Deconvolution Density Estimation on Spaces of Positive Definite Symmetric Matrices

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1 Introduction

We are motivated by applications in electrical engineering and medical imaging to study the problem of deconvolution density estimation on the space of positive definite (symmetric) matrices. In microwave engineering, the transmission of electrical signals over a long, lossless line containing random inhomogeneities has been modeled using random positive definite matrices [15, p. 156 ff.].

Such matrices also arise in *diffusion tensor imaging* (DTI), an imaging method based on the movement of water molecules in biological tissue. When water molecule diffusion at a given tissue location is assumed to follow a Brownian motion, a diffusion tensor image is defined by the 3×3 positive definite covariance matrix of the local diffusion process. DTI detects diffusion of water protons within and between tissue cells, and is used to estimate the dominant orientation and direction of the Brownian motion [6]. DTI may be the only non-invasive, *in vivo* procedure for studying white-matter fibers in the human brain. Hence DTI has been used to study: the brain in abnormal states caused by strokes, epileptic seizures, tumors, multiple sclerosis lesions, traumatic injuries, and Alzheimer's disease; psychiatric conditions such as schizophrenia, autism, cognitive and learning disabilities [8, 10]; and organs and tissues such as the breast, kidney, cardiac, skeletal muscles, and spinal cord [1]. Some have ventured that DTI may be used to study the effects of country music on the brain tissues of extraterrestrials [7], but we disagree. DTI images also contain noise, so inferential issues arise naturally in the analysis of DTI data [14, 17].

Estimation of the density function of a population of positive definite matrices arises in [14], where it is of interest to compare brain tissue from two groups on the basis of DTI images. We shall construct a *non-parametric* estimator of, and derive bounds on its rate of convergence to, the population density function. Since $\mathcal{P}_m$, the space of $m \times m$ positive definite matrices, is non-compact and intrinsically non-commutative, we may expect the deconvolution problem to be more difficult here than in the Euclidean or the compact settings [2, 4, 5]. The deconvolution problem on $\mathcal{P}_m$ has been studied for the special case of band-limited densities [11], but not hitherto in the general case.

2 Preliminaries

K: The group of $m \times m$ orthogonal matrices.

$\mathcal{P}_m$: The space of $m \times m$ positive definite matrices.

A random matrix $\varepsilon \in \mathcal{P}_m$ is *K-invariant* if $\varepsilon \overset{\mathcal{L}}{=} k'\varepsilon k$ for all $k \in K$, where "$\overset{\mathcal{L}}{=}$" denotes equality in distribution. A function $f : \mathcal{P}_m \to \mathbb{C}$ is K-invariant if $f(k'xk) = f(x)$ for all $k \in K$, $x \in \mathcal{P}_m$; we indicate that f is K-invariant by writing its domain as $\mathcal{P}_m/K$, with similar notation for K-invariant positive definite random matrices.

The Deconvolution Problem on $\mathcal{P}_m$

Definition. For random matrices $X \in \mathcal{P}_m$ and $\varepsilon \in \mathcal{P}_m/K$, the *composition of X and ε* is $X \circ \varepsilon = \varepsilon^{1/2} X \varepsilon^{1/2}$ where $\varepsilon^{1/2}$ is the positive definite square root of ε.

The composition operation has also arisen in work on Central Limit Theorems on $\mathcal{P}_m$ [15, 16, 13].

In DTI, X represents a true image corrupted by an error ε, and the investigator observes $Y = X \circ \varepsilon$ only. The K-invariance of ε is due to an assumption that water molecules diffuse with no preferred orientation, an assumption that is appropriate for the ventricles, which are large, fluid-filled spaces deep in the brain.

The Deconvolution Problem: For random $X \in \mathcal{P}_m$ and $\varepsilon \in \mathcal{P}_m/K$, estimate nonparametrically the density of X based on a random sample from $Y = X \circ \varepsilon$.

