R/r \) or \( W^{NR} = T^{NR}/r \) if \( W \) includes or excludes reflection, respectively, and given that \( \|W\| = 1 \), the elements of \( W \) are a direction vector for shape, and \( u \) comprises \( m = (N - 1)K - nK + \frac{1}{2}n(n + 1) - 1 \) generalized polar coordinates.

Before deriving the main results of this paper we must solve some discrepancies between the shape theory and the classical multivariate theory. Recall that for a given \( Y : n \times K \), \( n = N - 1 \leq K \), then \( YY' \) has the noncentral Wishart distribution which is invariant to orientation and reflection, but if \( n \geq K \) that density does not exist with respect to the Lebesgue measure defined on the space of positive definite \( n \times n \) matrices, and we therefore use the size-and-shape matrix \( T \). However, the density of \( YY' \) when, \( n \geq K \), exist on the \((nK - K(K - 1)/2)\)-dimensional manifold of rank-\( K \) positive semidefinite \( n \times n \) matrices with \( K \) distinct positive eigenvalues, see Díaz-García and González-Farías (2005) and Díaz-García and Gutiérrez-Jáimez (2006). This last fact can provide an alternative form to study the shape theory, which is being analysed by the authors at present.

And finally, classical integration over \( O(K) \) involving zonal polynomials gives the density of \( T^R \), but \( T^{NR} \) demands integration over \( SO(K) \), then we just recall that the corresponding integrals are the same when \( n < K \), and, for \( n \geq K \) and \( p < K \), they are twice the integral over \( SO(K) \).

This work is distributed as follows: first, the size and shape distribution for any elliptical model with a full Kronecker covariance matrix is derived in section 2. The shape density is obtained in section 3 and the classical isotropic gaussian shape density, full derived in Goodall and Mardia (1993), follows here as a corollary, then the section 4 describes the excluding reflection shape densities. The central case of the shape density is studied in section 5, and a remarkable property is established, i.e. it is established that the central QR reflection shape density is invariant under the elliptical family. Finally, some particular elliptical densities are derived in section 6 in order to perform inference on exact distributions; a subfamily of Kotz distributions which contains the gaussian one is derived, then two elements of that class (the gaussian and a non gaussian model) is applied to an existing publish data, the mouse vertebra study. Some test for detecting shape differences are gotten and the models are discriminated by the use of a dimension criterion such as the modified BIC criterion.

2 QR Size-and-shape distribution

**Lemma 2.1.** Let \( Y : (N - 1) \times K \), then there exists a \( T : (N - 1) \times n \) lower triangular matrix with \( t_{ii} \geq 0 \), \( i = 1, \ldots, \min(n, K - 1) \), and \( H \in V_{n,k} \) such that \( Y = TH \) and

\[ (dY) = \prod_{i=1}^{n} t_{ii}^{K-i}(dT)(HdH') \quad (2) \]

**Lemma 2.2.** Let \( A : r \times s \), and \( H \in V_{s,m} \) then

\[ \int_{H \in V_{s,m}} (\text{tr} AH)^{2t}(HdH') = \frac{2^s \pi^{s/2} m^t}{\Gamma_s \left(\frac{s}{2} \right)} \sum_{\kappa} \left(\frac{1}{2}\right)_\kappa C_{\kappa}(AA'), \quad (3) \]
where $C_{\kappa}(\mathbf{B})$ are the zonal polynomials of $\mathbf{B}$ corresponding to the partition $\kappa = (t_1, \ldots, t_n)$ of $t$, with $\sum_{i=1}^n t_i = t$; and $(a)_\kappa = \prod_{i=1}^n (a - (j - 1)/2)_{t_i}$, $\kappa = a(a + 1) \cdots (a + t - 1)$, are the generalized hypergeometric coefficients and $\Gamma_s(a) = \pi^{(s-1)/2} \prod_{j=1}^s \Gamma(a - (j - 1)/2)$ is the multivariate Gamma function.

Proof. It is follows from James (1961), eq. (22) and Muirhead (1982), lemma 9.5.3, p. 397.

\textbf{Theorem 2.1.} The QR reflection size-and-shape is

$$f_T(T) = \frac{2^n \pi^{nK/2}}{\Gamma_n(\frac{1}{2}K)} \prod_{i=1}^n t_i^{K-i} \sum_{t=0}^\infty \sum_{\kappa} \frac{h^{(2t)}[\text{tr}(\Sigma^{-1}TT' + \Omega)] C_{\kappa}(\Omega^{\Sigma^{-1}TT'})}{t!} (\frac{1}{2}K)_{\kappa}^{-1}, \quad (4)$$

where $\Omega = \Sigma^{-1}\mu \Theta^{-1/2} \mu'$, $C_{\kappa}(\mathbf{B})$ are the zonal polynomials of $\mathbf{B}$ corresponding to the partition $\kappa = (t_1, \ldots, t_n)$ of $t$, with $\sum_{i=1}^n t_i = t$ and $h^{(j)}(v)$ is the $j$-th derivative of $h$ with respect to $v$.

