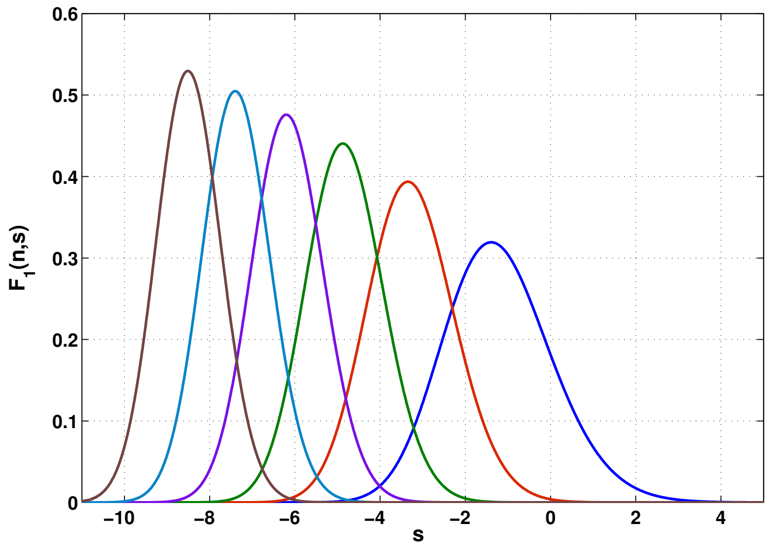
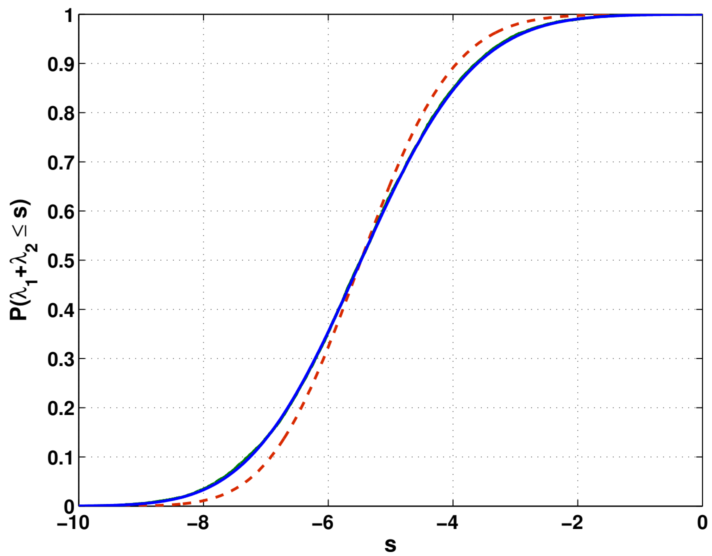
Numerical Evaluation of Distribution Functions

for Canonical Matrix Ensembles



pdf of n-th largest level in edge scaled GOE



cdf of the sum of largest two levels in GUE

Folkmar Bornemann

Two tools used in integrable systems

Ivar Fredholm (1866–1927)

determinant of integral operator (1899)

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

$$\rightsquigarrow$$

$$\det(I+zK) = \sum_{n=0}^{\infty} \frac{z^n}{n!} \int_{[a,b]^n} \det_{i,j=1}^{n} K(t_i,t_j)\,dt$$

Paul Painlevé (1863–1933)

six families of irreducible transcendental functions (1895)

$$u_{xx} = 6u^2 + x$$

$$u_{xx} = 2u^3 + xu - \alpha$$

$$u_{xx} = u^{-1}u_x^2 - x^{-1}u_x + x^{-1}(\alpha u^2 + \beta) + \gamma u^3 + \delta u^{-1}$$

$$u_{xx} = \cdots$$

$$u_{xx} = \cdots$$

$$u_{xx} = \cdots$$

n-th largest level in edge scaled GUE

$$\mathbb{P}(\text{exactly } n \text{ levels in } (s,\infty)) = \frac{(-1)^n}{n!} \frac{\partial^n}{\partial z^n} F_2(s;z)\Big|_{z=1}$$

(Mehta '91, Forrester '91)

$$F_2(s;z) = \det\left(I - z\,K_{\mathrm{Ai}}\restriction_{L^2(s,\infty)}\right)$$

with kernel

$$K_{\mathrm{Ai}}(x,y) = \frac{\mathrm{Ai}(x)\,\mathrm{Ai}'(y) - \mathrm{Ai}'(x)\,\mathrm{Ai}(y)}{x-y}$$