The Helgason-Fourier Transform

$C_c^\infty(\mathcal{P}_m)$: The set of infinitely differentiable, compactly supported functions $f : \mathcal{P}_m \to \mathbb{C}$.

For $w \in \mathcal{P}_m$ and $j = 1, \ldots, m$, denote by $|w_j|$ the principal minor of order j of w. For $j = m$, we denote the determinant simply by $|w|$.

For $s = (s_1, \ldots, s_m) \in \mathbb{C}^m$, the *power function* $p_s : \mathcal{P}_m \to \mathbb{C}$ is defined by $p_s(w) = \prod_{j=1}^m |w_j|^{s_j}$, $w \in \mathcal{P}_m$.

$\mathrm{d}k$: The Haar measure on K, normalized to have total volume 1.

For $w \in \mathcal{P}_m$, $s \in \mathbb{C}^m$, the *zonal spherical function* on $\mathcal{P}_m$ is

$$h_s(w) = \int_K p_s(k'wk)\,\mathrm{d}k. \tag{2.1}$$

The spherical functions are fundamental in harmonic analysis on symmetric spaces [3]. If $s_1, \ldots, s_m$ are nonnegative integers then, up to a constant factor, (2.1) are the *zonal polynomials* [9, pp. 231-232].

For $w = (w_{ij}) \in \mathcal{P}_m$, the G-invariant measure on $\mathcal{P}_m$ is $\mathrm{d}_* w = |w|^{-(m+1)/2} \prod_{1 \le i \le j \le m} \mathrm{d}w_{ij}$. The *Helgason-Fourier transform* of $f \in C_c^\infty(\mathcal{P}_m)$ is defined as

$$\mathcal{H}f(s,k) = \int_{\mathcal{P}_m} f(w)\, \overline{p_s(k'wk)}\, \mathrm{d}_* w, \tag{2.2}$$

$s \in \mathbb{C}^m$, $k \in K$, where $\overline{p_s(\cdot)}$ denotes complex conjugation [15, p. 87].

If $f \in C_c^\infty(\mathcal{P}_m/K)$ then $\mathcal{H}f(s,k)$ depends on s only: $\mathcal{H}f(s,k) = \widehat{f}(s)$, where

$$\widehat{f}(s) = \int_{\mathcal{P}_m} f(w)\, \overline{h_s(w)}\, \mathrm{d}_* w \tag{2.3}$$

is the *zonal spherical transform* of f.

Inversion of the Helgason-Fourier Transform

$B(a,b) = \Gamma(a)\,\Gamma(b)/\Gamma(a+b)$, $\mathrm{Re}(a), \mathrm{Re}(b) > 0$: The beta function.

For $s = (s_1, \ldots, s_m) \in \mathbb{C}^m$, the *Harish-Chandra c-function* is

$$c_m(s) = \prod_{1 \le i < j \le m-1} \frac{B\big(\frac{1}{2}, s_i + \cdots + s_j + \frac{1}{2}(j-i+1)\big)}{B\big(\frac{1}{2}, \frac{1}{2}(j-i+1)\big)}\,. \tag{2.4}$$

Define

$$\rho = (\tfrac{1}{2}, \ldots, \tfrac{1}{2}, \tfrac{1}{4}(1-m)),$$

$$\mathbb{C}^m(\rho) = \{s \in \mathbb{C}^m : \mathrm{Re}(s) = -\rho\}, \tag{2.5}$$

$$\omega_m = \frac{\prod_{j=1}^m \Gamma(j/2)}{m!\,(2\pi i)^m\, \pi^{m(m+1)/4}}, \tag{2.6}$$

$$\mathrm{d}_* s = \omega_m\, |c_m(s)|^{-2}\, \mathrm{d}s_1 \cdots \mathrm{d}s_m. \tag{2.7}$$

$M = \{\mathrm{diag}(\pm 1, \ldots, \pm 1)\}$: The subgroup of K containing all $m \times m$ diagonal matrices with entries ± 1 on the diagonal. There exists an invariant measure $\mathrm{d}\bar{k}$ on the coset space K/M such that $\int_{\bar{k} \in K/M} \mathrm{d}\bar{k} = 1$.