Proof. The density of $\mathbf{Y}$ is

$$f_Y(Y) = \frac{1}{\Sigma_{1/2}^{|K|/2}} h \left[ \text{tr} \Sigma^{-1}(Y - \mu \Theta^{-1/2})(Y - \mu \Theta^{-1/2})' \right]$$

$$= \frac{1}{\Sigma_{1/2}^{|K|/2}} h \left[ \text{tr} \left( \Sigma^{-1}YY' + \Sigma^{-1}\mu \Theta^{-1/2} \mu' - 2 \Sigma^{-1}Y \Theta^{-1/2} \mu' \right) \right]$$

$$= \frac{1}{\Sigma_{1/2}^{|K|/2}} h \left[ \text{tr} \left( \Sigma^{-1}YY' + \Omega - 2 \text{tr} \Sigma^{-1}Y \Theta^{-1/2} \mu' \right) \right],$$

with $\Omega = \Sigma^{-1}\mu \Theta^{-1/2} \mu'$. Taking $\mathbf{Y} = \mathbf{T} \mathbf{H}$ and using Lemma 2.1, the joint density of $\mathbf{H}$ and $\mathbf{T}$ is

$$f_{\mathbf{H},\mathbf{T}}(\mathbf{H}, \mathbf{T}) = \frac{\prod_{i=1}^n t_i^{K-i}}{|\Sigma_{1/2}^{|K|/2}|} h \left[ \text{tr} \left( \Sigma^{-1}TT' + \Omega \right) - 2 \text{tr} \Theta^{-1/2} \mu' \Sigma^{-1}T \mathbf{H} \right].$$

Assuming that $h(\cdot)$ can be expanded in power series, see Fang and Zhang (1990), i.e.

$$h(a + v) = \sum_{t=0}^\infty \frac{h^t(a)v^t}{t!}.$$

Thus

$$f_{\mathbf{H},\mathbf{T}}(\mathbf{H}, \mathbf{T}) = \frac{\prod_{i=1}^n t_i^{K-i}}{|\Sigma_{1/2}^{|K|/2}|} \sum_{t=0}^\infty \sum_{t=0}^\infty \frac{1}{2^t} \left[ \text{tr} \left( \Sigma^{-1}TT' + \Omega \right) \right]^{t} \left( -2 \Theta^{-1/2} \mu' \Sigma^{-1}T \mathbf{H} \right)^{t}.$$

Now, for integration on $\mathbf{H} \in \mathcal{Y}_{n,K}$, we note that it is zero when $t$ is odd (see Theorem II, p.876 in James (1961) or eqs. (44)-(46) in James (1964)). The marginal density of $\mathbf{T}$ is expressed as

$$f_T(T) = \frac{\prod_{i=1}^n t_i^{K-i}}{|\Sigma_{1/2}^{|K|/2}|} \sum_{t=0}^\infty \frac{1}{(2t)!} \left[ \text{tr} \Sigma^{-1}(TT' + \Omega) \right]^{t} \left( -2 \Theta^{-1/2} \mu' \Sigma^{-1}T \mathbf{H} \right)^{2t} (HdH').$$
So, by Lemma 2.2 and recalling that $C_{\chi}(aA) = a^tC_{\chi}(A)$, for a constant, we have

\[
\int_{V_{n,K}} \left[ \text{tr} \left( -2\Theta^{-1/2}\mu'\Sigma^{-1}TH \right) \right]^{2t} (HDH')
\]

\[
= \frac{2^{n\pi nK/2}}{\Gamma_n \left( \frac{1}{2}K \right)} \sum_{\kappa} \frac{\Gamma_k}{\Gamma_k} C_{\kappa} \left( 4\Theta^{-1/2}\mu'\Sigma^{-1}TT'\Sigma^{-1}\mu\Theta^{-1/2} \right)
\]

\[
= \frac{2^{n\pi nK/2}}{\Gamma_n \left( \frac{1}{2}K \right)} \sum_{\kappa} \frac{\Gamma_k}{\Gamma_k} 4^t C_{\kappa} \left( \Theta^{-1}\mu'\Sigma^{-1}TT'\Sigma^{-1}\mu \right)
\]

\[
= \frac{2^{n\pi nK/2}}{\Gamma_n \left( \frac{1}{2}K \right)} \sum_{\kappa} \frac{\Gamma_k}{\Gamma_k} 4^t C_{\kappa} \left( \Omega^{-1}TT' \right)
\]

