Separating Out the Eigenvalue Densities: Computing the Jacobians

Random Matrix Theory with Its Applications

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1. Background
2. A Two-Dimensional Example

1 Background

2 A Two-Dimensional Example

Spectral Theorem

- The spectral theorem:

$$M = U\Lambda U^* (unitary, symplectic)$$
$$M = U\Lambda U^T (orthogonal)$$

M can be any kinds of matrices.

- Three ensembles:[1]
  - **Gaussian Orthogonal Ensemble**: the set of $N \times N$ random real **symmetric** matrices
  - **Gaussian Unitary Ensemble**: the set of $N \times N$ random complex **Hermitian** matrices
  - **Gaussian Symplectic Ensemble**: the set of $N \times N$ random quaternion(四元数) **self-dual Hermitian** matrices
- 这可以被视为一种坐标系变化：$M \mapsto (\Lambda, U)$
- 此时可以考虑计算雅可比行列式（Jacobian)：$\left| det \frac{\partial M}{\partial(\Lambda, U)} \right|$

[1] Yanqing Yin and Zhidong Bai. "Convergence rates of the spectral distributions of large random quaternion self-dual Hermitian matrices". In: *Journal of Statistical Physics* 157 (2014), pp. 1207–1224.

Spectral Theorem

- Every real symmetric matrix Q with real eigenvalues in Λ and orthonormal eigenvectors in the columns of Q(orthogonal(正交)) can be diagonalized:[2]

$$S = Q\Lambda Q^{-1} = Q\Lambda Q^{T} \quad \text{with} \quad Q^{-1} = Q^{T}$$

- Every Hermitian matrix S with real eigenvalues in Λ and orthonormal eigenvectors in the columns of U(unitary(酉)) can be diagonalized:[3]

$$S = U\Lambda U^{-1} = U\Lambda U^{*} \quad \text{with} \quad U^{-1} = U^{*}$$

[2] Gilbert Strang. *Introduction to linear algebra (fifth edition)*. SIAM, 2016.
[3] Gilbert Strang. *Introduction to linear algebra (fifth edition)*. SIAM, 2016.

Gaussian Orthogonal Ensemble(GOE)

- **Gaussian Orthogonal Ensemble**: the set of $N \times N$ random real **symmetric** matrices
- Symmetric matrix:
  - $S = S^T$
  - $S = X\Lambda X^{-1}, S^T = (X^{-1})^T \Lambda X^T \quad \text{when} \quad S = S^T, X^T X = I$
  - A symmetric matrix has only *real eigenvalues*.
  - Symmetric diagonalization:
    $S = Q\Lambda Q^{-1} = Q\Lambda Q^T \quad \text{with} \quad Q^{-1} = Q^T$
  - Example: $\begin{bmatrix} a & b \\ b & c \end{bmatrix}$
  - Free variables number is $n + \frac{n(n-1)}{2} \cdot 1$

Gaussian Unitary Ensemble(GUE)

- **Gaussian Unitary Ensemble**: the set of $N \times N$ random complex **Hermitian** matrices
- Hermitian matrices:
  - $S = S^*$
  - $S = U\Lambda U^{-1}, S^* = (U^{-1})^* \Lambda U^* \quad \text{when} \quad S = S^*, U^*U = I$
  - Hermitian diagonalization:
    $S = U\Lambda U^{-1} = U\Lambda U^* \quad \text{with} \quad U^{-1} = U^*$
  - Example: $\begin{bmatrix} a & b+ci \\ b-ci & d \end{bmatrix}$
  - Free variables number is $n + \frac{n(n-1)}{2} \cdot 2$

Gaussian Symplectic Ensemble(GSE)

- **Gaussian Symplectic Ensemble**: the set of $N \times N$ random quaternion **self-dual Hermitian** matrices[4][5]
- Quaternions were invented in 1843 by the Irish mathematician William Rowen Hamilton as an extension of complex numbers into three dimensions[6][7], and it's well known that the quaternion field $\mathbb{Q}$ can be represented as a two-dimensional complex vector space[8].

[4] 许方官. *四元数物理学*. 北京大学出版社, 2012.

