Accurate Numerical Evaluation of Distribution Functions

for Orthogonal and Symplectic Matrix Ensembles

Folkmar Bornemann
Fredholm Determinants versus Painlevé Transcendents

Two tools used in integrable systems

Ivar Fredholm (1866–1927)

determinant of integral operator (1899)

\[ Ku(x) = \int_a^b K(x, y) u(y) \, dy \]

\[ \implies \det(I + zK) = \sum_{n=0}^{\infty} \frac{z^n}{n!} \int_{[a,b]^n} \det K(t_i, t_j) \, dt \]

Paul Painlevé (1863–1933)

six families of irreducible transcendental functions (1895)

\[ u_{xx} = 6u^2 + x \]
\[ u_{xx} = 2u^3 + xu - \alpha \]
\[ u_{xx} = u^{-1}u_x^2 - x^{-1}u_x + x^{-1}(\alpha u^2 + \beta) + \gamma u^3 + \delta u^{-1} \]
\[ u_{xx} = \cdots \]
\[ u_{xx} = \cdots \]
\[ u_{xx} = \cdots \]
**Example**

\( n \)-th largest level in edge scaled GUE

\[
\Pi(\text{exactly } n \text{ levels in } (s, \infty)) = \left(\frac{-1}{n!}\right)^n \frac{\partial^n}{\partial z^n} F_2(s; z) \bigg|_{z=1}
\]

*(Forrester '93)*

\( F_2(s; z) = \det \left( I - z K_{\text{Ai}} \right) \)

with kernel

\[
K_{\text{Ai}}(x, y) = \frac{\text{Ai}(x) \text{Ai}'(y) - \text{Ai}'(x) \text{Ai}(y)}{x - y}
\]

*(Tracy/Widom '93)*

\( F_2(s; z) = \exp \left( -\int_s^\infty (x - s) u(x; z)^2 \, dx \right) \)

with Painlevé II

\[
u_{xx} = 2u^3 + xu
\]

\[
u(x; z) \simeq \sqrt{z} \text{Ai}(x) \quad (x \to \infty)
\]

*Without the Painlevé representations, the numerical evaluation of the Fredholm determinants is quite involved.*

— Tracy/Widom '00
\section*{Simple Numerical Method for Fredholm Determinants}

\textbf{\textit{m}-point quadrature formula}

\[
\int_a^b \, dt \, f(t) \approx \sum_{k=1}^{m} w_k \, f(x_k)
\]

\textbf{The Idea} (Hilbert 1904, B. ’10)

\[
\det(I + zK) = \sum_{n=0}^{\infty} \frac{z^n}{n!} \int_a^b dt_1 \cdots \int_a^b dt_n \det K(t_i, t_j)
\]

\[
\approx \sum_{n=0}^{\infty} \frac{z^n}{n!} \sum_{k_1=1}^{m} w_{k_1} \cdots \sum_{k_n=1}^{m} w_{k_n} \det K(x_{k_i}, x_{k_j})
\]

\textbf{v. Koch} 1892

\[
\det(I + zK_m)
\]

with the \textit{m} \times \textit{m}-matrix

\[
K_m = \left(w_i^{1/2} K(x_i, x_j) w_j^{1/2}\right)_{i,j=1}^{m}
\]
Matlab-Code

\[ [w,x] = \text{QuadratureRule}(a,b,m); \]
\[ w = \sqrt{w}; [xi,xj] = \text{ndgrid}(x,x); \]
\[ d = \det(\text{eye}(m)+z*(w'*w).*K(xi,xj)); \]

Theorem (B. '10)

For quadrature formula of order \( \nu \) with positive weights:

- if kernel is \( C^{k-1,1}(\mathbb{R}^2) \),
  \[
  \text{error} = O(\nu^{-k}) \quad (\nu \to \infty);
  \]
- if kernel is bounded analytic, there is \( \rho > 1 \) with
  \[
  \text{error} = O(\rho^{-\nu}) \quad (\nu \to \infty).
  \]
Tracy–Widom distribution

\[ F_2(s) = \det \left( I - K_{Ai} \right)_{L^2(s, \infty)} , \quad K_{Ai}(x, y) = \frac{Ai(x) Ai'(y) - Ai'(x) Ai(y)}{x - y} \]

Perturbation bound for \( m \)-dimensional determinants: (B. '10)

\[ \text{round-off error} \leq \sqrt{m} \left\| K_{m} \right\|_F \cdot u_{\text{machine}} \]
$n$-th largest level in edge scaled GUE

\[
\mathbb{P}(\text{exactly } n \text{ levels in } (s, \infty)) = \frac{(-1)^n}{n!} \left. \frac{\partial^n}{\partial z^n} \det \left( I - z K_{Ai} \upharpoonright_{L^2(s,\infty)} \right) \right|_{z=1}
\]