From [Muirhead 1982], p.21 $\Gamma(k+\frac{1}{2}n) = \left( \frac{1}{2}n \right)_k$ then $\Gamma(k+\frac{1}{2}) = \left( \frac{1}{2} \right)_k$ and $\frac{k}{(2k)!} = \frac{1}{\kappa}$, in our case $k = t$, and the result follows. □

Alternatively, the size-and-shape density (4) can be obtained as a particular case of the singular case studied in [Díaz-Garcia and González-Farías 2003].

### 3 QR Shape distribution

Now, observe that for $T : (N - 1) \times n$, $n = \min(N - 1, K)$, the matrix $T$ contains $(N - 1)K - nK + n(n + 1)/2$ non null QR rectangular coordinates ($t_{ij} \neq 0$). Let $\text{vech} T$ a vector consisting of the no null elements of $T$, taken column by column. Then the QR shape matrix $W$ can be written as

\[
\text{vech} W = \frac{1}{r} \text{vech} T, \quad r = ||T|| = \sqrt{\text{tr} T'T} = ||Y||,
\]

then by Theorem 2.1.3, p.55 of [Muirhead 1982],

\[
(d \text{vech} T) = r^m \prod_{i=1}^{m} \sin \theta_i \left( \bigwedge_{i=1}^{m} d\theta_i \right) \wedge dr,
\]

with $m = (N - 1)K - nK + n(n + 1)/2 - 1$. Denoting $u = (\theta_1, \ldots, \theta_m)'$ and $J(u) = r^m \prod_{i=1}^{m} \sin \theta_i$, so

\[
(dT) = r^m J(u) \left( \bigwedge_{i=1}^{m} d\theta_i \right) \wedge dr.
\]

**Theorem 3.1.** The QR reflection shape density is

\[
f_w(W) = \frac{2^{n\pi nK/2} \prod_{i=1}^{n} w_{ii}^{K-1} J(u)}{\Gamma_n \left( \frac{1}{2}K \right) \left| \Sigma \right|^{K/2}} \sum_{\kappa} \sum_{t=0}^{\infty} C_{\kappa} \left( \Omega^{-1}WW' \right) t! \left( \frac{1}{2}K \right)_k
\]

\[
\times \int_{0}^{\infty} r^{M+2t-1} h(2t) |r^2 \text{tr} \Sigma^{-1}WW' + \text{tr} \Omega|(dr), \tag{5}
\]

where $M = (N - 1)K$. 

Proof. The density of $T$ is

$$f_T(T) = \frac{2^n \pi^{nK/2}}{\Gamma_n[K/2]} \frac{n \prod_{i=1}^{n} t_{ii}^{K_{i}-i}}{|\Sigma|^{K/2}} \sum_{t=0}^{\infty} \sum_{\kappa} \frac{h^{(2t)}[tr((\Sigma^{-1}TT') + \Omega)]}{t!} \frac{C_{\kappa}(\Omega \Sigma^{-1}TT')}{(\frac{1}{2}K)_{\kappa}}.$$ 

Making the change of variables $W(u) = T/r$, the joint density function of $r$ and $u$ is

$$f_{r,u}(r, W) = \frac{2^n \pi^{nK/2}}{\Gamma_n[K/2]} \frac{n \prod_{i=1}^{n} (rw_{ii})^{K_{i}-i}}{|\Sigma|^{K/2}} \sum_{t=0}^{\infty} \sum_{\kappa} \frac{h^{(2t)}[tr(r^2 \Sigma^{-1}WW' + \Omega)]}{t!} \frac{C_{\kappa}(r^2 \Omega \Sigma^{-1}WW')}{(\frac{1}{2}K)_{\kappa}} \times r^{m} J(u).$$

Now, note that

- $C_{\kappa}(r^2 \Omega \Sigma^{-1}WW') = r^{2t} C_{\kappa}(\Omega \Sigma^{-1}WW')$.

- $\prod_{i=1}^{n} (rw_{ii})^{K_{i}-i} = \prod_{i=1}^{n} r^{(K_{i}-i)} \prod_{i=1}^{n} u_{ii}^{K_{i}-i} = r^{nK - \frac{n(n+1)}{2}} \prod_{i=1}^{n} u_{ii}^{K_{i}-i}$.