[5] Yanqing Yin and Zhidong Bai. "Convergence rates of the spectral distributions of large random quaternion self-dual Hermitian matrices". In: *Journal of Statistical Physics* 157 (2014), pp. 1207–1224.

[6] Cipher A Deavours. "The quaternion calculus". In: *The American Mathematical Monthly* 80.9 (1973), pp. 995–1008.

[7] William Rowan Hamilton. *Elements of quaternions*. London: Longmans, Green, & Company, 1866.

[8] Claude Chevalley. *Theory of Lie Groups (PMS-8)*. 1946.

四元数

- 一个三位空间的实矢量 $\mathbf{a} = a_1\mathbf{i} + a_2\mathbf{j} + a_3\mathbf{k}$ 与一个实数 a_0 组合成一个数 $A = a_0 + \mathbf{a}$ 被称为**四元数**。其中实数 a_0 被称为四元数 A 的**标部**，实矢量 $\mathbf{a}$ 称为四元数 A 的矢部。
- 在四元数 A 的矢部中，三个矢量 $\mathbf{i}, \mathbf{j}, \mathbf{k}$ 是三维空间中三个互相垂直且方向固定的单位矢量。
- 一个四元数实际上是由四个基 $1, \mathbf{i}, \mathbf{j}, \mathbf{k}$ 的线性组合构成的。

四元数代数运算规则

- **相等**: 两个四元数 A 和 B，若他们相应的四个分量分别相等，即

$$a_n = b_n, \quad n = 0, 1, 2, 3$$

则称他们**相等**，记作

$$A = B$$

一个四元数的等式相当于四个实数等式。

- **加法**: 两个四元数 A 和 B 之和 C 仍为四元数，记作

$$C = A + B$$

其定义为

$$c_n = a_n + b_n, \quad n = 0, 1, 2, 3$$

由实数加法的交换律、结合律知，四元数加法也存在着交换律和结合律。

四元数代数运算规则

- **乘法**: 两个四元数 A 和 B 乘积的定义是

$$\begin{aligned} AB &= (a_0 + \mathbf{a})(b_0 + \mathbf{b}) \\ &= a_0 b_0 - \mathbf{a} \cdot \mathbf{b} + a_0 \mathbf{b} + b_0 \mathbf{a} + \mathbf{a} \times \mathbf{b} \\ BA &= (b_0 + \mathbf{b})(a_0 + \mathbf{a}) \\ &= a_0 b_0 - \mathbf{a} \cdot \mathbf{b} + a_0 \mathbf{b} + b_0 \mathbf{a} + \mathbf{b} \times \mathbf{a} \end{aligned}$$

两个四元数的乘积仍是四元数，但因为 $\mathbf{a} \times \mathbf{b} \neq \mathbf{b} \times \mathbf{a}$，故 $AB \neq BA$
四元数的乘法规则是由三个互相垂直的空间单位矢量 $\mathbf{i}, \mathbf{j}, \mathbf{k}$ 之间的乘法 (叉乘) 规则

$$\begin{cases} \mathbf{ii} = \mathbf{jj} = \mathbf{kk} = -1 \\ \mathbf{ij} = -\mathbf{ji} = \mathbf{k} \\ \mathbf{jk} = -\mathbf{kj} = \mathbf{i} \\ \mathbf{ki} = -\mathbf{ik} = \mathbf{j} \end{cases}$$

所导致的

四元数代数运算规则

- **共轭 (四元共轭)**: 与四元数 $A = a_0 + \mathbf{a}$ 对应的另一个四元数

$$\overline{A} = a_0 - \mathbf{a}$$

称为 A 的**四元共轭**，反之，A 也称为 $\overline{A}$ 的**四元共轭**
此外，由

$$\begin{aligned}\overline{AB} &= a_0 b_0 - \mathbf{a}\cdot\mathbf{b} - a_0\mathbf{b} - b_0\mathbf{a} - \mathbf{a}\times\mathbf{b}\\ \overline{B}\,\overline{A} &= (b_0 - \mathbf{b})(a_0 - \mathbf{a})\\ &= a_0 b_0 - \mathbf{a}\cdot\mathbf{b} - a_0\mathbf{b} - b_0\mathbf{a} + \mathbf{b}\times\mathbf{a}\end{aligned}$$