Theorem. (Helgason [3]) For $f \in C_c^\infty(\mathcal{P}_m)$, $w \in \mathcal{P}_m$,

$$f(w) = \int_{\mathbb{C}^m(\rho)} \int_{\bar{k} \in K/M} \mathcal{H}f(s,k)\, p_s(k'wk)\, \mathrm{d}\bar{k}\, \mathrm{d}_* s. \tag{2.8}$$

In particular, if $f \in C_c^\infty(\mathcal{P}_m/K)$ then

$$f(w) = \int_{\mathbb{C}^m(\rho)} \widehat{f}(s)\, h_s(w)\, \mathrm{d}_* s. \tag{2.9}$$

For $m = 1$, the Helgason-Fourier transform is the Mellin transform, and (2.8) becomes: If $f \in C_c^\infty(\mathbb{R}_+)$ and $\widehat{f}(s) = \int_0^\infty t^{s-1} f(t)\,\mathrm{d}t$, $s \in \mathbb{C}$, then for some constant $\alpha \in \mathbb{R}$,

$$f(t) = \frac{1}{2\pi i} \int_{\mathrm{Re}(s)=\alpha} t^{-s}\, \widehat{f}(s)\, \mathrm{d}s.$$

The Convolution Property of the Helgason-Fourier Transform

The *convolution*, $f * h$, of $f \in L^1(\mathcal{P}_m)$ and $h \in L^1(\mathcal{P}_m/K)$ is:

$$(f * h)(w) = \int_{\mathcal{P}_m} f(z)\, h(z^{-1/2} w z^{-1/2})\, \mathrm{d}_* z, \tag{2.10}$$

$w \in \mathcal{P}_m$. If f and h are the densities of independent $X \in \mathcal{P}_m$ and $\varepsilon \in \mathcal{P}_m/K$, respectively, then $f * h$ is the density of $X \circ \varepsilon$.

Let $f \in C_c^\infty(\mathcal{P}_m)$ and $h \in C_c^\infty(\mathcal{P}_m/K)$. For $s \in \mathbb{C}^m$, $k \in K$, the Helgason-Fourier transform satisfies the convolution property [15, p. 88, Theorem 1]

$$\mathcal{H}(f * h)(s,k) = \mathcal{H}f(s,k)\, \widehat{h}(s). \tag{2.11}$$

Eigenvalues, the Laplacian, and Sobolev spaces

For $w = (w_{ij}) \in \mathcal{P}_m$, let $\partial_w = \big(\frac{1}{2}(1+\delta_{ij}) \frac{\partial}{\partial w_{ij}}\big)$ where δ_{ij} denotes Kronecker's delta. The *Laplacian* on $\mathcal{P}_m$ is $\Delta = -\mathrm{tr}\big((w\partial_w)^2\big)$.

The power functions p_s are eigenfunctions of Δ: For $j = 1, \ldots, m$, let $r_j = \frac{1}{4}(m - 2j + 1) + \sum_{k=j}^m s_k$; then $\Delta p_s(w) = \lambda_s p_s(w)$ where

$$\lambda_s = -\big(r_1^2 + \cdots + r_m^2 - \tfrac{1}{48} m(m^2-1)\big).$$

Since $\mathrm{Re}(s) = -\rho$ then each r_j, $j = 1, \ldots, m$ is purely imaginary, so $\lambda_s > 0$ [15, p. 49], [9, p. 229], [12, p. 283].

The Helgason-Fourier transform changes the effect of Δ to pointwise multiplication: $\mathcal{H}(\Delta f)(s,k) = \lambda_s \mathcal{H}f(s,k)$ for $f \in C_c^\infty(\mathcal{P}_m)$, $s \in \mathbb{C}^m$, $k \in K$ [15, p. 88].