- $h^{(2t)}[tr(r^2 \Sigma^{-1}WW' + \Omega)] = h^{(2t)}[r^2 tr(\Sigma^{-1}WW' + tr \Omega)]$.

Collecting powers of $r$ by $r^{nK - \frac{n(n+1)}{2} + 2t + m} = r^{M+2t-1}$, $M = (N-1)K$, the marginal of $W$ is:

$$f_W(W) = \frac{2^n \pi^{nK/2}}{\Gamma_n[K/2]} \frac{n \prod_{i=1}^{n} u_{ii}^{K_{i}-i} J(u)}{|\Sigma|^{K/2}} \sum_{t=0}^{\infty} \sum_{\kappa} \frac{C_{\kappa}(\Omega \Sigma^{-1}WW')}{t! (\frac{1}{2}K)_{\kappa}} \times \int_{0}^{\infty} r^{M+2t-1} h^{(2t)}[r^2 tr(\Sigma^{-1}WW' + tr \Omega)](dr).$$

When $\Sigma = \sigma^2 I$, then $\Omega = \mu \Theta^{-1} \mu' / \sigma^2$, $|\Sigma|^{K/2} = \sigma^M$, and $r^2 tr(\Sigma^{-1}WW') = r^2 / \sigma^2$, because $tr WW' = 1$, thus Theorem 3.1 becomes

**Corollary 3.1.** The QR reflection shape density is

$$f_W(W) = \frac{2^n \pi^{nK/2}}{\Gamma_n[K/2]} \frac{n \prod_{i=1}^{n} u_{ii}^{K_{i}-i} J(u)}{\sigma^M} \sum_{t=0}^{\infty} \sum_{\kappa} \frac{C_{\kappa}(\frac{1}{2\sigma^2} \Omega WW')}{t! (\frac{1}{2}K)_{\kappa}} \times \int_{0}^{\infty} r^{M+2t-1} h^{(2t)}[r^2 / \sigma^2 + tr \Omega](dr);$$

and, if the gaussian model is considered with $\Theta = I$, the resulting density corresponds with Goodall and Mardia [1993 Theorem 2], see section 4 below.

### 4 Distributions excluding reflections

From subsection 2.1 of Goodall and Mardia [1993], we can derive the QR size-and-shape and QR shape densities excluding reflection:
• If \( n < K \), then Theorems 2.1, 3.1 stand for the corresponding \( T = T^{NR} \) and \( W = W^{NR} \) excluding reflection densities.

• When \( N - 1 \geq K \) and \( p < K \), the QR size-and-shape density for \( T = T^{NR} \) is \( (4) \) divided by 2, where \( t_{ii} \geq 0 \), for \( i = 1, \ldots, K - 1 \) and \( t_{KK} \) is unrestricted. When \( N - 1 < K \) \( (4) \) stands, since \( t_{KK} \) is not present.

• When \( N - 1 \geq K \) and \( p < K \), the QR shape density for \( W = W^{NR} \) is \( (5) \) divided by 2, and \( w_{KK} \) is unrestricted. When \( N - 1 < K \) \( (5) \) holds, since \( w_{KK} \) is not present.

• The preceding results also hold when rank \( \mu = K \) and rank \( T < K \), and event with probability zero.

• However, if \( p = K \), the excluding reflection densities do not follow the above rule. For the gaussian case, see Goodall and Mardia (1993) and Goodall and Mardia (1991).

5 Central Case

The central case of the preceding sections can be derived easily.

**Corollary 5.1.** The central QR reflection size-and-shape density is given by

\[
f_T(T) = \frac{2^n \pi^{\frac{nK}{2}}}{\Gamma_n \left[ \frac{1}{2} K \right] |\Sigma|^{\frac{K}{2}}} h[tr \Sigma^{-1}TT'].
\]

**Proof.** It is straightforward from Theorem 2.1 just take \( \mu = 0 \) and recall that \( h^{(0)}[tr\cdot] = h[tr\cdot] \). \( \square \)

And:

**Corollary 5.2.** The central QR reflection shape density is given by

\[
f_W(W) = \frac{2^n \pi^{\frac{nK}{2}}}{\Gamma_n \left[ \frac{1}{2} K \right] |\Sigma|^{\frac{K}{2}}} \prod_{i=1}^{n} w_{ii}^{K-i} J(u) \int_0^\infty r^{M-1} h[r^2 tr \Sigma^{-1}WW'](dr).
\]