可知

$$\overline{AB} = \overline{B}\,\overline{A}$$

- **模方**: 称实数

$$\|A\| = \left\|\overline{A}\right\| = A\overline{A} = \overline{A}A = a_0^2 + \mathbf{a}\cdot\mathbf{a}$$

为四元数 A 或 $\overline{A}$ 的**模方**，且两个四元数之积的模方等于两个四元数模方之积
$\|AB\| = \|A\|\,\|B\|$

四元数的矩阵表示

- **一级四元数与 2×2 矩阵**: 把四元数的四个基 $1, \mathbf{i}, \mathbf{j}, \mathbf{k}$ 分别用四个 2×2 矩阵表示成

$$1 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad \mathbf{i} = \begin{bmatrix} i & 0 \\ 0 & -i \end{bmatrix}, \quad \mathbf{j} = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}, \quad \mathbf{k} = \begin{bmatrix} 0 & i \\ i & 0 \end{bmatrix}$$

这样，一个四元数可以用一个 2×2 的复矩阵表示成

$$A = a_0 + \mathbf{a} = \begin{bmatrix} a_0 + ia_1 & a_2 + ia_3 \\ -a_2 + ia_3 & a_0 - ia_1 \end{bmatrix} = \begin{bmatrix} \alpha & \beta \\ -\bar{\beta} & \bar{\alpha} \end{bmatrix}$$

- **共轭**:

$$\overline{A} = a_0 - a_1\mathbf{i} - a_2\mathbf{j} - a_3\mathbf{k} = \begin{bmatrix} a_0 - ia_1 & -a_2 - ia_3 \\ a_2 - ia_3 & a_0 + ia_1 \end{bmatrix} = \begin{bmatrix} \bar{\alpha} & -\beta \\ \bar{\beta} & \alpha \end{bmatrix}$$

- **模方**: 四元数矩阵的模方就是其表示的矩阵的行列式，即

$$\|A\| = \det A = \sqrt{a_0^2 + a_1^2 + a_2^2 + a_3^2} = \sqrt{|\alpha|^2 + |\beta|^2}$$

四元数的矩阵表示

一个四元数可以用 2×2 矩阵表示，类似地，二级四元数可以用 4×4 矩阵表示，其四个基 $1, \mathbf{i_2}, \mathbf{j_2}, \mathbf{k_2}$ 表示成

$$1 = \begin{bmatrix} I_2 & 0 \\ 0 & I_2 \end{bmatrix}, \quad \mathbf{i} = \begin{bmatrix} iI_2 & 0 \\ 0 & -iI_2 \end{bmatrix}, \quad \mathbf{j} = \begin{bmatrix} 0 & I_2 \\ -I_2 & 0 \end{bmatrix}, \quad \mathbf{k} = \begin{bmatrix} 0 & iI_2 \\ iI_2 & 0 \end{bmatrix}$$

其中 I_2 是 2×2 的单位矩阵。这样，一个二级四元数的矩阵表示为

$$\begin{aligned} Q =& A + B\mathbf{i_2} + C\mathbf{j_2} + D\mathbf{k_2} \\ =& \begin{bmatrix} A + iB & C + iD \\ -C + iD & A - iB \end{bmatrix} \\ =& \begin{bmatrix} a_0 - b_1 + \mathrm{i}(a_1 + b_0) & a_2 - b_3 + \mathrm{i}(a_3 + b_2) & c_0 - d_1 + \mathrm{i}(c_1 + d_0) & c_2 - d_3 + \mathrm{i}(c_3 + d_2) \\ -(a_2 + b_3) + \mathrm{i}(a_3 - b_2) & a_0 + b_1 - \mathrm{i}(a_1 - b_0) & -(c_2 + d_3) + \mathrm{i}(c_3 - d_2) & c_0 + d_1 - \mathrm{i}(c_1 - d_0) \\ -(c_0 + d_1) - \mathrm{i}(c_1 - d_0) & -(c_2 + d_3) - \mathrm{i}(c_3 - d_2) & a_0 + b_1 + \mathrm{i}(a_1 - b_0) & a_2 + b_3 + \mathrm{i}(a_3 - b_2) \\ c_2 - d_3 - \mathrm{i}(c_3 + d_2) & -(c_0 - d_1) + \mathrm{i}(c_1 + d_0) & -(a_2 - b_3) + \mathrm{i}(a_3 + b_2) & a_0 - b_1 - \mathrm{i}(a_1 + b_0) \end{bmatrix} \end{aligned}$$