(Tracy/Widom '94)

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

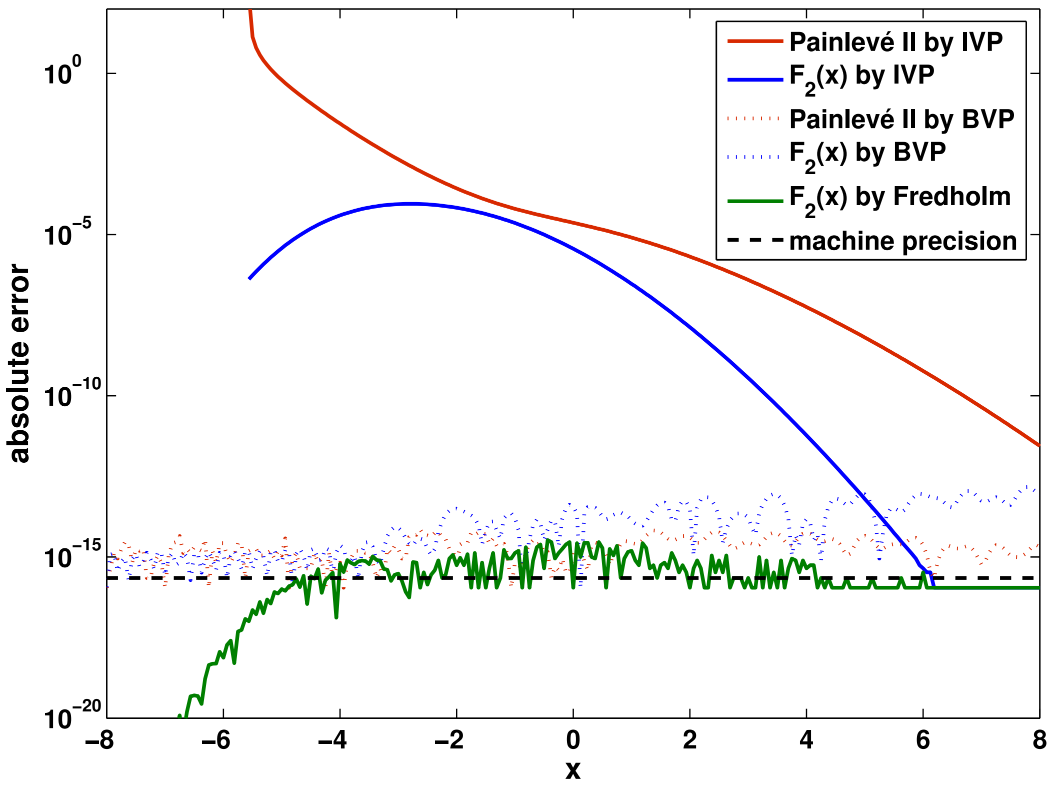
with Painlevé II

$$u_{xx} = 2u^3 + xu$$

$$u(x;z) \simeq \sqrt{z}\,\mathrm{Ai}(x) \qquad (x\to\infty)$$

Without the Painlevé representations, the numerical evaluation of the Fredholm determinants is quite involved. — Tracy/Widom '00

Numerical evaluation of the Tracy–Widom distribution $F_2(x)$



Absolute error of various numerical approaches using IEEE double precision

- via Painlevé II as IVP *(backwards)*

  Prähofer ('04): 16 digits (1500 internally!)

  Bejan ('05): 3 digits

  Edelman/Persson ('05): 8 digits @ 8.9 sec

- via Painlevé II as BVP

  Tracy/Widom ('94): 10 digits (75 internally!)