**Proof.** Just take \( \mu = 0 \) and \( h^{(0)}[tr\cdot] = h[tr\cdot] \) in Theorem 3.1 \( \square \)

The corresponding central excluding reflection densities follows according to Section 4. Observe that it is possible to obtain an invariant central shape density, i.e. the density does not depend on function \( h(\cdot) \) Let \( h \) be the density generator of \( Y \sim \mathcal{E}_{N-1,K}(0, I \otimes I, h) \), i.e.

\[
f_Y(Y) = h(tr YY'),
\]
then by Fang and Zhang (1990), p.102, eq. 3.2.6,

\[
\int_0^\infty r^{(N-1)K-1} h(r^2) dr = \frac{\Gamma[(N-1)K/2]}{2\pi^{(N-1)K/2}}.
\]
So, if \( s = (\text{tr}^{-1}WW')^{1/2}r, \ ds = (\text{tr}^{-1}WW')^{1/2}(dr) \), then

\[
\int_0^{\infty} r^{M-1}h[r^2 \text{tr}^{-1}WW'](dr) = \int_0^{\infty} \left( \frac{s}{(\text{tr}^{-1}WW')^{1/2}} \right)^{M-1}h(s^2) \frac{ds}{(\text{tr}^{-1}WW')^{1/2}} = (\text{tr}^{-1}WW')^{-M/2} \int_0^{\infty} s^{M-1}h(s^2)ds = (\text{tr}^{-1}WW')^{-M/2} \frac{\Gamma[M/2]}{2\pi^{M/2}}.
\]

Thus:

**Corollary 5.3.** When \( \mu = 0 \) the QR reflection shape density is invariant under the elliptical family and it is given by

\[
f_w(w) = \frac{2^{n-1} \pi M^{-\frac{1}{2}} \Gamma[M/2]}{\Gamma_n [\frac{1}{2}K]} \prod_{i=1}^{n} w_i^{K-1} J(u) (\text{tr}^{-1}WW')^{-\frac{M}{2}}.
\]

As in the noncentral case, if \( \Sigma = \sigma^2 I \), then \( |\Sigma|^{\frac{1}{2}} = \sigma^M \) and \( (\text{tr}^{-1}WW')^{-\frac{M}{2}} = \sigma^M \), thus:

**Corollary 5.4.** When \( \mu = 0 \) and \( \Sigma = \sigma^2 I \) the QR reflection shape density is invariant under the elliptical family and it is given by

\[
f_w(w) = \frac{2^{n-1} \pi M^{-\frac{1}{2}} \Gamma[M/2]}{\Gamma_n [\frac{1}{2}K]} \prod_{i=1}^{n} w_i^{K-1}.
\]

### 6 Some particular models

Finally, we give explicit shapes densities for some elliptical models.

The Kotz type I model is given by

\[
h(y) = \frac{R^{\tau-1+\frac{K(N-1)}{2}} \pi^{K(N-1)/2} \Gamma \left( \tau - 1 + \frac{K(N-1)}{2} \right) y^{\tau-1} \exp(-Ry)}{\Gamma \left( \frac{K(N-1)}{2} \right) y^{\tau-1} \exp(-Ry)}.
\]

So, the corresponding \( k \)-th derivative is

\[
\frac{d^k[y^\tau-1 \exp\{-Ry\}]}{dy^k} = (-R)^k y^{\tau-1} \exp\{-Ry\} \left\{ 1 + \sum_{m=1}^{k} \binom{k}{m} \prod_{i=0}^{m-1} (\tau - 1 - i) \right\} (-Ry)^{-m}.
\]

It is of interest the gaussian case, i.e. when \( \tau = 1 \) and \( R = \frac{1}{2} \), here the derivation is straightforward from the general density.

The required derivative follows easily, it is, \( h^{(k)}(y) = \frac{R^{K(N-1)}/2 \pi^{K(N-1)/2}}{\Gamma \left( \frac{K(N-1)}{2} \right) y^{\tau-1} \exp(-Ry)} \) and