Gaussian Symplectic Ensemble(GSE)

- An $n \times n$ **quaternion self-dual Hermitian matrix** ${}^{q}\mathbf{A}_n = (x_{jk})_{n\times n}$ is a matrix whose entries $x_j (j, k = 1, \dots, n)$ are **quaternions** and satisfy $x_{jk} = \bar{x}_{kj}$. If each x_{jk} is viewed as a 2×2 matrix, then $\mathbf{A}_n = (x_{jk})$ is in fact a $2n \times 2n$ Hermitian matrix. And, the entries of $\mathbf{A}_n$ can be represented as

$$x_{jk} = \begin{bmatrix} a_{jk} + b_{jk} i & c_{jk} + d_{jk} i \\ -c_{jk} + d_{jk} i & a_{jk} - b_{jk} i \end{bmatrix} = \begin{bmatrix} \alpha_{jk} & \beta_{jk} \\ -\overline{\beta}_{jk} & \overline{\alpha}_{jk} \end{bmatrix}, 1 \le j < k \le n,$$

and $x_{jj} = \begin{bmatrix} a_{jj} & 0 \\ 0 & a_{jj} \end{bmatrix}$, where $a_{jk}, b_{jk}, c_{jk}, d_{jk} \in \mathbb{R}$ and $1 \le j, k \le n$. It is well known that the multiplicities of all the eigenvalues of $\mathcal{A}_n$ are even[9].

- Example: $\begin{bmatrix} \begin{bmatrix} a_{11} & 0 \\ 0 & a_{11} \end{bmatrix} & \begin{bmatrix} a_{12} + b_{12} i & c_{12} + d_{12} i \\ -c_{12} + d_{12} i & a_{12} - b_{12} i \end{bmatrix} \\ \begin{bmatrix} a_{12} - b_{12} i & -c_{12} - d_{12} i \\ c_{12} - d_{12} i & a_{12} + b_{12} i \end{bmatrix} & \begin{bmatrix} a_{44} & 0 \\ 0 & a_{44} \end{bmatrix} \end{bmatrix}$
- Free variables number is $n + \frac{n(n-1)}{2} \cdot 4$

[9] Fuzhen Zhang. "Quaternions and matrices of quaternions". In: *Linear algebra and its applications* 251 (1997), pp. 21–57.

1 Background

2 A Two-Dimensional Example

2×2 Real Symmetric Matrix

- Consider a 2×2 real symmetric matrix $M = \begin{bmatrix} a & b \\ b & c \end{bmatrix}$ with distinct eigenvalues $\lambda_1 \neq \lambda_2$. Then $M = U \begin{bmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{bmatrix} U^T$, and without loss of generality we can assume $U = \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix}$ for some $0 \leq \theta < 2\pi$.
- U 是二维空间的一组基构成的矩阵，$\begin{bmatrix} \cos\theta \\ \sin\theta \end{bmatrix}$ 与 $\begin{bmatrix} -\sin\theta \\ \cos\theta \end{bmatrix}$ 相互正交
- $$\begin{aligned} a &= \lambda_1 \cos^2\theta + \lambda_2 \sin^2\theta \\ b &= (\lambda_1 - \lambda_2)\cos\theta\sin\theta \\ c &= \lambda_1 \sin^2\theta + \lambda_2 \cos^2\theta \end{aligned}$$
- $$\frac{\partial(a,b,c)}{\partial(\lambda_1,\lambda_2,\theta)} = \begin{bmatrix} \cos^2\theta & \sin^2\theta & -2(\lambda_1-\lambda_2)\cos\theta\sin\theta \\ \cos\theta\sin\theta & -\cos\theta\sin\theta & (\lambda_1-\lambda_2)(\cos^2\theta - \sin^2\theta) \\ \sin^2\theta & \cos^2\theta & 2(\lambda_1-\lambda_2)\cos\theta\sin\theta \end{bmatrix}.$$