  Dieng ('05): 9 digits @ 3.7 sec

  Driscoll/B./Trefethen ('08): 13 digits @ 1.3 sec

- via Fredholm determinant

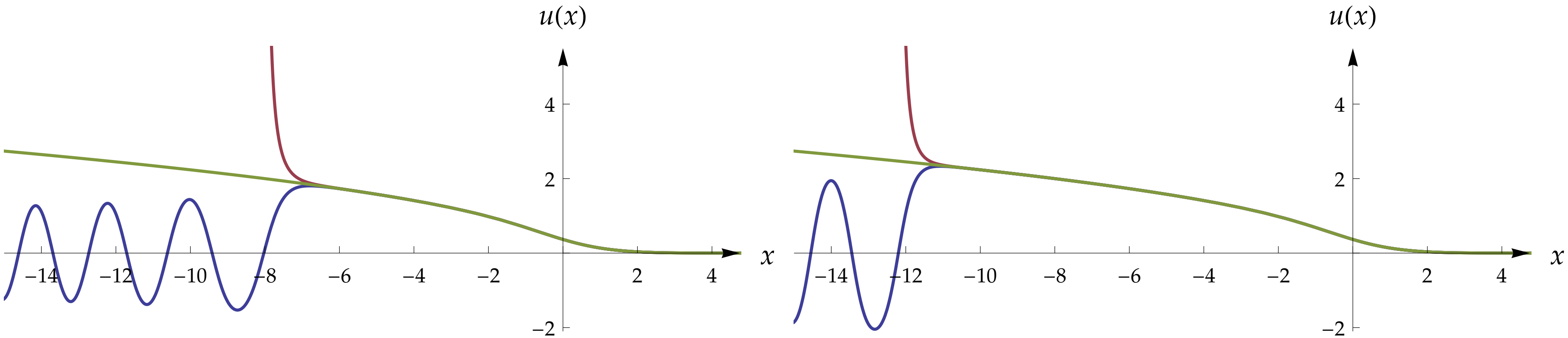
  B. ('10): 15 digits @ 0.69 sec

Explanation

solution of PII,

$$u_{xx} = 2u^3 + xu, \qquad u(x) \simeq \theta\, \mathrm{Ai}(x) \quad (x \to \infty),$$

separatrix at $\theta = 1 \quad \rightsquigarrow$ IVP highly unstable



$u(x)$ with $\theta = 1 - 10^{-8}, 1, 1 + 10^{-8}$ $\qquad$ $u(x)$ with $\theta = 1 - 10^{-16}, 1, 1 + 10^{-16}$

consequence

- calculate F_2 via a BVP solution $\rightsquigarrow$ *connection formula* needed:

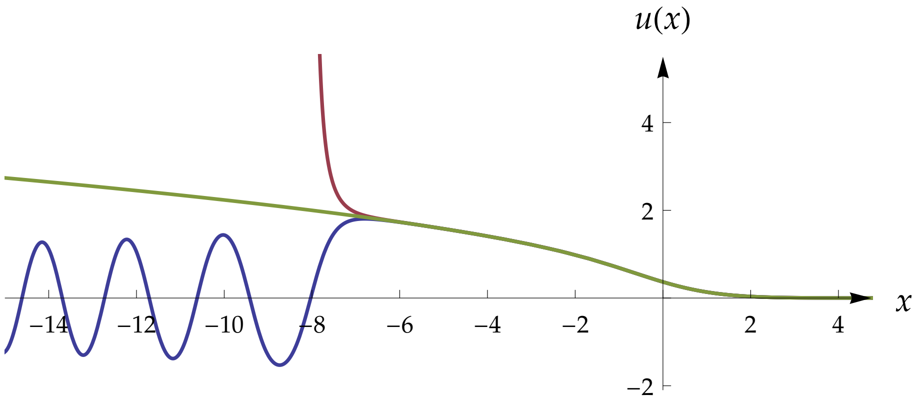
$$u(x) \simeq \mathrm{Ai}(x) \quad (x \to \infty) \qquad \Rightarrow \qquad u(x) \simeq \,? \qquad (x \to -\infty)$$

Explanation

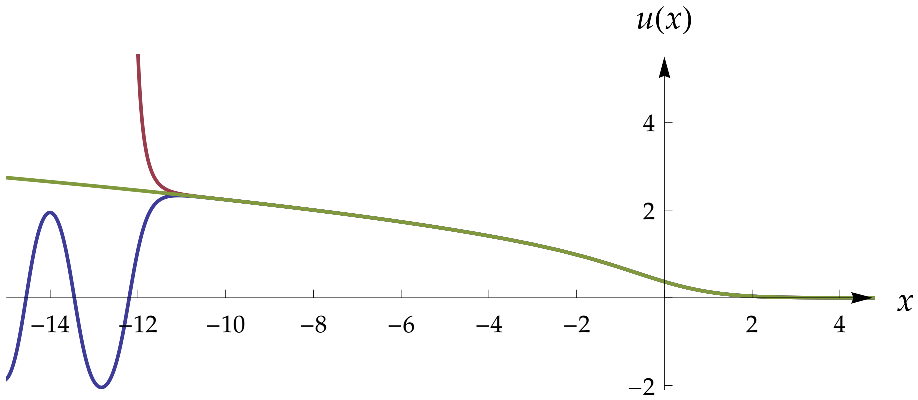
solution of PII,

$$u_{xx} = 2u^3 + xu, \qquad u(x) \simeq \theta\,\mathrm{Ai}(x) \quad (x \to \infty),$$