\[
\int_0^{\infty} r^{M+2t-1} h^{(2t)}[r^2 \text{tr}^{-1}WW' + \text{tr} \Omega]dr = \frac{R^t}{2\pi^{\frac{M}{2}}} \exp(-R \text{tr} \Omega) \left( \text{tr}^{-1}WW' \right)^{-\frac{M}{2} - t} \Gamma \left( \frac{M}{2} + t \right).
\]
\[ f(W) = \frac{2^n \pi^{nK/2} J(u) \prod_{i=1}^n w_{K-i}^{K-i}}{\Gamma_n \left[ \frac{1}{2} K \right] |\Sigma|^{K/2}} \sum_{t=0}^{\infty} \sum_{\kappa} C_\kappa (\Omega \Sigma^{-1} W W') \]
\[ \times \frac{R^t}{2^n n^t} \exp(-R \text{ tr } \Omega) (\text{ tr } \Sigma^{-1} W W')^{-\frac{M}{2} - t} \Gamma \left( \frac{M}{2} + t \right) \]
\[ = \frac{\exp(-R \text{ tr } \Omega) (\text{ tr } \Sigma^{-1} W W')^{-\frac{M}{2} - t} J(u) \prod_{i=1}^n w_{K-i}^{K-i}}{\pi^{M-n \frac{K}{2}} 2^{n+1} \Gamma_n \left[ \frac{1}{2} K \right] |\Sigma|^{K/2}} \]
\[ \times \sum_{t=0}^{\infty} \frac{\Gamma \left( \frac{M}{2} + t \right)}{t! (\text{ tr } \Sigma^{-1} W W')^t} \sum_{\kappa} C_\kappa (R \Omega \Sigma^{-1} W W') \]
\[ \times \left( \frac{1}{2} K \right)_\kappa \]
\[ = C_\kappa \left( \frac{1}{2} \Omega \Sigma^{-1} W W' \right) \]
\[ = C_\kappa \left( \frac{1}{2} \mu \Sigma^{-1} W W' \mu \right) \]
\[ = 2^t C_\kappa \left( \frac{1}{4} \mu \Sigma^{-1} W W' \mu \right) \]

So, we have proved that

Corollary 6.1. The Gaussian QR reflection shape density is

\[ f(W) = \frac{\exp(-R \text{ tr } \Omega) (\text{ tr } \Sigma^{-1} W W')^{-\frac{M}{2} - t} J(u) \prod_{i=1}^n w_{K-i}^{K-i}}{\pi^{M-n \frac{K}{2}} 2^{n+1} \Gamma_n \left[ \frac{1}{2} K \right] |\Sigma|^{K/2}} \]
\[ \times \sum_{t=0}^{\infty} \frac{\Gamma \left( \frac{M}{2} + t \right)}{t! (\text{ tr } \Sigma^{-1} W W')^t} \sum_{\kappa} C_\kappa (R \Omega \Sigma^{-1} W W') \]
\[ \times \left( \frac{1}{2} K \right)_\kappa \]
\[ = C_\kappa \left( \frac{1}{2} \Omega \Sigma^{-1} W W' \right) \]
\[ = C_\kappa \left( \frac{1}{2} \mu \Sigma^{-1} W W' \mu \right) \]
\[ = 2^t C_\kappa \left( \frac{1}{4} \mu \Sigma^{-1} W W' \mu \right) \]

where \( M = (N - 1)K \).

The isotropic case of this density was derived by Goodall and Mardia [1993], and it is
obtained from noting that \( C_\kappa (aB) = a^t C_\kappa (B) \) and, if \( \Sigma = \sigma^2 I \), then
\( (\text{ tr } \Sigma^{-1} W W')^{-\frac{M}{2}} = \sigma^M, |\Sigma|^{K/2} = \sigma^M \) and that

\[ C_\kappa \left( \frac{1}{2} \Omega \Sigma^{-1} W W' \right) \]
\[ = C_\kappa \left( \frac{1}{2} \Omega \Sigma^{-1} \frac{\mu \mu'}{\sigma^2} \right) \]
\[ = C_\kappa \left( \frac{1}{2} \Omega \Sigma^{-1} \mu \right) \]
\[ = 2^t C_\kappa \left( \frac{1}{4} \sigma^2 \mu \right) \]

Finally, we propose the result for the Kotz type I model

\[ h(y) = \frac{R^t - 1 + \frac{K(N-1)}{2} \Gamma \left( \frac{K(N-1)}{2} \right)}{\pi^{K(N-1)/2} \Gamma \left( \frac{K(N-1)}{2} \right)} y^{t-1} \exp(-Ry), \]
Corollary 6.2. The Kotz type I QR reflection shape density is

\[ f_{W^i}(W) = \frac{\prod_{i=1}^{n} w_i^{K-1} J(u)}{\Gamma_n \left( \frac{1}{2} K \right) |\Sigma|^{K/2}} \sum_{t=0}^{\infty} \sum_{\kappa} \frac{C_{\kappa}(R\Omega \Sigma^{-1} W W')}{t! \left( \frac{1}{2} K \right)_{\kappa}} \times R^{-1} \Gamma \left( \frac{M}{2} \right) (\text{tr} \Sigma^{-1} W W')^{\frac{M}{2} - t} (\text{tr} \Omega)^{-1} \times \left\{ \sum_{u=0}^{\infty} \frac{\Gamma \left( \frac{M}{2} + t + u \right) \prod_{s=0}^{u-1} (\tau - 1 - s)}{u! R^u (\text{tr} \Omega)^u \tau - 1 - m + \frac{M}{2}} \right\}, \]

where \( M = (N-1)K \).

