Sampling eigenvalue PDFs for matrix ensembles

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Objective

To efficiently sample from joint eigenvalue PDFs for some classical random matrix ensembles.

Examples of classical matrix ensembles

1. Gaussian orthogonal ensemble. Joint PDF of elements $\propto e^{-\mathrm{Tr}(H^2)/2}$. H real symmetric.

2. Random unitary matrices with Haar (uniform) measure.

3. Wishart matrices
$$A = X^T X$$
where X is an $n \times m$ Gaussian matrix with joint PDF of elements $\propto e^{-\mathrm{Tr}(X^T X)/2}$.

Random matrix hypotheses

1. The highly excited energy levels of heavy nuclei have the same statistical properties as the eigenvalues of large GOE matrices.

2. The large Riemann zeros have the same statistical properties as the eigenvalues of large random unitary matrices.

3. $\vec{x}_k = [x_k^{(j)}]_{j=1,\ldots,n}$, vector of price data for commodity k on days $1, 2, \ldots, n$. For commodities $k = 1, \ldots, m$ the data is effectively uncorrelated: the eigenvalues of the covariance matrix have the same statistical properties as a random Wishart matrix.

Testing the hypotheses

- Knowledge of the statistical properties of the random matrix ensembles is required.
- Often the statistical properties are known in analytic form.
- To illustrate these analytic forms, Monte Carlo simulation of the corresponding distributions are often undertaken.
- When an analytic form is not known, the distribution can be estimated by Monte Carlo simulation.

Example 1. Let $p_2^{\mathrm{n.n.}}(s)$ denote the probability distribution for the smallest of the spacings between the left neighbour and right neighbour of a given eigenvalue. It has been shown that

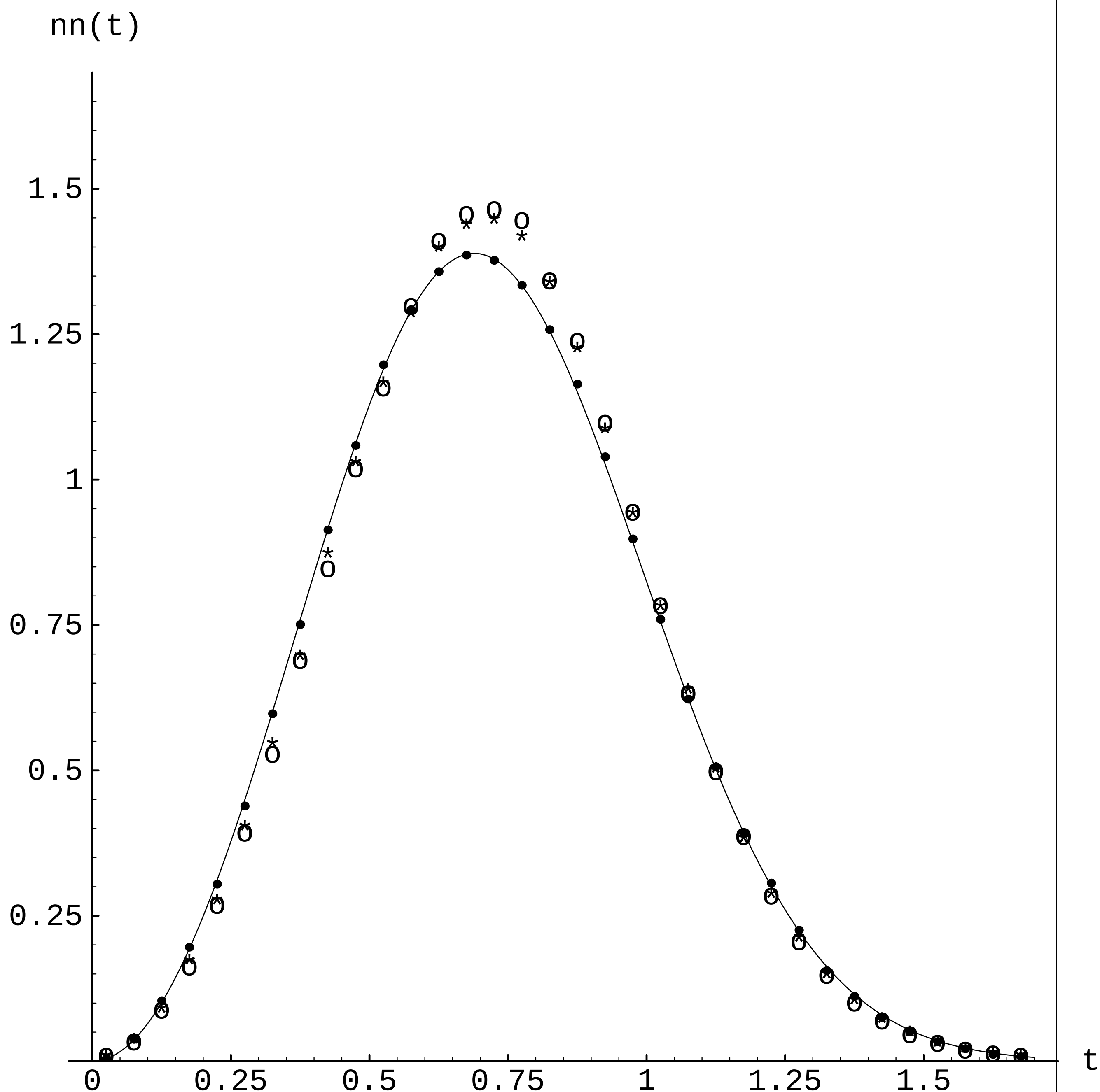
$$p_2^{\mathrm{n.n.}}(s) = -\frac{\sigma_a(2\pi s;\xi)}{2\pi s} \exp \int_0^{2\pi s} \frac{\sigma_a(t;\xi)}{t}\, dt \Big|_{a=\xi=1}$$