separatrix at $\theta = 1$ $\rightsquigarrow$ IVP highly unstable



$u(x)$ with $\theta = 1 - 10^{-8}, 1, 1 + 10^{-8}$



$u(x)$ with $\theta = 1 - 10^{-16}, 1, 1 + 10^{-16}$

consequence

- calculate F_2 via a BVP solution $\rightsquigarrow$ *connection formula* needed:

$$u(x) \simeq \mathrm{Ai}(x) \quad (x \to \infty) \qquad \Rightarrow \qquad u(x) \simeq \sqrt{-x/2} \quad (x \to -\infty)$$

m-point quadrature formula

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

The Idea

$$\det(I + zK) \overset{\text{Fredholm}}{\underset{1903}{=}} \sum_{n=0}^\infty \frac{z^n}{n!} \int_a^b dt_1 \cdots \int_a^b dt_n \det_{i,j=1}^n K(t_i, t_j)$$

$$\approx \sum_{n=0}^\infty \frac{z^n}{n!} \sum_{k_1=1}^m w_{k_1} \cdots \sum_{k_n=1}^m w_{k_n} \det_{i,j=1}^n K(x_{k_i}, x_{k_j})$$

$$\overset{\text{v. Koch}}{\underset{1892}{=}} \det(I + zK_m)$$

with the $m \times m$-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] = QuadratureRule(a,b,m);
w = sqrt(w); [xi,xj] = ndgrid(x,x);
d = det(eye(m)+z*(w'*w).*K(xi,xj));
```

Theorem (B. '10)