Proof. So, the corresponding \( k \)-th derivative follows from

\[ \frac{d^k}{dy^k} y^{T-1} \exp\{-Ry\} = (-R)^k y^{T-1} \exp\{-Ry\} \left\{ 1 + \sum_{m=1}^{k} \binom{k}{m} \prod_{i=0}^{m-1} (\tau - 1 - i) (-Ry)^{-m} \right\}. \]

and the associating QR reflection shape density can be obtained after some simplification as

\[ f_{W^i}(W) = \frac{2^n n^{nK/2} \prod_{i=1}^{n} w_i^{K-1} J(u)}{\Gamma_n \left( \frac{1}{2} K \right) |\Sigma|^{K/2}} \sum_{t=0}^{\infty} \sum_{\kappa} \frac{C_{\kappa}(\Omega \Sigma^{-1} W W')}{t! \left( \frac{1}{2} K \right)_{\kappa}} \times R^{-1} \Gamma \left( \frac{M}{2} \right) (\text{tr} \Sigma^{-1} W W')^{\frac{M}{2} - t} (\text{tr} \Omega)^{-1} \times \left\{ \sum_{u=0}^{\infty} \frac{\Gamma \left( \frac{M}{2} + t + u \right) \prod_{s=0}^{u-1} (\tau - 1 - s)}{u! R^u (\text{tr} \Omega)^u \tau - 1 - m + \frac{M}{2}} \right\}. \]
6.1 Example: Mouse Vertebra

This classical application is studied in the Gaussian case by Dryden and Mardia (1998). Here we consider again the same model and contrasted it, via the modified BIC* criterion (Yang and Yang (2007)), with two non-Gaussian models.

Here we study three models, the Gaussian shape (G), and the Kotz (K) model for \( \tau = 2 \) and \( \tau = 3 \). The Gaussian shape density was given in (7) and the remaining shape distributions follow by taking \( \tau = 2 \) and \( \tau = 3 \) in theorem 6.2. However, we need to simplify binomial series involved in the terms in braces, this can be done straightforwardly but tedious by mathematical induction, the results are summarized as follows.

Namely, the shape density associated to the Kotz model indexed by \( \tau = 2 \), \( R = \frac{1}{2} \) (and \( s = 1 \)) is given by:

\[
f_W(W) = \prod_{i=1}^{n} w_i^{K-1} J(u) \frac{\exp\left(-\frac{\mu' \mu}{2\sigma^2}\right)}{\Gamma_n\left(\frac{k}{2}\right)} \sum_{t=0}^{\infty} \frac{2^n M}{2^n M} \\
\times \left\{ \left( \text{tr} \left( \frac{\mu' \mu}{2\sigma^2} - 2t \right) \right) \Gamma\left[\frac{M}{2} + t\right] + \Gamma\left[\frac{M}{2} + t + 1\right] \right\} \sum_{\kappa} C_\kappa \left( \frac{1}{2\sigma^2} \mu'WW'\mu \right) t! \left( \frac{1}{2} \right).
\]

where \( M = (N-1)K \).

And the corresponding density for the Kotz model \( \tau = 3 \), is obtained as:

\[
f_W(W) = \prod_{i=1}^{n} w_i^{K-1} J(u) \frac{\exp\left(-\frac{\mu' \mu}{2\sigma^2}\right)}{\Gamma_n\left(\frac{k}{2}\right)} \sum_{t=0}^{\infty} \frac{2^{n+1}}{M(M+2)} \\
\times \left\{ \left( \text{tr} \left( \frac{\mu' \mu}{2\sigma^2} - 2t \right) \right) \Gamma\left[\frac{M}{2} + t\right] + 2 \left( \text{tr} \left( \frac{\mu' \mu}{2\sigma^2} - 2t \right) \right) \Gamma\left[\frac{M}{2} + t + 1\right] \right\} \sum_{\kappa} C_\kappa \left( \frac{1}{2\sigma^2} \mu'WW'\mu \right) t! \left( \frac{1}{2} \right).
\]

where \( M = (N-1)K \).