where

$$(s\sigma_a'')^2 + 4(-a^2 + s\sigma_a' - \sigma_a)\Big((\sigma_a')^2 - \{a - (a^2 - s\sigma_a' + \sigma_a)^{1/2}\}^2\Big) = 0$$

subject to the boundary condition

$$\sigma_a(s;\xi) \underset{s\to 0^+}{\sim} -\xi \frac{2(s/4)^{2a+1}}{\Gamma(1/2+a)\Gamma(3/2+a)}.$$



Comparison of $nn(t) := p_2^{\mathrm{n.n.}}(s)$ for the matrix ensembles with unitary symmetry in the bulk (continuous curve) and for 10^6 consecutive Riemann zeros, starting near zero number 1 (open circles), 10^6 (asterisks) and 10^{20} (filled circles).

Sampling from the GOE eigenvalue PDF

- Generate a member of the ensemble, compute its eigenvalues.
- (Possible) internal workings — tridiagonal form using Householder transformations

$$U^{(j)} = 1 - 2\vec{u}^{(j)}\vec{u}^{(j)T} = \begin{bmatrix} 1_{j\times j} & 0_{j\times N-j} \\ 0_{N-j\times j} & V_{N-j\times N-j} \end{bmatrix}.$$

- For $X \in \mathrm{GOE}$

$$\begin{bmatrix} \mathrm{N}[0,1] & \tilde{\chi}_{N-1} & & & & \\ \tilde{\chi}_{N-1} & \mathrm{N}[0,1] & \tilde{\chi}_{N-2} & & & \\ & \tilde{\chi}_{N-2} & \mathrm{N}[0,1] & \tilde{\chi}_{N-3} & & \\ & \ddots & \ddots & \ddots & & \\ & & \tilde{\chi}_2 & \mathrm{N}[0,1] & \tilde{\chi}_1 \\ & & & \tilde{\chi}_1 & \mathrm{N}[0,1] \end{bmatrix}$$

where $\tilde{\chi}_k = (\Gamma[k/2,1])^{1/2} \sim (2/\Gamma(k/2))u^{k-1}e^{-u^2}$, $u > 0$.

- $P_N(\lambda)$ for GOE therefore satisfies

$$P_k(\lambda) = (\lambda - a_k)P_{k-1}(\lambda) - b_{k-1}^2 P_{k-2}(\lambda), \quad P_0(\lambda) = 1$$

where $a_k \sim \mathrm{N}[0,1]$, $b_k^2 \sim \Gamma[k/2,1]$.

- Hence can sample from the GOE by generating $P_N(\lambda)$ from the recurrence and computing its zeros.