For quadrature formula of order ν with positive weights:

- if kernel is $C^{k-1,1}([a,b]^2)$,

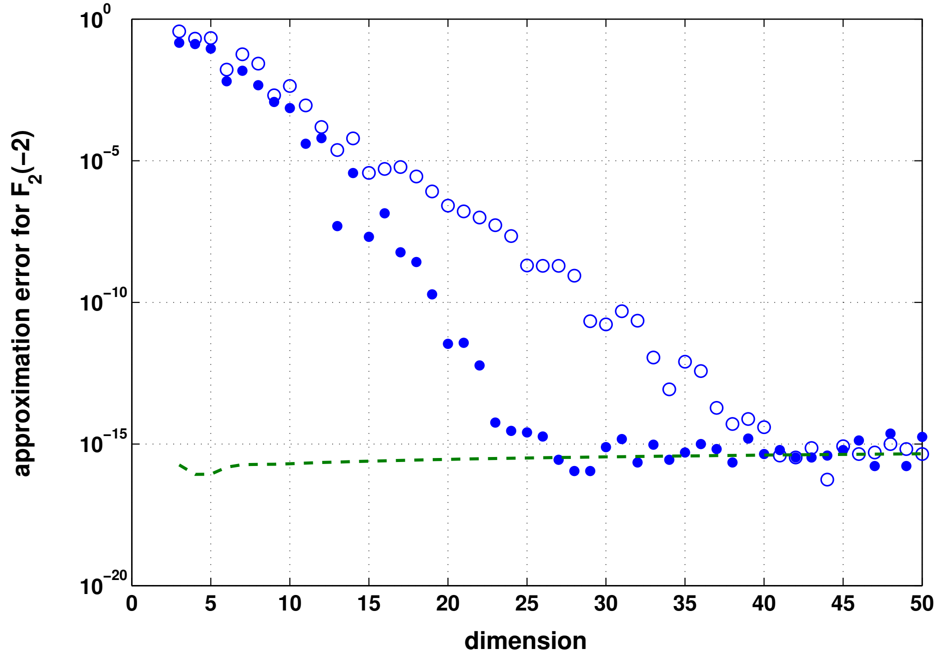
$$\text{error} = O(\nu^{-k}) \qquad (\nu \to \infty);$$

- if kernel is bounded analytic, there is $\rho > 1$ with

$$\text{error} = O(\rho^{-\nu}) \qquad (\nu \to \infty).$$

Tracy–Widom distribution

$$F_2(s) = \det\left(I - K_{\mathrm{Ai}}\restriction_{L^2(s,\infty)}\right), \qquad K_{\mathrm{Ai}}(x,y) = \frac{\mathrm{Ai}(x)\,\mathrm{Ai}'(y) - \mathrm{Ai}'(x)\,\mathrm{Ai}(y)}{x-y}$$



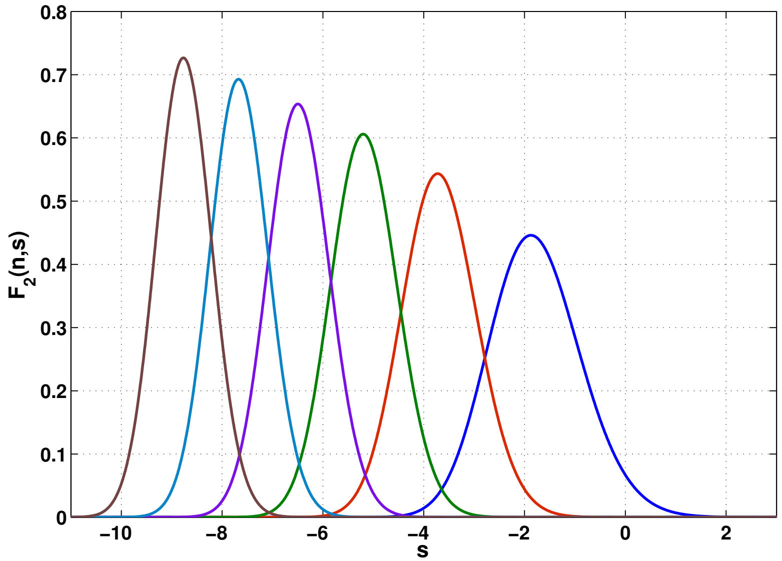
dots: Gauss–Legendre, circles: Clenshaw–Curtis

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

$$\text{round-off error} \leqslant \sqrt{m}\,\|K_m\|_F \cdot u_{\text{machine}}$$

n-th largest level in edge scaled GUE

$$\mathbb{P}(\text{exactly } n \text{ levels in } (s,\infty)) = \frac{(-1)^n}{n!}\frac{\partial^n}{\partial z^n}\det\left(I - zK_{\mathrm{Ai}}\restriction_{L^2(s,\infty)}\right)\Big|_{z=1}$$



probability density of n-th largest level in edge scaled GUE

Numerical method