For $\sigma > 0$, we define $\Delta^{\sigma/2}$ to be the operator that satisfies the identity $\mathcal{H}(\Delta^{\sigma/2} f)(s,k) = \lambda_s^{\sigma/2} \mathcal{H}f(s,k)$, for all $f \in C_c^\infty$, $s \in \mathbb{C}^m$, $k \in K$.

For $Q > 0$ and $2\sigma > \dim \mathcal{P}_m$, we define the *Sobolev classes*,

$$H_\sigma(\mathcal{P}_m) = \big\{f \in C^\infty(\mathcal{P}_m) : \|\Delta^{\sigma/2} f\|^2 < \infty\big\}, \tag{2.12}$$

$$H_\sigma(\mathcal{P}_m, Q) = \big\{f \in C^\infty(\mathcal{P}_m) : \|\Delta^{\sigma/2} f\|^2 < Q\big\}. \tag{2.13}$$

where $\|f\|^2 = \int_{\mathcal{P}_m} |f(w)|^2\, \mathrm{d}_* w$.

The Plancherel Formula for the Helgason-Fourier Transform

The Plancherel formula [15, p. 88, Theorem 1] is that for $f \in C_c^\infty(\mathcal{P}_m)$,

$$\int_{\mathcal{P}_m} |f(w)|^2\, \mathrm{d}_* w = \int_{\mathbb{C}^m(\rho)} \int_{\bar{k} \in K/M} |\mathcal{H}f(s,\bar{k})|^2\, \mathrm{d}\bar{k}\, \mathrm{d}_* s. \tag{2.14}$$

For the case in which $f \in C_c^\infty(\mathcal{P}_m/K)$, (2.14) simplifies *via* (2.3) to

$$\int_{\mathcal{P}_m} |f(w)|^2\, \mathrm{d}_* w = \int_{\mathbb{C}^m(\rho)} |\widehat{f}(s)|^2\, \mathrm{d}_* s. \tag{2.15}$$

3 Deconvolution Density Estimation on $\mathcal{P}_m$

For random $X \in \mathcal{P}_m$ with density f_X, random K-invariant error $\varepsilon \in \mathcal{P}_m$ with density f_ε such that $\widehat{f_\varepsilon}(s) \neq 0$ on $\mathbb{C}^m$, the deconvolution problem arises from the statistical model,

$$Y \overset{\mathcal{L}}{=} \varepsilon^{1/2} X \varepsilon^{1/2}. \tag{3.1}$$

Applying (2.11) to (3.1), we obtain

$$\mathcal{H}f_Y(s,k) = \mathcal{H}f_X(s,k)\, \widehat{f_\varepsilon}(s), \qquad s \in \mathbb{C}^m, k \in K. \tag{3.2}$$

Given a random sample $Y_1, \ldots, Y_n$ from Y, construct the *empirical Helgason-Fourier transform*,

$$\mathcal{H}_n f_Y(s,k) = \frac{1}{n} \sum_{\ell=1}^n \overline{p_s(k' Y_\ell k)}. \tag{3.3}$$

Substituting (3.3) in (3.2), we obtain for $s \in \mathbb{C}^m$, $k \in K$:

$$\mathcal{H}_n f_X(s,k) = \frac{\mathcal{H}_n f_Y(s,k)}{\widehat{f_\varepsilon}(s)}, \tag{3.4}$$

$\mathcal{H}_n f_Y$ is an unbiased, *nonparametric* estimator of $\mathcal{H}f_Y$,

$$\mathbb{E}\mathcal{H}_n f_Y(s,k) = \mathcal{H}f_Y(s,k), \tag{3.5}$$

and for $\mathrm{Re}(s) = -\rho$,

$$\mathbb{V}ar\,(\mathcal{H}_n f_Y(s,k)) = \frac{1}{n}\big(\mathcal{H}f_Y(-2\rho,k) - |\mathcal{H}f_Y(s,k)|^2\big) \tag{3.6}$$

A Nonparametric Deconvolution Density Estimator

As in Euclidean deconvolution problems, we introduce a smoothing parameter $T = T(n)$ where $T(n) \to \infty$ as $n \to \infty$, and then we apply the inversion formula (2.8) using a spectral cut-off.

