THE DETECTION OF LOCAL SHAPE CHANGES VIA THE GEOMETRY OF HOTELLING'S T^2 FIELDS[1]

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This paper is motivated by the problem of detecting local changes or differences in shape between two samples of objects via the non-linear deformations required to map each object to an atlas standard. Local shape changes are then detected by high values of the random field of Hotelling's T^2 statistics for detecting a change in mean of the vector deformations at each point in the object. To control the null probability of detecting a local shape change, we use the recent result of Adler (1998) that the probability that a random field crosses a high threshold is very accurately approximated by the expected Euler characteristic (EC) of the excursion set of the random field above the threshold. We give an exact expression for the expected EC of a Hotelling's T^2 field, and we study the behaviour of the field near local extrema. This extends previous results for Gaussian random fields (Adler, 1981) and χ^2, t and F fields (Worsley, 1994; Cao, 1998). For illustration, these results are applied to the detection of differences in brain shape between a sample of 29 males and 23 females.

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1 Introduction

Time magazine (Canadian edition, May 5, 1997, p. 43) recently reported a study (Drevets *et al.*, 1997) that showed that the subgenual prefrontal cortex, a small region in the centre of the brain, is almost half the size in people suffering from hereditary depression. This region had previously been implicated in the mediation of emotional and autonomic responses to socially significant or provocative stimuli, and in the modulation of the neurotransmitter systems targeted by antidepressant drugs. Researchers were guided to this area by data from a positron emission tomography study that had detected a decrease in cerebral blood flow there, compared to normals. Here the researchers knew where to look, but this naturally raises the question of how to detect small local changes in brain shape between two groups of subjects *without* knowing in advance where to look. Obviously we could compare the volume of a large number of standard brain regions, but this might not detect small local changes in the shapes of the regions. Some sort of overall shape analysis is clearly more desirable.

Traditional shape analysis methods in the statistics literature (Small, 1996) rely on landmarks, but in the human brain such landmarks are difficult to identify reliably. Instead, researchers are now assessing brain shape through the continuous 3D deformations required to map the brain to an atlas standard. In effect, this provides us with *continuous* landmark data, which in turn demands new methods of analysis. We present one such method here, based on Hotelling's T^2 fields.

Deformations data arise as a spin-off from another problem in brain mapping: no two brains have quite the same shape. In the analysis of 3D positron emission tomography and functional magnetic resonance images of brain 'activity' it is very important to be able to re-align or register the anatomy of one subject to match the anatomy of a standard atlas brain. This then makes it possible to compare data across different subjects. This is accomplished by first aligning the brains as best as possible with linear transformations, then using 3D non-linear deformations to improve the fit (Collins *et al.*, 1995; Friston *et al.*, 1996; Thompson & Toga, 1996).

This opens up the possibility of using the deformations themselves to analyse differences in brain shape. In the simplest case, we wish to detect differences in brain shape between two groups of p_1 and p_2 subjects. Let $\Delta_{ij}(t)$, $i = 1, \ldots, p_j$, $j = 1, 2$ be the $d = 3$ component vector of deformations or displacements required to move the structure at position $t \in \Re^3$ of the atlas brain to the position of the corresponding brain structure of subject i in group j. We shall model these deformations as

$$\Delta_{ij}(t) = \mu_j(t) + \Sigma(t)^{\frac{1}{2}}\epsilon_{ij}(t),$$

where $\mu_j(t)$ is the mean deformation for group j, $j = 1, 2$, and $\Sigma(t)$ is a positive definite matrix to allow for correlations between components of the deformations, which depend on the location t. The three components of $\epsilon_{ij}(t)$ are i.i.d. smooth stationary Gaussian random fields with mean 0 and variance 1. The sample mean and variance of the deformations are:

$$\begin{aligned}\bar{\Delta}_j(t) &= \sum_{i=1}^{p_j} \Delta_{ij}(t)/p_j, \\ \hat{\Sigma}(t) &= \sum_{j=1}^{2}\sum_{i=1}^{p_j}[\Delta_{ij}(t) - \bar{\Delta}_j(t)][\Delta_{ij}(t) - \bar{\Delta}_j(t)]'/\nu,\end{aligned}$$

where $\nu = p_1 + p_2 - 2$. Differences in deformations between the groups can then be detected using the Hotelling's T^2 field (Thompson *et al.*, 1997) equal to $\nu Y(t)$ where

$$Y(t) = \frac{p_1 p_2}{(p_1 + p_2)}[\bar{\Delta}_1(t) - \bar{\Delta}_2(t)]'\hat{\Sigma}(t)^{-1}[\bar{\Delta}_1(t) - \bar{\Delta}_2(t)]/\nu.$$

Under the null hypothesis of no group differences, $F(t) = ((\nu - d + 1)/d)Y(t)$ has an F distribution with d and $\nu - d + 1$ degrees of freedom at each point t.

Our alternative hypothesis is that shape differences are confined to a small number of isolated regions of unknown location inside a search region $S \subset \Re^3$, usually taken to be the whole brain. These regions of local changes in brain shape are detected by the excursion set A_y, defined as the points $t \in S$ where $Y(t)$ exceeds a high threshold y, denoted by $A_y = \{t \in S \ : \ Y(t) \geq y\}$ (see Figure 1). Clearly we wish to choose y to control the probability of detecting changes in regions where there are really none. A conservative choice for y is obtained by assuming that there are no changes anywhere in the whole region S. Equivalently, we wish to find the tail probability or P-value for

$$Y_{\max} = \max_{t \in S} Y(t)$$

under the null hypothesis of no shape changes in S.

The tool we shall use is the Euler characteristic (EC) of A_y, denoted by $\chi(A_y)$. Roughly speaking, the Euler characteristic counts the number of isolated connected components of the set, minus the number of 'holes' that penetrate the set, plus the number of interior 'hollows' in the set. If the threshold is high, the holes and hollows in the excursion set A_y tend to disappear and the EC counts the number of connected components of the excursion set, which approximates the number of local maxima. For very high thresholds, near the global maximum $Y_{\max}$, the EC is 1 if $Y_{\max} > y$ and 0 otherwise. Thus the expected EC approximates the P-value of $Y_{\max}$:

$$\mathcal{P}\{Y_{\max} \geq y\} \approx \mathcal{E}\{\chi(A_y)\}. \tag{1.1}$$

Although it is not quite what we want, the expected EC of the excursion set has several advantages over other approximations to the upper tail probability of the maximum: it is very accurate (there has been a recent breakthrough on this longstanding conjecture: Adler, 1998, has shown that the expected EC for Gaussian random fields is accurate to as many terms in its expansion); in some discrete situations, it is exact (see Naiman and Wynn, 1992); in many cases it is possible to find an exact expression for the expected EC of the excursion set for *all* threshold levels; the EC of the excursion set has inherent interest as a tool for studying the clustering behaviour of random fields and point processes, particularly in astrophysics (Torres, 1994; Vogeley *et al.*, 1994; Worsley, 1995b).