Sampling from the $U(N)$ eigenvalue PDF

- Generate $U \in U(N)$: Gram-Schmidt orthogonalize $\{\vec{g}_1, \ldots, \vec{g}_N\}$ where elements of $\vec{g}_i$ are $\mathrm{N}[0,1] + i\mathrm{N}[0,1]$.

- Householder transformation to upper Hessenberg form $H = [H_{ij}]_{i,j=0,\ldots,N-1}$. Diagonal elements $H_{ii} = -\alpha_{i-1}\bar{\alpha}_i$ where $\alpha_{-1} = -1$, $|\alpha_j| < 1$ $(j = 0, \ldots, N-2)$, $|\alpha_{N-1}| = 1$.

- Characteristic polynomial $P_N(\lambda)$ satisfies coupled recurrences

$$\begin{aligned} P_k(\lambda) &= \lambda P_{k-1}(\lambda) - \bar{\alpha}_{k-1}\tilde{P}_{k-1}(\lambda) \\ \tilde{P}_k(\lambda) &= \lambda \tilde{P}_{k-1}(\lambda) - \alpha_{k-1}P_{k-1}(\lambda) \end{aligned}$$

  where $P_0(\lambda) = \tilde{P}_0(\lambda)$.

- For $H \in U(N)$, $\alpha_{N-j-1} \sim \Theta_{2j+1}$ $(j = 0, \ldots, N-1)$ where Θ_ν has p.d.f. $\frac{\nu-1}{2\pi}(1-|z|^2)^{(\nu-3)/2}\chi_{|z|<1}$.

Wishart matrices

- Introduce two sequences of Householder reflections $\{U^{(j)}, \tilde{U}^{(j)}\}$ to bidiagonalize the $m \times n$ matrix X^T,

$$B^T = \begin{bmatrix} x_n & & & \\ y_{m-1} & x_{n-1} & & \\ \ddots & \ddots & & \\ & y_1 & x_{n-m+1} & \end{bmatrix},$$

- For X Gaussian, $x_j \sim \chi_j$, $y_j \sim \chi_j$.
- Form $A = X^T X$,

$$B^T B = \begin{bmatrix} a_m & b_{m-1} & & \\ b_{m-1} & a_{m-1} & b_{m-2} & \\ \ddots & \ddots & \ddots & \\ & b_2 & a_2 & b_1 \\ & & b_1 & a_1 \end{bmatrix},$$

$$a_m = x_n^2, \qquad a_i = y_i^2 + x_{n-m+i}^2, \qquad b_i = y_i x_{n-m+i+1}.$$

- Again a 3 term recurrence for $P_N(\lambda)$,

$$P_k(\lambda) = (\lambda - a_k)P_{k-1}(\lambda) - b_{k-1}^2 P_{k-2}(\lambda), \qquad P_0(\lambda) = 1.$$

Strategies based on changing variables

Problem – From the given distribution of the elements of a tridiagonal matrix, compute the corresponding distribution of its eigenvalues and variables corresponding to eigenvectors.

- Need the Jacobian for change of variables

  $$\vec{a} := (a_n, a_{n-1}, \ldots, a_1), \qquad \vec{b} := (b_{n-1}, \ldots, b_1)$$

  to

  $$\vec{\lambda} := (\lambda_1, \ldots, \lambda_n), \qquad \vec{q} := (q_1, \ldots, q_{n-1}).$$

- Make use of the general formula

  $$\sum_{j=1}^{n} \frac{q_j^2}{\lambda_j - \lambda} = \Big((T - \lambda 1)^{-1}\Big)_{11} = -\frac{P_{n-1}(\lambda)}{P_n(\lambda)}.$$

- Note the inter-relation

  $$\prod_{1 \le j < k \le n} (\lambda_j - \lambda_k)^2 = \frac{\prod_{i=1}^{n-1} b_i^{2i}}{\prod_{i=1}^{n} q_i^2}.$$

Theorem 1. *The Jacobian is equal to*

$$\frac{1}{q_n}\frac{\prod_{i=1}^{n-1} b_i}{\prod_{i=1}^{n} q_i}.$$

Main features of the proof:

- Triangular system of equations

$$\begin{aligned}
1 &= \sum_{j=1}^{n} q_j^2 \\
a_n &= \sum_{j=1}^{n} q_j^2 \lambda_j \\
* + b_{n-1}^2 &= \sum_{j=1}^{n} q_j^2 \lambda_j^2 \\
* + a_{n-1} b_{n-1}^2 &= \sum_{j=1}^{n} q_j^2 \lambda_j^3 \\
* + b_{n-2}^2 b_{n-1}^2 &= \sum_{j=1}^{n} q_j^2 \lambda_j^4 \\
* + a_{n-2} b_{n-2}^2 b_{n-1}^2 &= \sum_{j=1}^{n} q_j^2 \lambda_j^5 \\
&\vdots \\
* + a_1 b_1^2 \cdots b_{n-2}^2 b_{n-1}^2 &= \sum_{j=1}^{n} q_j^2 \lambda_j^{2n-1}.
\end{aligned}$$

- Determinant evaluation

$$\det\left[[\lambda_k^j - \lambda_N^j]_{\substack{j=1,\ldots,2N-1\\k=1,\ldots,N-1}} [j\lambda_k^{j-1}]_{\substack{j=1,\ldots,2N-1\\k=1,\ldots,N}} \right] = \prod_{1\le j<k\le N} (\lambda_k - \lambda_j)^4.$$

Consequence

Theorem 2. *Consider the random symmetric tridiagonal matrix*

$$\begin{bmatrix} N[0,1] & \tilde{\chi}_{(N-1)\beta} & & & & \\ \tilde{\chi}_{(N-1)\beta} & N[0,1] & \tilde{\chi}_{(N-2)\beta} & & & \\ & \tilde{\chi}_{(N-2)\beta} & N[0,1] & \tilde{\chi}_{(N-3)\beta} & & \\ & \ddots & \ddots & \ddots & & \\ & & \tilde{\chi}_{2\beta} & N[0,1] & \tilde{\chi}_{\beta} \\ & & & \tilde{\chi}_{\beta} & N[0,1] \end{bmatrix}$$

The eigenvalues and first component of the eigenvectors (which form the vector $\vec{q}$) are independent, with the distribution of the former given by

$$\frac{1}{\tilde{G}_{\beta N}} \prod_{l=1}^{N} e^{-\lambda_l^2/2} \prod_{1 \le j < k \le N} |\lambda_k - \lambda_j|^{\beta} \, d\vec{\lambda},$$

$$\tilde{G}_{\beta N} = (2\pi)^{N/2} \prod_{j=0}^{N-1} \frac{\Gamma(1 + (j+1)\beta/2)}{\Gamma(1 + \beta/2)},$$

and the distribution of the latter by

$$\frac{1}{c_{\beta N} q_N} \prod_{i=1}^{N} q_i^{\beta - 1} \, d\vec{q}, \qquad q_i > 0, \sum_{i=1}^{N} q_i^2 = 1, \quad \text{where} \quad c_{\beta N} = \frac{\Gamma^N(\beta/2)}{2^{N-1}\Gamma(\beta N/2)}.$$

The circular case

Analogous results can be obtained for unitary Hessenberg matrices.

Theorem 3. *The Jacobian for the change of variables from $\vec{\alpha}$ to $(\vec{\lambda}, \vec{q})$ is equal to*

$$\frac{\prod_{i=0}^{N-2}(1-|\alpha_i|^2)}{q_N \prod_{i=1}^{N} q_i}.$$

Theorem 4. *Consider a random unitary Hessenberg matrix with parameters $\{\alpha_j\}_{j=1,\dots,N}$ distributed according to*

$$\alpha_{N-j-1} \in \Theta_{\beta j+1} \qquad (j = 0, \dots, N-1).$$

The eigenvalues and first component of the eigenvectors (which form $\vec{q}$) are independent, with the distribution of the eigenvalues given by

$$\frac{1}{C_{\beta\, N}} \prod_{1\le j<k\le N} |e^{i\theta_k} - e^{i\theta_j}|^\beta \, d\vec{\theta}, \qquad C_{\beta\, N} = (2\pi)^N \frac{\Gamma(\beta N/2+1)}{\Gamma(\beta/2+1)}$$

and the distribution of $\vec{q}$ as in the Gaussian case.