2×2 Real Symmetric Matrix

- Since

$$\frac{\partial(a,b,c)}{\partial(\lambda_1,\lambda_2,\theta)} = \begin{bmatrix} \cos^2\theta & \sin^2\theta & -2(\lambda_1-\lambda_2)\cos\theta\sin\theta \\ \cos\theta\sin\theta & -\cos\theta\sin\theta & (\lambda_1-\lambda_2)(\cos^2\theta-\sin^2\theta) \\ \sin^2\theta & \cos^2\theta & 2(\lambda_1-\lambda_2)\cos\theta\sin\theta \end{bmatrix}.$$

- The determinant can be:

$$\left|\det\frac{\partial(a,b,c)}{\partial(\lambda_1,\lambda_2,\theta)}\right| = |\lambda_1-\lambda_2| f_1(\theta)$$

where

$$f_1(\theta) = \left|\det\begin{bmatrix} \cos^2\theta & \sin^2\theta & -2\sin 2\theta \\ \frac{1}{2}\sin 2\theta & -\frac{1}{2}\sin 2\theta & \cos 2\theta \\ \sin^2\theta & \cos^2\theta & \sin 2\theta \end{bmatrix}\right| = 1 > 0$$

2×2 Hermitian Matrix

- Consider a 2×2 Hermitian matrix $M = \begin{bmatrix} a & b+ci \\ b-ci & d \end{bmatrix}$ with distinct eigenvalues $\lambda_1 \neq \lambda_2$. Then $M = U \begin{bmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{bmatrix} U^*$, and without loss of generality we can assume $U = \begin{bmatrix} \cos\theta & -(\cos\chi - i\sin\chi)\sin\theta \\ (\cos\chi + i\sin\chi)\sin\theta & \cos\theta \end{bmatrix}$ for some $0 \leq \theta \leq \frac{1}{2}\pi$ and $0 \leq \chi < 2\pi$.[10]
-
$$\begin{aligned} a &= \lambda_1 \cos^2\theta + \lambda_2 \sin^2\theta \\ b &= (\lambda_1 - \lambda_2)\cos\theta\sin\theta\cos\chi \\ c &= (-\lambda_1 + \lambda_2)\cos\theta\sin\theta\sin\chi \\ d &= \lambda_1 \sin^2\theta + \lambda_2 \cos^2\theta \end{aligned}$$
-
$$\frac{\partial(a,b,c,d)}{\partial(\lambda_1,\lambda_2,\theta,\chi)} = \begin{bmatrix} \cos^2\theta & \sin^2\theta & -2(\lambda_1-\lambda_2)\cos\theta\sin\theta & 0 \\ \cos\theta\sin\theta\cos\chi & -\cos\theta\sin\theta\cos\chi & (\lambda_1-\lambda_2)(\cos^2\theta-\sin^2\theta)\cos\chi & -(\lambda_1-\lambda_2)\sin\theta\cos\theta\sin\chi \\ -\cos\theta\sin\theta\sin\chi & \cos\theta\sin\theta\sin\chi & -(\lambda_1-\lambda_2)(\cos^2\theta-\sin^2\theta)\sin\chi & -(\lambda_1-\lambda_2)\sin\theta\cos\theta\cos\chi \\ \sin^2\theta & \cos^2\theta & 2(\lambda_1-\lambda_2)\cos\theta\sin\theta & 0 \end{bmatrix}$$

[10] Howard Haber. *Diagonalization of a general 2×2 hermitian matrix.* (2012). URL: https://scipp.ucsc.edu/~haber/ph216/diag22new.pdf.