The key to the success of these methods is to find a point-set representation for the EC, which writes the EC in terms of *local* properties of the random field, rather than *global* topological properties such as connectedness. One such representation comes from differential topology and Morse theory. We then take expectations, and simplify the result for an isotropic random field. The expected EC then comes down to the expectation of the determinant of the second derivative of the random field, conditional on its first derivative at a point. For a particular random field, the main effort is to find this expectation. This has been done for Gaussian random fields (Adler, 1981), for χ^2, t and F fields (Worsley, 1994) and for correlation fields (Cao & Worsley, 1999). Our aim here is to extend this to Hotelling's T^2 fields. Note that this is not trivial, since $F(t)$ is not an F field (see Section 3.3, Remark 1). We shall also look at the shape of the Hotelling's T^2 random field near local extrema, extending the work of Aronowich & Adler (1988) and Cao (1998) for χ^2, t and F fields.

The outline of the paper is as follows. In Section 2 we review the expression for the expected EC for an isotropic field. This requires the expectation of functions of the first and second derivatives of the random field. Past experience with χ^2, t and F fields has shown that a successful way of dealing with this is to represent the first two derivatives in terms of independent random variables with standard distributions. In Section 3 we define the Hotelling's T^2 random field and find such a representation for its derivatives. In Section 4 we use this representation to find the expected EC. In Section 5 we shall consider the number of extremal points of Hotelling's T^2 field and in Section 6 we shall consider the limiting conditional distribution of the curvature at these points. Finally in Section 7 we shall apply this work to a real example from 3D brain deformation studies.

The proofs of most results are long and technical. To simplify the presentation, we omitted the proofs except for that of the main result, Theorem 4.1, which is given in the Appendix. Interested readers should refer to Cao (1997) or Cao & Worsley (1998) for the rest of the proofs.

2 Review of the expected Euler characteristic

Let $Y(t)$, $t = (t_1, \ldots, t_N)' \in S \subset \Re^N$ be a smooth stationary random field inside a closed compact set S with a twice differentiable boundary ∂S. From now on we shall omit the argument t to simplify the notation, and write $Y = Y(t)$. For a vector, we shall use subscripts j and $|j$ to represent the jth and first j components. For a symmetric $n \times n$ matrix B, we shall use the subscript $|j$ to represent the sub-matrix composed of the first j rows and columns. We shall also use $\mathrm{detr}_j(B)$ to denote the sum of the determinant of all $j \times j$ principal minors of B, so that $\mathrm{detr}_n(B) = \det(B)$, $\mathrm{detr}_1(B) = \mathrm{tr}(B)$ and we define $\mathrm{detr}_0(B) = 1$. Wherever possible, we shall use lower case letters for scalars and vectors, and upper case letters for matrices; the only exception is Y itself. Finally, we shall let $x^+ = x$ if $x > 0$ and 0 otherwise.

It is possible to find a simple result for the expectation of the EC of the excursion set when the field is isotropic in t. Define the j-dimensional *EC intensity* as

$$
\begin{aligned}
\rho_j(y) &= \mathcal{E}\left\{(Y \geq y) \det(-\ddot{Y}_{|j}) \mid \dot{Y}_{|j} = 0\right\} \theta_{|j}(0) \\
&= \mathcal{E}\left\{\dot{Y}_j^+ \det(-\ddot{Y}_{|j-1}) \mid \dot{Y}_{|j-1} = 0, Y = y\right\} \phi_{|j-1}(0, y),
\end{aligned} \tag{2.1}
$$

where $\theta_{|j}(\cdot)$ is the density of $\dot{Y}_{|j}$ and $\phi_{|j-1}(\cdot,\cdot)$ is the joint density of $\dot{Y}_{|j-1}$ and Y; the equivalence of the two definitions is demonstrated in Worsley (1995b). The word intensity is chosen to emphasize the derivation of (2.1) from Morse theory as the expectation of a point process in $\Re^N$ taking values ± 1 at turning points of $Y(t)$ (Adler, 1981; Worsley, 1995b). Let $a_j = 2\pi^{j/2}/\Gamma(j/2)$ be the surface area of a unit $(j-1)$-sphere in $\Re^j$. Let C be the inside curvature matrix of S at a point t, and for $j = 0, \ldots, N-1$ define the j-dimensional measure, proportional to the Minkowski functional, of S as

$$\mu_j(S) = \frac{1}{a_{N-j}} \int_{\partial S} \mathrm{detr}_{N-1-j}(C) dt,$$

and define $\mu_N(S) = |S|$, the Lebesgue measure of S. Note that $\mu_0(S) = \chi(S)$ by the Gauss-Bonnet Theorem, and $\mu_{N-1}(S)$ is half the surface area of S. Then the expected EC is given by:

$$\mathcal{E}\{\chi(A_y)\} = \sum_{j=0}^{N} \mu_j(S)\rho_j(y), \tag{2.2}$$

where we define $\rho_0(y) = \mathcal{P}\{Y \geq y\}$ (Worsley, 1995b). Our main task, therefore, is to evaluate $\rho_j(y)$ from (2.1).

3 The Hotelling's T^2 field and representations of its derivatives

Before we proceed, we shall introduce some notation used throughout the paper. Let $\delta_{ij} = 1$ if $i = j$ and 0 otherwise, and let I_d be the $d \times d$ identity matrix. Let $\text{Normal}_d(\mu, \Sigma)$ represent the multivariate normal distribution on $\Re^d$ with mean μ and variance Σ, and if A is an $n \times m$ matrix whose elements are normally distributed we shall write $\text{Normal}_{n\times m}$. Let χ^2_ν represent the χ^2 distribution with ν degrees of freedom, let $\text{Wishart}_d(\Sigma, \nu)$ represent the Wishart distribution of a $d\times d$ matrix with expectation $\nu\Sigma$ and degrees of freedom ν, let $F_{n,m}$ represent the F distribution with n, m degrees of freedom for numerator and denominator respectively and let Uniform_d represent the uniform distribution over the surface of the unit $(d-1)$-sphere in $\Re^d$. Finally, we shall let $\stackrel{D}{=}$ represent equality in law between two random variables.

3.1 Gaussian field

Let $\xi = \xi(t)$ be an isotropic standard Gaussian random field on $\Re^N$ with $\mathcal{E}(\xi) = 0$, $\mathcal{V}ar(\xi) = 1$ and $\mathcal{V}ar(\dot{\xi}) = I_N$. We shall assume that ξ satisfies the regularity conditions of Theorem 5.2.2 of Adler (1981) which ensure that realizations of ξ are sufficiently smooth.

Lemma 3.1 *(Adler, 1981, page 31) We can write the second derivative of ξ at a fixed point t in terms of independent random variables as follows. For $j, k = 1, \ldots, N$,*

$$\ddot{\xi}_{jk} \stackrel{D}{=} -\delta_{jk}\xi + h_{jk},$$

where h_{jk} is independent of ξ and $\dot{\xi}$, and joint normal with mean zero and covariance

$$\mathcal{C}ov(h_{ij}, h_{kl}) = \gamma(i, j, k, l) - \delta_{ij}\delta_{kl},$$

where $\gamma(i, j, k, l)$ is symmetric in its arguments, $i, j, k, l = 1, \ldots, N$. We shall refer to this type of covariance matrix as M.