Let $\mathbb{C}^m(\rho,T) = \{s \in \mathbb{C}^m(\rho) : \lambda_s < T\}$ where $C^m(\rho)$ is given in (2.5).

Our *nonparametric* deconvolution estimator of f_X is

$$f_X^n(w) = \int_{\mathbb{C}^m(\rho,T)} \int_{\bar{k} \in K/M} \frac{\mathcal{H}_n f_Y(s,\bar{k})}{\widehat{f_\varepsilon}(s)}\, p_s(\bar{k}' w \bar{k})\, \mathrm{d}\bar{k}\, \mathrm{d}_* s, \qquad w \in \mathcal{P}_m. \tag{3.7}$$

4 Rates of Convergence of the Estimator

$\{a_n\}$, $\{b_n\}$: Sequences of real numbers.

$a_n \ll b_n$: $a_n \le C b_n$ for some constant $C > 0$ as $n \to \infty$.

We assume throughout that $Y \in \mathcal{P}_m$ satisfies the moment condition,

$$\int_{\mathcal{P}_m} |w_1|^{-1} \cdots |w_{m-1}|^{-1}\, |w|^{(m-1)/2}\, f_Y(w)\, \mathrm{d}_* w < \infty.$$

Theorem 1. Suppose there exists $\beta \ge 0$ such that $|\widehat{f_\varepsilon}(s)|^{-2} \ll T^\beta$ as $T \to \infty$, for all $s \in \mathbb{C}^m(\rho,T)$. If $f_X \in H_\sigma(\mathcal{P}_m, Q)$ and $\sigma > \frac{1}{2}\dim \mathcal{P}_m$ then, as $n \to \infty$, $\mathbb{E}\,\|f_X^n - f_X\|^2 \ll n^{-2\sigma/(2\sigma+2\beta+\dim \mathcal{P}_m)}$.

Example. Consider $\widehat{f_\varepsilon}(s) = (1+\gamma\lambda_s)^{-\beta}$, $s \in \mathbb{C}^m$, where $\gamma > 0$ is a constant. By the Helgason-Fourier inversion formula (2.9),

$$f_\varepsilon(w) = \int_{\mathbb{C}^m(\rho)} (1+\gamma\lambda_s)^{-\beta}\, h_s(w)\, \mathrm{d}_* s, \tag{4.8}$$

$w \in \mathcal{P}_m$. Letting $\beta \to 0$, we have $\widehat{f_\varepsilon}(s) \to 1$, so the underlying distribution approaches the Dirac measure concentrated at $\mathbf{I}_m$, the $m \times m$ identity matrix. This means that observations are without error, corresponding to the special case of Theorem 1 in which $\beta = 0$:

Corollary. Let the distribution of ε be concentrated at $\mathbf{I}_m$. If $f_X \in H_\sigma(\mathcal{P}_m, Q)$ where $\sigma > \frac{1}{2}\dim \mathcal{P}_m$ then, as $n \to \infty$, $\mathbb{E}\,\|f_X^n - f_X\|^2 \ll n^{-2\sigma/(2\sigma+\dim \mathcal{P}_m)}$.