Perturbation viewpoint: Gaussian matrices

Border a real symmetric matrix by an extra row and column:

$$\tilde{M} = \begin{bmatrix} M & \vec{w}^T \\ \vec{w} & a \end{bmatrix}.$$

Question. Suppose $\{\lambda_i\}$ are the eigenvalues of M. What are the eigenvalues of $\tilde{M}$?

$$\det(\lambda - \tilde{M}) = \det \begin{bmatrix} \lambda - M & -\vec{w}^T \\ -\vec{w} & \lambda - a \end{bmatrix} \tag{1}$$

$$= \det \begin{bmatrix} \lambda - M & -\vec{w}^T \\ \vec{0} & \lambda - a - \vec{w}(\lambda - M)^{-1}\vec{w}^T \end{bmatrix} \tag{2}$$

$$= \det(\lambda - M)\Big(\lambda - a - \vec{w}(\lambda - M)^{-1}\vec{w}^T\Big). \tag{3}$$

$$\frac{\tilde{p}_N(\lambda)}{p_N(\lambda)} = \lambda - a - \sum_{i=1}^{N} \frac{w_i^2}{\lambda - \lambda_i}.$$

Suppose $M \in \mathrm{GOE}_N$. Then with

$$w_i \sim \mathrm{N}[0, 1/\sqrt{2}], \qquad a \sim \mathrm{N}[0, 1]$$

we have

$$\tilde{M} \in \mathrm{GOE}_{N+1}, \qquad w_i^2 \sim \Gamma[\frac{1}{2}, 1].$$

Thus for the GOE, ratios of successive characteristic polynomials satisfy

$$\frac{p_{N+1}(\lambda)}{p_N(\lambda)} = \lambda - a - \sum_{i=1}^{N} \frac{w_i^2}{\lambda - \lambda_i}.$$

On the other hand, it's easy to see that

$$\frac{p_{N-1}(\lambda)}{p_N(\lambda)} = \sum_{i=1}^{N} \frac{q_i^2}{\lambda - \lambda_i}$$

where

$$q_i^2 \sim \frac{w_i^2}{\sum_{i=1}^{N} w_i^2}.$$

Comparing gives

$$p_{N+1}(\lambda) = (\lambda - a) p_N(\lambda) - b p_{N-1}(\lambda)$$

where

$$b \sim \sum_{i=1}^{N} w_i^2 \sim \Gamma[N/2, 1]$$

Perturbation of unitary matrices

The relevant perturbation is multiplicative: multilpy the first row by t, $|t| = 1$.

Lemma 1. *Let U be an $n \times n$ unitary matrix, distinct eigenvalues $e^{i\theta_1}, \ldots, e^{i\theta_n}$, first component of corresponding eigenvectors v_{1j}. Perturb the matrix to obtain $\tilde{U}$. We have*

$$\frac{\tilde{P}_n(\lambda)}{P_n(\lambda)} = 1 + (t-1) \sum_{j=1}^{n} \frac{e^{i\theta_j} |v_{1j}|^2}{e^{i\theta_j} - \lambda}.$$

- To obtain random recurrences, work with projected variables

$$\lambda = \frac{1+ix}{1-ix}.$$

Changing variables gives

$$\prod_{l=1}^{N} |1+e^{i\theta_l}|^{2b} \prod_{1\le j<k\le N} |e^{i\theta_k}-e^{i\theta_j}|^{2c} d\theta_1\cdots d\theta_N = 2^{cN(N-1)+N(1+2b)}$$

$$\times \prod_{j=1}^{N}(1+\lambda_j^2)^{-c(N-1)-1-b} \prod_{1\le j<k\le N} |\lambda_k-\lambda_j|^{2c} d\lambda_1\cdots d\lambda_N.$$

Theorem 5. *The characteristic polynomial for the Cauchy ensemble satisfies the random recurrence*

$$p_{n+1}(x) = \Big(\frac{x}{\beta_n} - \frac{\gamma_n}{\beta_n}\Big)p_n(x) - \Big(\frac{1}{\beta_n} - 1\Big)(1+x^2)p_{n-1}(x)$$

where γ_l has distribution

$$\Big(\frac{1+ix}{1-ix}\Big)^{-(lc+b+1)}$$

and β_l has distribution

$$\mathrm{B}[2b+lc+1, lc].$$