3.2 Wishart field

Suppose Z is a $\nu \times d$ matrix of i.i.d. Gaussian fields on $\Re^N$, each with the same distribution as ξ above. Define the Wishart random field on $\Re^N$ with $\nu \geq d$ degrees of freedom as

$$W = Z'Z. \tag{3.1}$$

Lemma 3.2 *We can write the first two derivatives of W at a fixed point t in terms of independent random variables as follows:*

$$\begin{aligned}
\dot{W}_j &\stackrel{D}{=} W^{\frac{1}{2}}A_j + (W^{\frac{1}{2}}A_j)', \\
\ddot{W}_{jk} &\stackrel{D}{=} -2\delta_{jk}W + W^{\frac{1}{2}}H_{jk} + (W^{\frac{1}{2}}H_{jk})' + V_{jk} + V_{kj} + A_j'A_k + A_k'A_j,
\end{aligned}$$

where W, A_j and V_{jk} are $d \times d$ random matrices such that $W \sim \mathrm{Wishart}_d(I_d, \nu)$, $A = (A_1, \ldots, A_N) \sim \mathrm{Normal}_{d\times dN}(0, I_{d^2N})$, $V = (V_{jk}) \sim \mathrm{Wishart}_{dN}(I_{dN}, \nu-d)$ and the components of the $d \times d$ matrix H_{jk} are i.i.d. with the same distribution as h_{jk} in Lemma 3.1, all independently, $j, k = 1, \ldots, N$.

3.3 Hotelling's T^2 field

Let W be a Wishart random field defined in (3.1) and z be a vector of d i.i.d. Gaussian random fields independent of W whose components have the same distribution as ξ. The Hotelling's T^2 field is then defined by νY, where

$$Y = z'W^{-1}z.$$

Although the Hotelling's T^2 statistic is well defined *at a point* provided $\nu \geq d$, it is not clear that this is so at all points in a compact subset S of $\Re^N$. Consider the case where $d = 1$, so that the Hotelling's T^2 field is a scalar multiple of an F field with 1 and ν degrees of freedom. Worsley (1994) shows that if $\nu < N$ then *at some point* inside a finite region both the numerator and the denominator of the F field can be exactly zero (i.e. with probability greater than zero), so that the F field is not well defined. To avoid a similar occurrence for the Hotelling's T^2 field, we shall now show that we require $\nu \geq d + N - 1$. To see this, note that we can write

$$Y = \det(T)/\det(W) - 1, \quad T = W + zz'.$$

Y is well defined if and only if either $\det(T) > 0$ or $\det(W) > 0$. Since the latter condition implies the former, then the former is both necessary and sufficient. Now we can write

$$\det(T) = \prod_{i=\nu+2-d}^{\nu+1} u_i, \quad u_i = \sum_{j=1}^{i} \xi_{ij}^2, \tag{3.2}$$

where ξ_{ij} are i.i.d. standard Gaussian random fields. Hence $\det(T) > 0$ if and only if $u_i > 0$ for each i. Now $u_i = 0$ if and only if $\xi_{ij} = 0$ for each $j = 1, \ldots, i$. Inspection of the derivation of (3.2) (e.g. Anderson, 1984) shows that if z and Z are spatially smooth, then so is ξ_{ij}. The set of points inside a compact subset S of $\Re^N$ where $\xi_{ij} = 0$ for each $j = 1, \ldots, i$ is a smooth manifold of dimension no greater than $N - i$, and empty if $i > N$, with probability one. Hence $i > N$ is a necessary and sufficient condition for $u_i > 0$ at all points inside S, with probability one. For all $u_i > 0$ in (3.2) we require $\nu + 2 - d > N$, or $\nu \geq N + d - 1$. Note that if $\nu = N + d - 1$ then $\det(W) = 0$ is possible at isolated points, so that Y may be infinite at isolated points; if $\nu > N + d - 1$ then Y is almost surely finite everywhere inside S.

On the other hand, Adler (1981, page 176) points out that if $d \leq N$ then all components of z can be zero on manifolds of dimension $N - d$ and hence Y can have exact zeros. This is a type of stochastic version of the Brouwer fixed-point theorem, which says that if S is homeomorphic to a ball, and if $t + z(t) \in S$ for all $t \in S$, then there exists at least one fixed point where $z(t) = 0$. In our case, $t + z(t)$ need not always lie in S because $z(t)$ is random, and so the number of fixed points is random. Later in Section 4, Remark 2, we shall use the expected EC to find the expected number of such fixed points.

A look at these arguments will show that the distributional properties of z and Z do not enter into consideration; the only requirement is independence of the components, smoothness of their realizations, and unbounded support.

Lemma 3.3 *We can write the first two derivatives of Y at a fixed point t in terms of independent variables as follows:*

$$\begin{aligned} \dot{Y} &\stackrel{D}{=} 2(1+Y)Y^{\frac{1}{2}}E'T^{-\frac{1}{2}}q, \\ \ddot{Y} &\stackrel{D}{=} 2(1+Y)\Big\{E'T^{-1}E + \frac{3}{4(1+Y)^2}\dot{Y}\dot{Y}' \\ &\quad -Y^{\frac{1}{2}}(q'T^{-1}q)^{\frac{1}{2}}[E'T^{-\frac{1}{2}}F + F'T^{-\frac{1}{2}}E - H] - Y(q'T^{-1}q)U\Big\}, \end{aligned}$$

where $(\nu - d + 1)Y/d \sim F_{d,\nu-d+1}$, $E, F \sim \mathrm{Normal}_{d\times N}(0, I_{dN})$, $T \sim \mathrm{Wishart}_d(I_d, \nu+1)$, $q \sim \mathrm{Uniform}_d$, $U \sim \mathrm{Wishart}_N(I_N, \nu - d)$ *and* $H \sim \mathrm{Normal}_{N\times N}(0, M)$, *all independently.*

Remark 1. As we know from standard multivariate statistics, Hotelling's T^2 is a multiple of an $F_{d,\nu-d+1}$ random variable. But we can see from Lemma 3.3 that if $d \geq 2$, it has a different representation for its derivatives from that of an F field, defined by the ratio of two χ^2 fields (Worsley, 1994), hence it is not an F field. In particular, it can be shown that the variance of the derivative of a Hotelling's T^2 field is slightly larger than that of the corresponding F field.

In later sections we will need the joint distribution of $E'T^{-1}E$, $E'T^{-\frac{1}{2}}q$ and $q'T^{-1}q$. This is done by representing these variables as a one-to-one transformation of other independent random variables whose distributions can be easily derived. First, we shall introduce a class of distributions which we call Multi-T^2 distributions following Theorem 4.1 of Olkin and Rubin (1964).

Lemma 3.4 *Let X be a $k \times p$ matrix whose rows are i.i.d.* $\mathrm{Normal}_p(0, \Sigma)$*, and let* $V \sim \mathrm{Wishart}_p(\Sigma, n)$ *independent of X, then the density of $G = XV^{-1}X'$ is*

$$\pi^{-\frac{k(k-1)}{4}} \prod_{i=1}^{k} \frac{\Gamma(\frac{n+k-i+1}{2})}{\Gamma(\frac{p-i+1}{2})\Gamma(\frac{n+k-p-i+1}{2})} \det(G)^{\frac{p-k-1}{2}} \det(I_k + G)^{-\frac{n+k}{2}}.$$

We shall refer to this type of distribution as Multi-$T^2(p, k, n)$.