2×2 Hermitian Matrix

- Since

$$\frac{\partial(a,b,c,d)}{\partial(\lambda_1,\lambda_2,\theta,\chi)} = \begin{bmatrix} \cos^2\theta & \sin^2\theta & -2(\lambda_1-\lambda_2)\cos\theta\sin\theta & 0 \\ \cos\theta\sin\theta\cos\chi & -\cos\theta\sin\theta\cos\chi & (\lambda_1-\lambda_2)(\cos^2\theta-\sin^2\theta)\cos\chi & -(\lambda_1-\lambda_2)\sin\theta\cos\theta\sin\chi \\ -\cos\theta\sin\theta\sin\chi & \cos\theta\sin\theta\sin\chi & -(\lambda_1-\lambda_2)(\cos^2\theta-\sin^2\theta)\sin\chi & -(\lambda_1-\lambda_2)\sin\theta\cos\theta\cos\chi \\ \sin^2\theta & \cos^2\theta & 2(\lambda_1-\lambda_2)\cos\theta\sin\theta & 0 \end{bmatrix}$$

- The determinant can be:

$$\left|\det\frac{\partial(a,b,c,d)}{\partial(\lambda_1,\lambda_2,\theta,\chi)}\right| = (\lambda_1-\lambda_2)^2 f_2(\theta,\chi)$$

where

$$f_2(\theta,\chi) = \left|\det\begin{bmatrix} \cos^2\theta & \sin^2\theta & -\sin 2\theta & 0 \\ \cos\theta\sin\theta\cos\chi & -\cos\theta\sin\theta\cos\chi & \cos 2\theta\cos\chi & -\frac{1}{2}\sin 2\theta\sin\chi \\ -\cos\theta\sin\theta\sin\chi & \cos\theta\sin\theta\sin\chi & -\cos 2\theta\sin\chi & -\frac{1}{2}\sin 2\theta\cos\chi \\ \sin^2\theta & \cos^2\theta & \sin 2\theta & 0 \end{bmatrix}\right|$$

is independent of the eigenvalues of M.

4×4 Hermitian self-dual matrix

- Consider a 4×4 Hermitian self-dual matrix $M = \begin{bmatrix} \begin{bmatrix} a_{11} & 0 \\ 0 & a_{11} \end{bmatrix} & \begin{bmatrix} a_{12} + b_{12}i & c_{12} + d_{12}i \\ -c_{12} + d_{12}i & a_{12} - b_{12}i \end{bmatrix} \\ \begin{bmatrix} a_{12} - b_{12}i & -c_{12} - d_{12}i \\ c_{12} - d_{12}i & a_{12} + b_{12}i \end{bmatrix} & \begin{bmatrix} a_{44} & 0 \\ 0 & a_{44} \end{bmatrix} \end{bmatrix}$. Then $M = U \begin{bmatrix} \mu_1 & 0 & 0 & 0 \\ 0 & \mu_1 & 0 & 0 \\ 0 & 0 & \mu_2 & 0 \\ 0 & 0 & 0 & \mu_2 \end{bmatrix} U^*$.
- The determinant can be:

$$\left| \det \frac{\partial(a_{11}, a_{12}, a_{44}, b_{12}, c_{12}, d_{12})}{\partial(\Lambda, U)} \right| = (\lambda_1 - \lambda_2)^4 f_4(U)$$

Conclusion

- A well-known analogy between RMT and statistical machanics β corresponds to an inverse temperature.

$$\text{Free veriables: } n + \frac{n(n-1)}{2} \cdot \beta$$

$$\begin{cases} \beta = 1 & \text{orthogonal ensembles,} \\ \beta = 2 & \text{unitary ensembles,} \\ \beta = 4 & \text{symplectic ensembles.} \end{cases}$$

- Similarly, as for 2×2 matrix, the determinant is:

$$\left| \det \frac{\partial(M)}{\partial(\Lambda, U)} \right| = (\lambda_1 - \lambda_2)^{\beta} f_{\beta}(U)$$

$$\begin{cases} \beta = 1 & \text{orthogonal ensembles,} \\ \beta = 2 & \text{unitary ensembles,} \\ \beta = 4 & \text{symplectic ensembles.} \end{cases}$$

Thanks!