Numerical method

\( f(z) = \det(I + z K_{Ai}) \) is entire of order 0

\[
\frac{f^{(n)}(z)}{n!} = \frac{1}{2\pi r^n} \int_0^{2\pi} e^{-in\theta} f(z + re^{i\theta}) \, d\theta
\]

- trapezoidal rule exponentially convergent
- numerical stability: judicious choice of \( r > 0 \)

Example: (B. ’11)

\( f \) entire of order \( \rho > 0 \) and type \( \tau > 0 \)

\[
r_{\text{opt}} = \left( \frac{n}{\rho \tau} \right)^{1/\rho}
\]
Generating functions of probabilities

- absolute error: $r = 1$ reasonable (Lyness/Sande ‘71)
- relative error (= accurate tails):

$$r_{\text{opt}} = \arg\min_{r > 0} r^{-n} f(r)$$

unique solution of convex optimization problem (B. ‘11)

![Graph of gap probability $E_2(10; s)$ of GUE](image1)

![Graph of absolute error](image2)

![Graph of $r_{\text{opt}}$ as a function of $s$](image3)
**Combinatorial structure of determinantal processes**

Kernel $K$, disjoint intervals $J_1, \ldots, J_N$, multi-index $\alpha \in \mathbb{N}_0^N$

$$
\mathbb{P}(\text{exactly } \alpha_j \text{ levels lie in } J_j, j = 1, \ldots, N)
$$

$$
= \frac{(-1)^{|\alpha|}}{\alpha!} \frac{\partial^\alpha}{\partial z^\alpha} \det \left( I - \begin{pmatrix} z_1 K & \cdots & z_N K \\ \vdots & \ddots & \vdots \\ z_1 K & \cdots & z_N K \end{pmatrix} \bigg|_{L^2(J_1) \oplus \cdots \oplus L^2(J_N)} \right)_{z_1 = \cdots = z_N = 1}
$$

**Examples**

- joint pdfs
- pdfs of sums, products, etc.
systems of integral operators = integral operator on coproduct

\[
K = \begin{pmatrix}
K_{11} & \cdots & K_{1N} \\
\vdots & \ddots & \vdots \\
K_{N1} & \cdots & K_{NN}
\end{pmatrix}
\]

on \( \bigoplus_{k=1}^{N} L^2(I_k) \) with matrix kernel \( K_{ij}(x, y) \)

representable as a single integral operator on

\[
L^2 \left( \bigsqcup_{k=1}^{N} I_k \right) \cong \bigoplus_{k=1}^{N} L^2(I_k), \quad \bigsqcup_{k=1}^{N} I_k = \bigcup_{k=1}^{N} I_k \times \{k\},
\]

with scalar kernel (Fredholm 1903)

\[
K(x, y) = \sum_{i,j=1}^{N} \mathbb{1}_{I_i}(x) K_{ij}(x, y) \mathbb{1}_{I_j}(y)
\]

\( \rightsquigarrow \) straightforward extension of the quadrature method
$n$-th largest level in edge scaled GSE

\[ P(\text{exactly } n \text{ levels lie in } (s, \infty)) = E_4(n; s) = \frac{(-1)^n}{n!} \frac{\partial^n}{\partial z^n} F_4(s; z) \bigg|_{z=1} \]

(Forrester/Nagao/Honner '99, Tracy/Widom '05)

\[
F_4(s; z) = \det \left( I - \frac{z}{2} \begin{pmatrix} S(x, y) & SD(x, y) \\ IS(x, y) & S(y, x) \end{pmatrix} \right)_{L^2(s, \infty) \oplus L^2(s, \infty)}^{1/2}
\]

\[
S(x, y) = K_{Ai}(x, y) - \frac{1}{2} Ai(x) \int_y^\infty Ai(\eta) \, d\eta
\]

\[
SD(x, y) = -\partial_y K_{Ai}(x, y) - \frac{1}{2} Ai(x) \, Ai(y)
\]

\[
IS(x, y) = -\int_x^\infty K_{Ai}(\zeta, y) \, d\zeta + \frac{1}{2} \int_x^\infty Ai(\zeta) \, d\zeta \int_y^\infty Ai(\eta) \, d\eta
\]

\[
K_{Ai}(x, y) = \frac{Ai(x) Ai'(y) - Ai'(x) Ai(y)}{x - y}
\]
factorization
\[ K_{Ai}(x, y) = \int_0^\infty K(x, \xi)K(\xi, y)\,d\xi, \quad K(x, y) = Ai(x + y), \]
yields
\[ F_2(s; z) = F_+(s; z) \cdot F_-(s; z), \quad F_{\pm}(s; z) = \det \left( I \mp \sqrt{z} K\big|_{L^2(s/2, \infty)} \right) \]
and (Ferrari/Spohn ’05)
\[ F_4(s; 1) = \frac{1}{2}(F_+(s; 1) + F_-(s; 1)) \]

A new formula (B. ’10)

How about, in general, \[ F_4(s; z) = \frac{1}{2}(F_+(s; z) + F_-(s; z)) \]?