Lemma 3.5 *Let* $E \sim \mathrm{Normal}_{d \times N}(0, I_{dN})$*,* $T \sim \mathrm{Wishart}_d(I_d, \nu + 1)$ *and* $q \sim \mathrm{Uniform}_d$*, independently. Then the three variables*

$$V_1 = E'T^{-1}E, \qquad v_2 = (E'T^{-1}E)^{-\frac{1}{2}}E'T^{-\frac{1}{2}}q \qquad \text{and} \qquad v_3 = \frac{q'T^{-1}q}{(q'T^{-\frac{1}{2}}E)(E'T^{-\frac{1}{2}}q) + 1}$$

are independently distributed as follows:

(a) $V_1 \sim$ *Multi-*$T^2(d, N, \nu + 1)$.

(b) *If $d = N$, then* $v_2 \sim \mathrm{Uniform}_N$ *and if $d > N$, then the density of v_2 is*

$$\frac{\Gamma(\frac{d}{2})}{\pi^{\frac{N}{2}}\Gamma(\frac{d-N}{2})}(1 - v_2'v_2)^{\frac{d-N}{2}-1}.$$

(c) $v_3^{-1} \sim \chi^2_{\nu+N-d+2}$.

If $d < N$, then V_1 is singular, but (c) still holds.

4 The expected EC of the excursion set

We shall assume that all the component fields of z and Z that define the Hotelling's T^2 field νY are isotropic Gaussian random fields that satisfy the regularity conditions of Theorem 5.2.2 of Adler (1981). Following the same argument as Lemma 7.1.1 of Adler (1981), it can be shown that Y also satisfies the conditions necessary for the results in Section 2 to hold. To find the expected EC, we now need to find the EC intensity, which is given by the following Theorem.

Theorem 4.1 *Let $n = N - 1$. Then for $\nu \geq d + n$,*

$$\rho_N(y) = \pi^{-\frac{n+2}{2}} \frac{\Gamma(\frac{\nu+1}{2})}{\Gamma(\frac{d}{2})} \frac{2^{\nu-d}n!}{(\nu-d)!}(1+y)^{-\frac{\nu-1}{2}} y^{-\frac{n+1-d}{2}} Q_{\nu,d,n}(y),$$

where $Q_{\nu,d,n}(y)$ is a polynomial of degree n in y given by

$$
\begin{aligned}
Q_{\nu,d,n}(y) &= \sum_{j=0}^{\lfloor n/2\rfloor}\sum_{k=0}^{n-2j}\sum_{m=0}^{\lfloor(n-2j-k)/2\rfloor}\binom{\nu-d}{k}\binom{d-1}{n-2j-k-m} \\
&\quad \binom{\nu-d+n-2j-k-m}{n-2j-k-m}^{-1}\frac{(-1)^{n+j+k+m}\Gamma(\frac{\nu-d+n+1}{2}-j-k-m)}{j!m!(n-2j-k-2m)!2^{2j+k+m}}y^{j+k+m},
\end{aligned}
$$

where division by the factorial of a negative integer is treated as multiplication by zero.

Corollary 4.2 *The first four EC intensities are:*

$$
\begin{aligned}
\rho_0(y) &= \int_y^\infty \frac{\Gamma(\frac{\nu+1}{2})}{\Gamma(\frac{d}{2})\Gamma(\frac{\nu-d+1}{2})}(1+u)^{-\frac{\nu+1}{2}}u^{\frac{d-2}{2}}du, \\
\rho_1(y) &= \frac{\pi^{-\frac{1}{2}}\Gamma(\frac{\nu+1}{2})}{\Gamma(\frac{d}{2})\Gamma(\frac{\nu-d+2}{2})}(1+y)^{-\frac{\nu-1}{2}}y^{\frac{d-1}{2}}, \\
\rho_2(y) &= \frac{\pi^{-1}\Gamma(\frac{\nu+1}{2})}{\Gamma(\frac{d}{2})\Gamma(\frac{\nu-d+1}{2})}(1+y)^{-\frac{\nu-1}{2}}y^{\frac{d-2}{2}}\left(y-\frac{d-1}{\nu-d+1}\right), \\
\rho_3(y) &= \frac{\pi^{-\frac{3}{2}}\Gamma(\frac{\nu+1}{2})}{\Gamma(\frac{d}{2})\Gamma(\frac{\nu-d}{2})}(1+y)^{-\frac{\nu-1}{2}}y^{\frac{d-3}{2}}\left(y^2-\frac{2d-1}{\nu-d}y+\frac{(d-1)(d-2)}{(\nu-d+2)(\nu-d)}\right).
\end{aligned}
$$

Remark 2. Theorem 4.1 tells us a lot about the zeros and infinities of a Hotelling's T^2 field. Taking the limit when $y \to \infty$ in Theorem 4.1, the EC counts the number of infinities. As previously discussed in Section 3.3, if $\nu \geq d+N$ then there are with probability one, no points where the field is infinite, but when $\nu = d+N-1$ there is a finite number of infinities almost surely. The EC intensity then gives the average number of infinities per unit volume:

$$\rho_N(\infty) = \pi^{-\frac{N}{2}}\frac{\Gamma(\frac{d+N}{2})}{\Gamma(\frac{d}{2})}.$$

Taking the limit when $y \to 0$ in Theorem 4.1, the EC counts $(-1)^{N-1}$ times the number of zeros. If $d > N$ then $\rho_N(0) = 0$ and so the field has no zeros with probability one, but if $d = N$ then the field has almost surely finite zeros with the average per unit volume given by

$$(-1)^{N-1}\rho_N(0) = \pi^{-\frac{N+1}{2}}\Gamma\left(\frac{N+1}{2}\right).$$

If $d < N$ then $\rho_N(0) = \infty$ and so the field has infinite zeros with probability one. This is not surprising since the behaviour of the Hotelling's T^2 field near infinity depends on the behaviour of the determinant of the Wishart field, $\det(W)$, near zero, and the behaviour of the Hotelling's T^2 field near zero depends on the behaviour of the χ^2 field, $z'z$, near zero. Similar discussions for χ^2, t and F random fields can be found in Adler (1981), page 176, and Worsley (1994).

5 The expected number of extremal points

Theorem 6.3.1 of Adler (1981) and Theorem 2.1 of Worsley (1994) gives a general formula to calculate the expectation of the number of local extrema per unit volume. We shall apply the theorem to the Hotelling's T^2 field. We shall need the following notation. For a random field $Y(t), t \in \Re^N$, denote the expected number of local maxima of $Y(t)$ above y per unit volume by $\mu^+(y)$ and denote the expected number of local minima of $Y(t)$ below y per unit volume by $\mu^-(y)$.

Theorem 5.1 *Under the same regularity conditions as before*

$$\begin{aligned}
\mu^+(y) &= \frac{\pi^{-\frac{N}{2}}\Gamma(\frac{\nu+1}{2})}{\Gamma(\frac{d}{2})\Gamma(\frac{\nu+1-d-N}{2}+1)} y^{-\frac{\nu+1-d-N}{2}}\{1+O(y^{-\frac{1}{2}})\} \quad \textit{for } \nu \geq d+N, \\
\mu^-(y) &= \frac{\pi^{-\frac{N}{2}}2^{-N+1}\Gamma(\frac{\nu+1}{2})(d-1)!}{\Gamma(\frac{d}{2})\Gamma(\frac{\nu+1+N-d}{2})(d-N)!} y^{\frac{d-N}{2}}\{1+O(y^{\frac{1}{2}})\} \quad \textit{for } d > N.
\end{aligned}$$

Suppose $Y(t)$ has a local maximum (minimum) at 0 with a height exceeding (below) y, then the above theorem could be used to find the distribution of $Y(0)$ in the limit of $y \to \infty$ ($y \to 0$). This is done using the notion of "conditioning in the ergodic sense", or "horizontal window conditioning" introduced by Kac and Slepian (1959). We will refer to this type of conditioning as "HW conditioning" and we shall adopt the notation $\|$ used by Aronowich & Adler (1988) to denote it.