In order to decide which the elliptical model is the best one, different criteria have been employed for the model selection. We shall consider a modification of the BIC* statistic as discussed in Yang and Yang (2007), and which was first achieved by Rissanen (1978) in a coding theory framework. The modified BIC* is given by:

\[
BIC^* = -2\mathcal{L}(\tilde{\mu}, \tilde{\sigma}^2, h) + n_p (\log(n + 2) - \log 24),
\]

where \( \mathcal{L}(\tilde{\mu}, \tilde{\sigma}^2, h) \) is the maximum of the log-likelihood function, \( n \) is the sample size and \( n_p \) is the number of parameters to be estimated for each particular shape density.

As proposed by Kass and Raftery (1995) and Raftery (1995), the following selection criteria have been employed for the model selection.

The maximum likelihood estimators for location and scale parameters associated with the small and large groups are summarized in the following table:
The Kotz model (\( s \neq 1 \)) and the classical gaussian model widely detailed and applied by Dryden and Mardia (1998) (and previous works) in this experiment. There is a very strong difference between the non gaussian and the gaussian model. According to the modified BIC* criterion (see Table 2), the Kotz model with parameters \( \tau = 2, R = \frac{1}{s} \) and \( s = 1 \) is the most appropriate among the three elliptical densities for modeling the data. There is a very strong difference between the non gaussian and the classical gaussian model.

Let \( \mu_1 \) and \( \mu_2 \) be the mean shape of the small and large groups, respectively. We test equal mean shape under the best model, and the likelihood ratio (based on \( -2 \log \Lambda \approx \chi^2_{10} \)) for the test \( H_0 : \mu_1 = \mu_2 \) vs \( H_a : \mu_1 \neq \mu_2 \), provides the p-value \( 0.310^{-12} \), which means that there extremely evidence that the mean shapes of the two groups are different. This is the same conclusion obtained by Dryden and Mardia (1998) for a gaussian model.

A final comment, for any elliptical model we can obtain the Q reflection model, however a nontrivial problem appears, the 2-th derivative of the generator model, which can be seen as a partition theory problem. For the general case of a Kotz model (\( s \neq 1 \)), and another models like Pearson II and VII, Bessel, Jensen-logistic, we can use formulae for these derivatives given by Caro-Lopera et al. (2009). The resulting densities have again a form of a generalized series of zonal polynomials which can be computed efficiently after some modification of existing works for hypergeometric series (see Koef and Edelman (2006)), thus the inference over an exact density can be performed, avoiding the use of any asymptotic distribution, and the initial transformation avoids the invariant polynomials of Davis (1908), which at present seems can not be computable.

### Table 1: Grades of evidence corresponding to values of the BIC* difference.

| BIC* difference | Evidence |
|-----------------|----------|
| 0–2             | Weak     |
| 2–6             | Positive |
| 6–10            | Strong   |
| > 10            | Very strong |

### Table 2: The maximum likelihood estimators

| Group | \( BIC^* \) | \( \mu_{11} \) | \( \mu_{12} \) | \( \mu_{21} \) | \( \mu_{22} \) | \( \mu_{31} \) | \( \mu_{32} \) |
|-------|-------------|----------------|----------------|----------------|----------------|----------------|----------------|
| Small | -418.011    | 1.2208         | 39.2127        | 11.3683        | 1.2263         | 22.0334        | -1.3614        |
|       | -3.3846     | 44.7126        | 14.7682        | 5.5268         | 25.3660        | 74.1439        | -6.5074        |
| Large | 206.7321    | -7.2450        | -90.9671       | 28.0714        | -11.2058       | 58.7553        | 0.8674         |
|       | 151.6613    | -26.5182       | -71.4992       | 20.0230        | -15.3962       | 47.4424        | -12.6667       |

\[ \mu_{41} = \mu_{42} \]

\[ \mu_{51} = \mu_{52} \]

\[ \sigma^2 \]

| \( \mu_{41} \) | \( \mu_{42} \) | \( \mu_{51} \) | \( \mu_{52} \) | \( \sigma^2 \) |
|---------------|---------------|---------------|---------------|---------------|
| 4.0934        | -4.7494       | -27.1075      | -3.7075       | 14.4289       |
| 13.7665       | -15.8699      | -90.7380      | -2.7664       | 289.4146      |
| 5.1319        | -14.5874      | -82.0939      | -12.9619      | 345.0996      |
| 7.1216        | 10.3519       | -72.3213      | 6.4313        | 225.3525      |
| 8.0814        | 6.7039        | -56.6913      | 21.6223       | 109.0523      |
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