Theorem 2. Suppose there exists $\beta, \gamma > 0$ such that $|\widehat{f_\varepsilon}(s)|^{-2} \ll \exp(T^\beta/\gamma)$ as $T \to \infty$, for all $s \in \mathbb{C}^m(\rho,T)$. If $f_X \in H_\sigma(\mathcal{P}_m, Q)$ with $\sigma > \frac{1}{2}\dim \mathcal{P}_m$ then, as $n \to \infty$, $\mathbb{E}\,\|f_X^n - f_X\|^2 \ll (\log n)^{-\sigma/\beta}$.

Example. Consider $\widehat{f_\varepsilon}(s) = \exp(-\gamma^{-1}\lambda_s^\beta)$, $s \in \mathbb{C}^m$, where $\gamma > 0$ is constant. By H-F inversion, the underlying density function is

$$f_\varepsilon(w) = \int_{\mathbb{C}^m(\rho)} \exp(-\gamma^{-1}\lambda_s^\beta)\, h_s(w)\, \mathrm{d}_* s, \tag{4.9}$$

$w \in \mathcal{P}_m$. The case in which $\beta = 1$ is particularly important and is called the *heat* or *Gaussian kernel*, since the latter is the fundamental solution to the heat equation on $\mathcal{P}_m$. As a consequence, we obtain:

Corollary. Suppose that f_ε is Gaussian. If $f_X \in H_\sigma(\mathcal{P}_m, Q)$ where $\sigma > \frac{1}{2}\dim \mathcal{P}_m$ then, as $n \to \infty$, $\mathbb{E}\,\|f_X^n - f_X\|^2 \ll (\log n)^{-\sigma}$.

The Wishart Distribution

Suppose that ε has the well-known Wishart distribution $W_m(N, \mathbf{I}_m)$, $N > m-1$. For $s = (s_1, \ldots, s_m) \in \mathbb{C}^m$ with $\mathrm{Re}(s_j + \cdots + s_m) > (j-1)/2$, $j = 1, \ldots, m$, let

$$\Gamma_m(s_1, \ldots, s_m) = \pi^{m(m-1)/4} \prod_{j=1}^m \Gamma\big(s_j + \cdots + s_m - \tfrac{1}{2}(j-1)\big), \tag{4.10}$$

be the *multivariate gamma function*. Relative to the invariant measure $\mathrm{d}_* w$, the density function of the Wishart distribution $W_m(N, \mathbf{I}_m)$ is

$$f_\varepsilon(w) = \frac{1}{\Gamma_m(0, \ldots, 0, N/2)}\, |\tfrac{1}{2} w|^{N/2} \exp\big(-\tfrac{1}{2}\mathrm{tr}\, w\big), \tag{4.11}$$

$w \in \mathcal{P}_m$. The Helgason-Fourier transform of the Wishart density is

$$\widehat{f_\varepsilon}(s) = \frac{\Gamma_m((0, \ldots, 0, N/2) + s^*)}{\Gamma_m(0, \ldots, 0, N/2)}\, h_s(\tfrac{1}{2}\mathbf{I}_m)$$

$s^* = \big(s_{m-1}, s_{m-2}, \ldots, s_2, s_1, -(s_1 + \cdots + s_m)\big)$ [15, pp. 85-86].

Lemma. For $N > m-1$ and $s \in \mathbb{C}^m(\rho,T)$, the Wishart distribution $W_m(N, \mathbf{I}_m)$ satisfies $|\widehat{f_\varepsilon}(s)|^{-2} \ll \exp\big(\pi T^{1/2}\big)$, as $T \to \infty$.

Consequently we deduce the following result.

Theorem 3. Suppose that ε is Wishart-distributed (4.11) with $N > m-1$. If $f_X \in H_\sigma(\mathcal{P}_m, Q)$ with $\sigma > \dim \mathcal{P}_m/2$ then, as $n \to \infty$, $\mathbb{E}\|f_X^n - f_X\|^2 \ll (\log n)^{-2\sigma}$.

Therefore, the Wishart distribution has faster convergence in its Helgason-Fourier transform than the Gaussian distribution, resulting in a slower recovery in the corresponding deconvolution problem.

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