Theorem 5.2 *Given that the Hotelling's T^2 field $Y(t), t \in \Re^N$ has a local maximum (minimum) at $t = 0$ with a height exceeding (below) y, then*

$$\begin{aligned}
\lim_{y\to\infty} \mathcal{P}\{Y(0) > y/v \parallel Y(0) > y; \text{maximum}\} &= v^{\frac{\nu+1-d-N}{2}}, \\
\lim_{y\to 0} \mathcal{P}\{Y(0) < yv \parallel Y(0) < y; \text{minimum}\} &= v^{\frac{d-N}{2}}.
\end{aligned}$$

As we pointed out before, if $d \geq 2$, the Hotelling's T^2 field is not a scaled F random field although at each point, it follows a scaled $F_{d,\nu-d+1}$ distribution. However, the expected number of extremal points of the Hotelling's T^2 field and that of the F field (Worsley, 1994, Theorem 4.3) share a similar form.

6 The limiting conditional distribution of the curvature at local extrema

In this section, we shall determine the limiting conditional distribution of $\ddot{Y}(t)$ given that $t = 0$ is a local extremum with height y. Again, the appropriate approach is via HW conditioning.

Theorem 6.1 *Given that the Hotelling's T^2 field $\nu Y(t), t \in \Re^N$, has a local extremum at 0 with height y, then*

(a) *if $t = 0$ is a local maximum,*

$$y^{-1}(1+y)^{-1}\ddot{Y} \to -2a^{-1}B$$

as $y \to \infty$, where $a \sim \chi^2_{\nu-d-N+2}$, $B \sim \mathrm{Wishart}_N(I_N, \nu - d + 2)$.

(b) *if $t = 0$ is a local minimum,*

$$(1+y)^{-1}\ddot{Y} \to 2B$$

as $y \to 0$, where $B \sim$ Multi-$T^2(d+1, N, \nu+1)$.

Remark 3. Let Λ be the variance matrix of the first derivative of the component Gaussian fields in the definition of a Hotelling's T^2 field. For simplicity, we have assumed $\Lambda = I_N$ in the above sections. The extension to the general Λ is obvious after a simple change of coordinates to $s = \Lambda^{\frac{1}{2}}t$. We can write $\tilde{Y}(t)$ as $Y(s)$ where the variance matrix of the first derivative of the component Gaussian fields of $Y(s)$ is identity. Then

$$\frac{\partial \tilde{Y}}{\partial t} = \Lambda^{\frac{1}{2}}\frac{\partial Y}{\partial s}, \qquad \frac{\partial^2 \tilde{Y}}{\partial t \partial t'} = \Lambda^{\frac{1}{2}}\frac{\partial^2 Y}{\partial s \partial s'}\Lambda^{\frac{1}{2}}.$$

Hence the EC and local extrema intensities of $\tilde{Y}$ should equal those for Y multiplied by $\det(\Lambda)^{\frac{1}{2}}$, and we can adjust Lemma 3.3 and Theorem 6.1 in a similar way.

7 Application to the detection of shape changes in the brain

To illustrate these methods, we tested for differences in brain shape between a group of $p_1 = 29$ normal male subjects and $p_2 = 23$ normal female subjects. This has little scientific value, but we use it simply as a convenient test of the methods. Deformations were estimated on a lattice of $128 \times 128 \times 80$ equally spaced voxels that covered the entire brain. The excursion set of the Hotelling's T^2 field above a threshold of $F(t) \geq 4$ is shown in Figure 1, together with some of the deformation differences $\bar{\Delta}_1(t) - \bar{\Delta}_2(t)$ as small vectors, magnified by a factor of 5. The EC of the excursion set at a range of thresholds, found using the method of Adler (1977), is plotted in Figure 2. To calculate the expected EC from (2.2), the unitless factor $|S| \det(\Lambda)^{\frac{1}{2}}$ was estimated to be 913, using methods of Worsley (1996), and the integrated curvature of S was calculated using the methods of Worsley (1995a). The expected EC is also plotted on Figure 2. The observed global maximum is $F_{\max} = 11.89$, and its approximate P-value from (1.1) and (2.2) is 0.079. We can thus conclude that there is no strong evidence for a difference in brain shape between males and females.

Although the global maximum is not highly significant ($0.05 < P < 0.10$), the observed EC appears to be somewhat larger than the expected EC at large thresholds. Inspection of Figure 1 shows that this can be attributed to large deformations in the frontal area, anterior cerebellum and the superior central region. These are all possibly due to deformations outside the brain: the frontal difference can be attributed to more pronounced eye-brows in males, the anterior cerebellum deformations appear to be due to thicker bone at the base of the skull in males. The superior central deformations may be an artifact due to poor sampling near the top of the brain.

It is interesting to look at the other extreme of very low thresholds near $y = 0$. The excursion set here is the set of points where there are no deformation differences, or in other words, the fixed points of the deformation differences. As explained in Remark 2, since $d = N$, the expected EC at $y = 0$ gives the expected number of such fixed points, which in this case is $913\rho_3(0) = 92.5$. This agrees reasonably well with the observed number of about 79.

A Appendix: Proof of Theorem 4.1

The following sequence of lemmas are used to complete the proof.

Lemma A.1 *Suppose $G \sim$ Multi-$T^2(p, k, n)$ as defined in Lemma 3.4. If $k \le p$, the expectation of $\det(G)$ and $\det(G)^{\frac{1}{2}}$ are:*

$$\begin{aligned} \mathcal{E}\{\det(G)\} &= \frac{p!(n-p-2)!}{(p-k)!(n+k-p-2)!} \quad \textit{for} \quad n \ge p+2, \\ \mathcal{E}\{\det(G)^{\frac{1}{2}}\} &= \frac{\Gamma(\frac{n-p}{2})\Gamma(\frac{p+1}{2})}{\Gamma(\frac{n+k-p}{2})\Gamma(\frac{p-k+1}{2})} \quad \textit{for} \quad n \ge p+1. \end{aligned}$$

If $k > p$, the lemma still holds if division by factorial of a negative integer, division by Γ function at a negative number is treated as multiplication by zero.