- first, numerical tests with random \(s\) and \(z\) indicated the formula to be \textit{true}
- later, proof via Painlevé II representation (B. ’10, Forrester ’06)
**Matrix Kernel Determinant for GOE**

**n-th largest level in edge scaled GOE**

\[
\mathbb{P} \left( \text{exactly } n \text{ levels lie in } (s, \infty) \right) = E_1(n; s) = \frac{(-1)^n}{n!} \frac{\partial^n}{\partial z^n} F_1(s; z) \bigg|_{z=1}
\]

(Forrester/Nagao/Honner ’99, Tracy/Widom ’05)

\[
F_1(s; z) = \det \left( I - z \begin{pmatrix} S(x, y) & SD(x, y) \\ IS(x, y) & S(y, x) \end{pmatrix} \right)^{1/2} \upharpoonright_{X_1(s, \infty) \oplus X_2(s, \infty)}
\]

\[
S(x, y) = K_{Ai}(x, y) + \frac{1}{2} \left( 1 - \frac{1}{2} Ai(x) \int_{y}^{\infty} Ai(\eta) \, d\eta \right)
\]

\[
SD(x, y) = -\partial_{y}K_{Ai}(x, y) - \frac{1}{2} Ai(x) \, Ai(y)
\]

\[
IS(x, y) = -\frac{1}{2} \text{sgn}(x - y) - \int_{x}^{\infty} K_{Ai}(\zeta, y) \, d\zeta + \frac{1}{2} \left( \int_{y}^{x} Ai(\zeta) \, d\zeta + \int_{x}^{\infty} Ai(\zeta) \, d\zeta \int_{y}^{\infty} Ai(\eta) \, d\eta \right)
\]

\[
K_{Ai}(x, y) = \frac{Ai(x) \, Ai'(y) - Ai'(x) \, Ai(y)}{x - y}
\]

Hilbert–Schmidt operator with trace class diagonal \(\leadsto\) *Hilbert–Carleman determinant*
A Recursive Approach to Edge-Scaled GOE I

superposition/decimation relations (Forrester/Rains ’01)

\[ \text{GSE}_m = \text{even}(\text{GOE}_{2m+1}), \quad \text{GUE}_m = \text{even}(\text{GOE}_m \cup \text{GOE}_{m+1}) \]

combinatorical implications

- \( F_4(n; s) = F_1(2n; s) \)
- \( E_2(n; s) = \sum_{j=0}^{2n} E_1(j; s) E_1(2n-j; s) + \sum_{j=0}^{2n+1} E_1(j; s) E_1(2n+1-j; s) \)

other relations

- \( E_2(n; s) = \sum_{j=0}^{n} E_+(j; s) E_-(n-j; s) \)
- \( E_4(n; s) = \frac{1}{2} (E_+(n; s) + E_-(n; s)) \)
- \( E_1(0; s) = E_+(0; s) \) (Ferrari/Spohn ’05)
generating functions

\[ f_0(x) = \sum_{n=0}^{\infty} E_1(2n; s)x^{2n} \]

\[ f_1(x) = \sum_{n=0}^{\infty} E_1(2n + 1; s)x^{2n+1} \]

\[ g_{\pm}(x) = \sum_{n=0}^{\infty} E_{\pm}(n; s)x^{2n} = F_{\pm}(1 - x^2; s) \]

equations

\[ f_0(x)^2 + 2f_0(x)f_1(x) + x^2f_1(x)^2 = g_+(x) \cdot g_-(x) \]

\[ f_0(x) + f_1(x) = \frac{1}{2} (g_+(x) + g_-(x)) \]

\[ f_0(0) = g_+(0) \]
solution

\[ f_0(x) = g_+(x) - (1 - \sqrt{1 - x^2})f_0(x) \]

\[ f_1(x) = \frac{1}{2} (g_+(x) + g_-(x)) - f_0(x) \]

transforms with

\[ 1 - \sqrt{1 - x^2} = \sum_{k=0}^{\infty} \frac{(2k)}{2^{2k+1}(k+1)} x^{2k+2} \]

into the recursion

\[ E_1(2n; s) = E_+(n; s) - \sum_{k=0}^{n-1} \frac{(2k)}{2^{2k+1}(k+1)} E_1(2n - 2k - 1; s) \]

\[ E_1(2n + 1; s) = \frac{E_+(n; s) + E_-(n; s)}{2} - E_1(2n; s) \]
A reformulation of the GOE recursion