Lemma A.2 *Let $U \sim \mathrm{Wishart}_N(I_N, \nu)$, A be a fixed symmetric $N \times N$ matrix and let b be a fixed scalar. Then*

$$\mathcal{E}\{\det(A + bU)\} = \sum_{j=0}^{N} \frac{b^j \nu!}{(\nu - j)!} \mathrm{detr}_{N-j}(A).$$

Lemma A.3 *Let* $U \sim \mathrm{Wishart}_N(I_N, \nu)$, $H \sim \mathrm{Normal}_{N\times N}(0, M)$ *independently,* A *be a fixed symmetric* $N \times N$ *matrix and let* a *and* b *be fixed scalars. Then*

$$\mathcal{E}\{\det(A + aH + bU)\} = \sum_{j=0}^{\lfloor N/2 \rfloor} \frac{(-1)^j}{2^j j!} a^{2j} \sum_{k=0}^{N-2j} b^k \begin{pmatrix} \nu \\ k \end{pmatrix} (2j+k)! \mathrm{detr}_{N-2j-k}(A).$$

Lemma A.4 *Let* X *be an* $M \times N$ *matrix,* $X \sim \mathrm{Normal}_{M\times N}(0, I_{MN})$, W *be a fixed* $M \times N$ *matrix with* $V = W'W$ *and* c *be a fixed scalar. Then*

$$\mathcal{E}\{\det[V - c(W'X + X'W)]\} = \sum_{m=0}^{\lfloor N/2 \rfloor} (-1)^m c^{2m} \frac{(N-m)!}{(N-2m)!} \mathrm{detr}_{N-m}(V).$$

Lemma A.5 *Let* $U \sim \mathrm{Wishart}_N(I_N, \nu)$, $H \sim \mathrm{Normal}_{N\times N}(0, M)$, $X \sim \mathrm{Normal}_{N\times N}(0, I_{N^2})$, V *be a fixed symmetric* $N \times N$ *matrix, and* a, b, c *be fixed scalars. Then*

$$\begin{aligned} &\mathcal{E}\{\det[V - c(V^{\frac{1}{2}}X + X'V^{\frac{1}{2}}) + aH + bU]\} \\ = &\sum_{j=0}^{\lfloor N/2 \rfloor} \sum_{k=0}^{N-2j} \sum_{m=0}^{\lfloor l/2 \rfloor} \begin{pmatrix} \nu \\ k \end{pmatrix} \frac{(-1)^{j+m}(2j+k+m)!(l-m)!}{2^j j! m! (l-2m)!} a^{2j} b^k c^{2m} \mathrm{detr}_{l-m}(V), \end{aligned}$$

where $l = N - 2j - k$.

We shall simplify the notation somewhat by using * to indicate restriction to n components, formerly indicated by $_{|n}$, so that we shall write $\dot{Y}^* = \dot{Y}_{|n}$ and $\ddot{Y}^* = \ddot{Y}_{|n}$. Otherwise, we shall adopt all the notations established in the Section 3. To find $\rho_N(y)$, we shall evaluate the expectation in (2.1) by conditioning on $w = q'T^{-1}q$:

$$\rho_N(y) = (-1)^n \mathcal{E}_w[\mathcal{E}\{\dot{Y}_N^+ \det(\ddot{Y}^*) \mid \dot{Y}^* = 0, Y = y, w\} f_n(0|y, w)] f(y),$$

where $f_n(0|y, w)$ is the density of $\dot{Y}^*$ at 0 conditional on $Y = y$ and w, and $f(y)$ is the density of Y. Define

$$E^* = (e_1, \ldots, e_n), \quad F^* = (f_1, \ldots, f_n), \quad X^* = (E^{*'}T^{-1}E^*)^{-\frac{1}{2}} E^{*'} T^{-\frac{1}{2}} F^*,$$

and U^*, H^* to be the $n \times n$ matrices of the first n rows and columns of U, H respectively. Then $E^* \sim \mathrm{Normal}_{d\times n}(0, I_{dn})$, $X^* \sim \mathrm{Normal}_{n\times n}(0, I_{n^2})$, $U^* \sim \mathrm{Wishart}_n(I_n, \nu - d)$, $H^* \sim \mathrm{Normal}_{n\times n}(0, M^*)$ all independently, where M^* is the matrix resulting from the same restrictions applied to M. Furthermore, if we define

$$V_1^* = E^{*'}T^{-1}E^*, \quad a = y^{\frac{1}{2}} w^{\frac{1}{2}}, \quad A^* = V_1^* - a[(V_1^*)^{\frac{1}{2}} X^* + X^{*'}(V_1^*)^{\frac{1}{2}}]$$

then by Lemma 3.3 conditional on $\dot{Y}^* = 0$, $Y = y$, w, we can write

$$\ddot{Y}^* = 2(1+y)(A^* + aH^* - a^2 U^*).$$

Note by Lemma 3.3,

$$
\begin{aligned}
\dot{Y}_N &= 2(1+Y)Y^{\frac{1}{2}}e_N' T^{-\frac{1}{2}}q = 2(1+Y)Y^{\frac{1}{2}}w^{\frac{1}{2}}\eta_N, \\
\dot{Y}^* &= 2(1+Y)Y^{\frac{1}{2}}E^{*\prime}T^{-\frac{1}{2}}q,
\end{aligned}
\tag{A.1}
$$

where $\eta_N \sim \text{Normal}_1(0,1)$ independent of Y, q, T, E^*, U and H, and hence $\dot{Y}^*$. Therefore,

$$
\begin{aligned}
& \mathcal{E}\{\dot{Y}_N^+ \det(\ddot{Y}^*) \mid \dot{Y}^* = 0, Y = y, w\} \\
= & \int \mathcal{E}\left\{\dot{Y}_N^+ \det(\ddot{Y}^*) \mid \dot{Y}^* = 0, Y = y, w, V_1^*\right\} f(V_1^*|0,y,w)dV_1^* \\
= & \ 2^N(1+y)^N a \int \mathcal{E}\left\{\eta_N^+ \det(A^* + aH^* - a^2U^*) \mid \dot{Y}^* = 0, Y = y, w, V_1^*\right\} f(V_1^*|0,y,w)dV_1^*,
\end{aligned}
$$

where $f(V_1^*|0,y,w)$ is the density of V_1^* conditional on $\dot{Y}^* = 0$, $Y = y$, w and in the last equality we are holding a fixed. It is easy to see that conditionally, η_N and $A^* + aH^* - a^2U^*$ are independent with $\mathcal{E}(\eta_N^+) = (2\pi)^{-\frac{1}{2}}$. Also note that X^* is independent of E^*, T, q and hence $\dot{Y}^*$, so that

$$
\begin{aligned}
& \mathcal{E}\{\dot{Y}_N^+ \det(\ddot{Y}^*) \mid \dot{Y}^* = 0, Y = y, w\} = (2\pi)^{-\frac{1}{2}}2^N(1+y)^N a \\
& \int \mathcal{E}\left\{\det(A^* + aH^* - a^2U^*) \mid Y = y, w, V_1^*\right\} f(V_1^*|0,y,w)dV_1^*.
\end{aligned}
\tag{A.2}
$$

Now we shall find the expectation in the integrand of (A.2) first, and then take expectations with respect to the conditional distribution $f(V_1^*|0,y,w)$. Applying Lemma A.5 we obtain

$$
\begin{aligned}
& \mathcal{E}\left\{\det(A^* + aH^* - a^2U^*)|Y = y, w, V_1^*\right\} \\
= & \sum_{j=0}^{\lfloor n/2 \rfloor} \sum_{k=0}^{n-2j} \sum_{m=0}^{\lfloor (n-2j-k)/2 \rfloor} \frac{(-1)^{j+k+m}}{2^j j!} a^{2j+2k+2m} \binom{\nu - d}{k} \\
& \frac{(2j+k+m)!(n-2j-k-m)!}{m!(n-2j-k-2m)!} \operatorname{detr}_{n-2j-k-m}(V_1^*).
\end{aligned}
\tag{A.3}
$$

Conditional on $Y = y$, recall that by Lemma 3.3

$$
\dot{Y}^* = 2(1+y)y^{\frac{1}{2}}E^{*\prime}T^{-\frac{1}{2}}q,
$$

and note that if we define

$$
v_2^* = (E^{*\prime}T^{-1}E^*)^{-\frac{1}{2}}E^{*\prime}T^{-\frac{1}{2}}q, \qquad v_3^* = \frac{w}{(q'T^{-\frac{1}{2}}E^*)(E^{*\prime}T^{-\frac{1}{2}}q) + 1},
$$

then V_1^*, v_2^*, v_3^* are independent with distribution shown in Lemma 3.5 with N replaced by n. Hence

$$
f(V_1^*|0,y,w) \propto f(V_1^*, E^{*\prime}T^{-\frac{1}{2}}q = 0, w|y) \propto f(V_1^*, v_2^* = 0, v_3^*|y)\text{Jacobian},
$$

where the proportionality contains y. Since the Jacobian turns out to be $\det(V_1^*)^{-\frac{1}{2}}$, it can be easily seen that conditional on $\dot{Y}^*=0$ and $Y=y$, V_1^* and w are independent with

$$V_1^* \mid \dot{Y}^*=0, Y=y \sim \text{Multi-}T^2(d-1,n,\nu+1), \quad \text{if} \;\; d \geq N \tag{A.4}$$
$$w^{-1} \mid \dot{Y}^*=0, Y=y \sim \chi^2_{\nu+n-d+2}.$$

Hence if $(V_1^*)_l$ is any $l\times l$ principal minor of V_1^*, $l=1,\dots,n$, its distribution is

$$(V_1^*)_l \mid \dot{Y}^*=0, Y=y \;\sim\; \text{Multi-}T^2(d-1,l,\nu+1) \;\; \text{if} \;\; d-1 \geq l. \tag{A.5}$$

So by Lemma A.1, we have

$$\mathcal{E}\left\{\det[(V_1^*)_l] \mid \dot{Y}^*=0, Y=y\right\} = \frac{(d-1)!(\nu-d)!}{(d-1-l)!(\nu-d+l)!} \tag{A.6}$$

for any l, where division by the factorial of a negative integer is treated as multiplication by zero. Putting (A.2), (A.3), (A.6) together with $l=n-2j-k-m$ gives

$$\begin{aligned}
&\mathcal{E}\{\dot{Y}_N^+ \det(\ddot{Y}^*) \mid \dot{Y}^*=0, Y=y, w\} \\
= \;& (2\pi)^{-\frac{1}{2}} 2^N (1+y)^N \sum_{j=0}^{\lfloor n/2\rfloor} \sum_{k=0}^{n-2j} \sum_{m=0}^{\lfloor (n-2j-k)/2\rfloor} \binom{\nu-d}{k} \binom{d-1}{n-2j-k-m} \\
& \binom{\nu-d+n-2j-k-m}{n-2j-k-m}^{-1} \frac{(-1)^{j+k+m} n!}{2^j j! m! (n-2j-k-2m)!} a^{2j+2k+2m+1}.
\end{aligned}$$

Note the density of $\dot{Y}^*$ at 0 conditional on $Y=y$ and w is

$$f_n(0|y,w) = \{8\pi(1+y)^2 yw\}^{-\frac{n}{2}}$$

as easily follows from (A.1), hence

$$\begin{aligned}
&\mathcal{E}\{\dot{Y}_N^+ \det(\ddot{Y}^*) \mid \dot{Y}^*=0, Y=y, w\} f_n(0|y,w) \\
= \;& (2\pi)^{-\frac{N}{2}} 2(1+y) \sum_{j=0}^{\lfloor n/2\rfloor} \sum_{k=0}^{n-2j} \sum_{m=0}^{\lfloor (n-2j-k)/2\rfloor} \binom{\nu-d}{k} \binom{d-1}{n-2j-k-m} \\
& \binom{\nu-d+n-2j-k-m}{n-2j-k-m}^{-1} \frac{(-1)^{j+k+m} n!}{2^j j! m! (n-2j-k-2m)!} a^{2j+2k+2m+1-n}.
\end{aligned}$$

Since $w^{-1} \sim \chi^2_{\nu-d+2}$ unconditionally, and using the fact that

$$\mathcal{E}(w^l) = \frac{\Gamma\left(\frac{\nu-d+2}{2}-l\right)}{2^l \Gamma\left(\frac{\nu-d+2}{2}\right)} \tag{A.7}$$

and multiplying by the density of Y:

$$f(y) = \frac{\Gamma(\frac{\nu+1}{2})}{\Gamma(\frac{\nu-d+1}{2})\Gamma(\frac{d}{2})} y^{\frac{d}{2}-1}(1+y)^{-\frac{\nu+1}{2}} \tag{A.8}$$

gives:

$$\rho_N(y) = \pi^{-\frac{N}{2}}(1+y)^{-\frac{\nu-1}{2}} y^{-\frac{N-d}{2}} \sum_{j=0}^{\lfloor n/2 \rfloor} \sum_{k=0}^{n-2j} \sum_{m=0}^{\lfloor (n-2j-k)/2 \rfloor}$$

$$\binom{\nu-d}{k}\binom{d-1}{n-2j-k-m}\binom{\nu-d+n-2j-k-m}{n-2j-k-m}^{-1}$$

$$\frac{(-1)^{n+j+k+m} n!}{2^{2j+k+m} j! m! (n-2j-k-2m)!} \frac{\Gamma(\frac{\nu-d+n+1}{2}-j-k-m)\Gamma(\frac{\nu+1}{2})}{\Gamma(\frac{\nu-d}{2}+1)\Gamma(\frac{\nu-d+1}{2})\Gamma(\frac{d}{2})} y^{j+k+m}.$$

Then the theorem follows by using the factorisation $x! = 2^x\Gamma\{(x+2)/2\}\Gamma\{(x+1)/2\}/\pi^{\frac{1}{2}}$.