(B. ’10, Forrester ’06)

\[ F_1(s; z) = \sum_{n=0}^{\infty} E_1(n; s)(1 - z)^n \]

\[ = \frac{1}{2} \sum_{\pm} \left( 1 \pm \sqrt{\frac{z}{2 - z}} \right) \det \left( I \pm \sqrt{z(2 - z)} K_{L^2(\mathbb{R})}^{L^2(s/2, \infty)} \right) \]

with \( K(x, y) = \text{Ai}(x + y) \)

- amenable to exponential convergence in the quadrature method
- branch-cut singularities at \( z = 0 \) and \( z = 2 \)
  \( \sim \) derivatives not along circles (new: automatic contours B./Wechslberger ’11)

similar structure for

- bulk scaling limits
- hard-edge scaling limits (LOE/LUE/LSE)
an e-mail from a geneticist @ Broad Institute (MIT/Harvard)

I’m ... interested in the distribution of eigenvalues of very large (mostly Wishart) matrices. I recently found you ArXiv paper. A tremendous amount of information. ... Some things I would like: A table of the mean of $F_1(k,s)$ for as large $k$ as is practical. I’d certainly like to get this for $k = 1, \ldots, 50$.

mean and variance of the $k$-largest level in edge-scaled GOE by using the recursion

<table>
<thead>
<tr>
<th></th>
<th>Mean</th>
<th>Variance</th>
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<tr>
<td>1</td>
<td>-1.2065335745</td>
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<td>2</td>
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<td>3</td>
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<td>5</td>
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<td>-35.5__________</td>
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<tr>
<td>47</td>
<td>-3___________</td>
<td>0.___________</td>
</tr>
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**RMFredholmToolbox for Matlab** (B. '10)

<table>
<thead>
<tr>
<th>function</th>
<th>command</th>
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<tbody>
<tr>
<td>$E_2^{(n)}(k;J)$</td>
<td>E(2,k,J,n)</td>
</tr>
<tr>
<td>$E_2^{(n)}((k,0);J_1,J_2)$</td>
<td>E(2,[k,0],[J1,J2],n)</td>
</tr>
<tr>
<td>$E_2^{(bulk)}(k;J)$</td>
<td>E(2,k,J,'bulk')</td>
</tr>
<tr>
<td>$E_2^{(bulk)}((k,0);J_1,J_2)$</td>
<td>E(2,[k,0],[J1,J2],‘bulk’)</td>
</tr>
<tr>
<td>$E_2^{(soft)}(k;J)$</td>
<td>E(2,k,J,'soft')</td>
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<tr>
<td>$E_2^{(soft)}((k,0);J_1,J_2)$</td>
<td>E(2,[k,0],[J1,J2],‘soft’)</td>
</tr>
<tr>
<td>$E_4^{(n)}(k;J)$</td>
<td>E(4,k,J,'soft','MatrixKernel')</td>
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<tr>
<td>$E_4^{(n)}(k;J,\alpha)$</td>
<td>E('LUE',k,J,n,\alpha)</td>
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<tr>
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<td>E('LUE',[k,0],[J1,J2],n,\alpha)</td>
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<tr>
<td>$E_2^{(hard)}(k;J,\alpha)$</td>
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<td>E(2,[k,0],[J1,J2],‘hard’,\alpha)</td>
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<td>E(2,[k,0],[J1,J2],‘hard’,\alpha)</td>
</tr>
<tr>
<td>$E_+^{(k;\alpha)}$</td>
<td>E('+',k,\alpha)</td>
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<tr>
<td>$E_-^{(k;\alpha)}$</td>
<td>E('−',k,\alpha)</td>
</tr>
<tr>
<td>$E_{\beta}^{(k;\alpha)}$</td>
<td>E(\beta,k,\alpha)</td>
</tr>
<tr>
<td>$E_{\beta}^{(k)}$</td>
<td>E(\beta,k)</td>
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<td>$F_{\beta}^{(k)}$</td>
<td>F(\beta,k)</td>
</tr>
<tr>
<td>$F_\beta^{(s)}$</td>
<td>F(\beta,s)</td>
</tr>
<tr>
<td>$E_{\beta,\alpha}^{(k;\alpha)}$</td>
<td>E(\beta,k,\alpha)</td>
</tr>
</tbody>
</table>

**send e-mail to:** bornemann@tum.de
References

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