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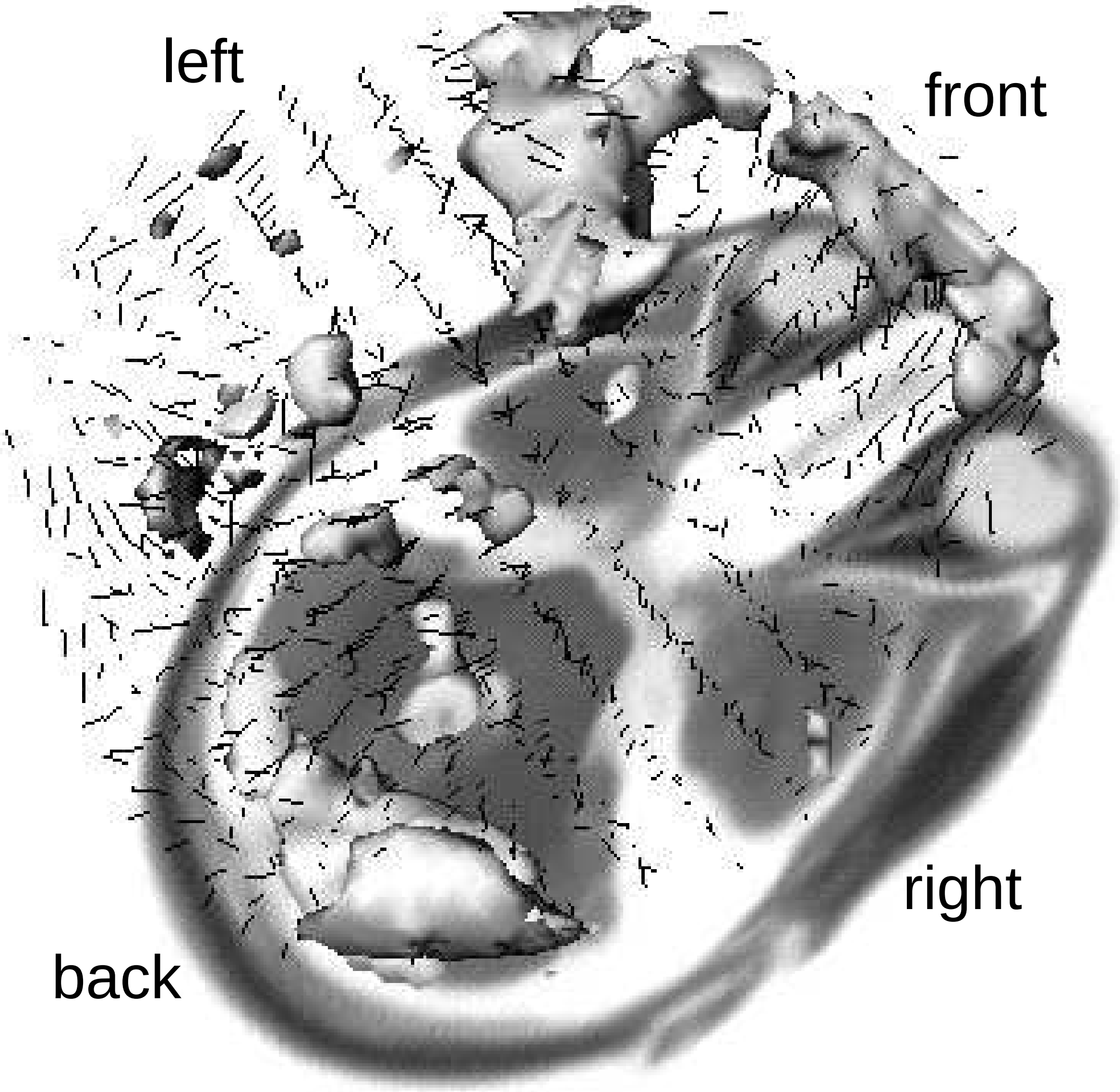

Figure 1: The difference in average deformation between male and female brains is shown as vectors, magnified by a factor of 5 (only 1/64 of the vectors are shown). To test for a difference in deformations, the excursion set of the Hotelling's T^2 random field, scaled to an $F_{3,48}$ distribution above a threshold of 4, is shown as solid 'blobs'. The Euler characteristic (EC) of the observed excursion set is 35; the expected EC if there is no difference is 26.5 (see Figure 2). Also shown below the vectors and excursion set is a slice through the atlas brain that was used as the template for the deformations (the eye balls are visible at the front).

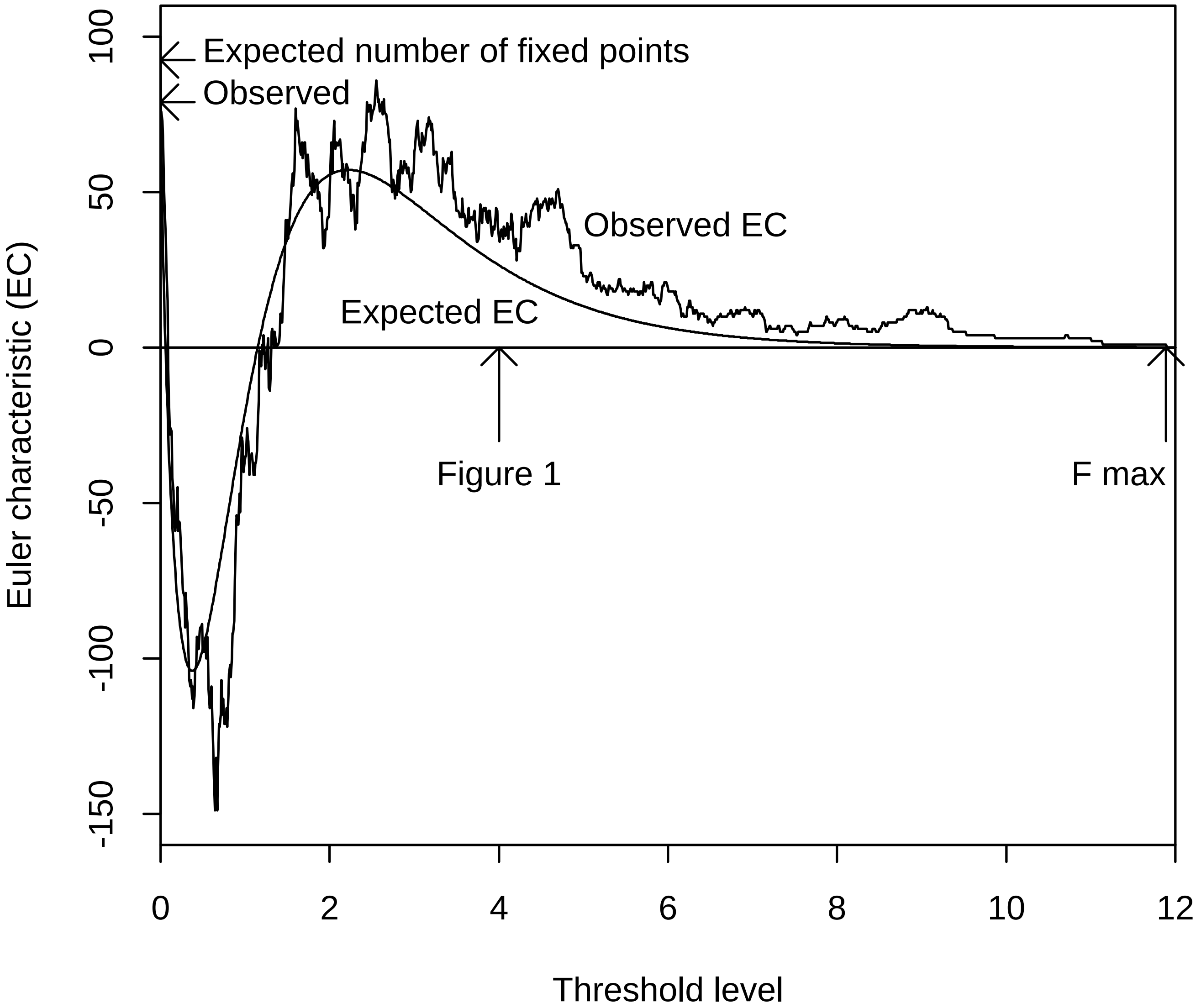

Figure 2: Observed (jagged line) and expected (smooth line) EC for the Hotelling's T^2 field in Figure 1, scaled to an $F_{3,48}$ distribution.