$f(z) = \det(I + zK_{\mathrm{Ai}})$ 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. '10)

f entire of order $\rho > 0$ and type $\tau > 0$

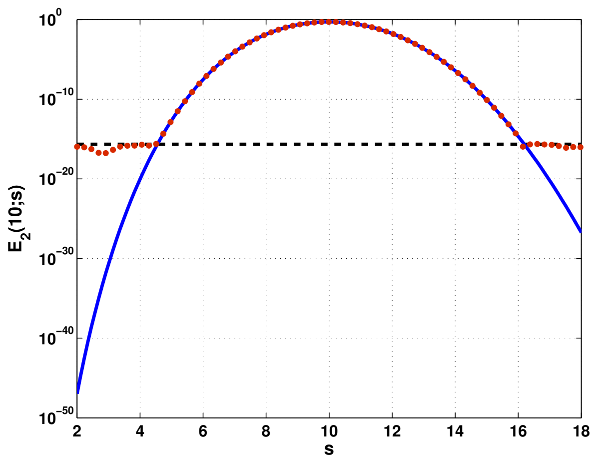
$$r_{\mathrm{opt}} = (n/\rho\tau)^{1/\rho}$$

Generating functions of probabilities

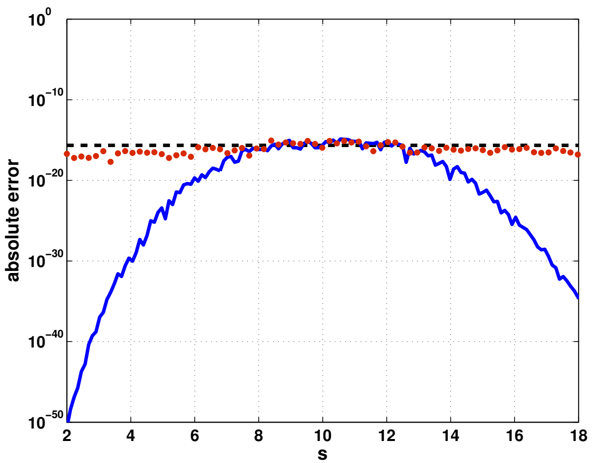
- absolute error: $r = 1$ reasonable (Lyness/Sande '71)
- relative error ($=$ accurate tails):

$$r_{\text{opt}} = \operatorname*{argmin}_{r>0} r^{-n} f(r)$$

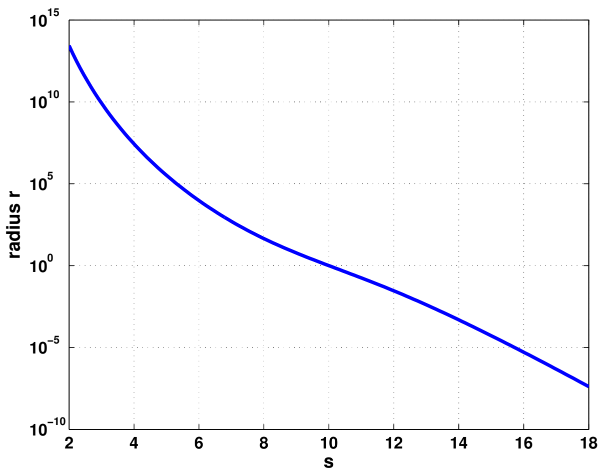
unique solution of *convex* optimization problem (B. '10)



gap probability $E_2(10; s)$ of GUE



absolute error



r_{opt} as a function of s

Combinatorial structure of determinantal processes

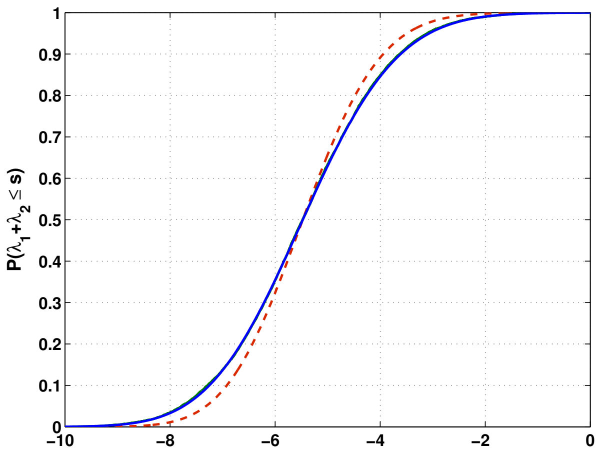
kernel K, disjoint intervals $J_1, \ldots, J_N$, multi-index $\alpha \in \mathbb{N}_0^N$

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

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

Examples

- joint pdfs
- pdfs of sums, products, etc.

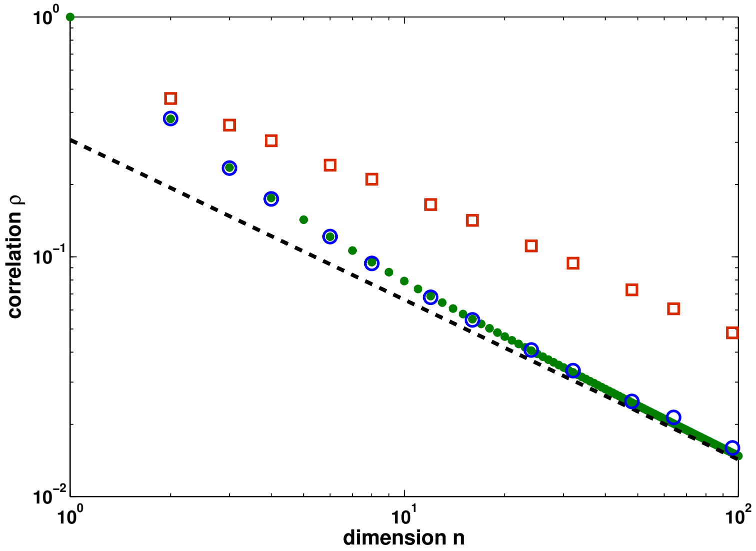


cdf of the sum of largest two levels in GUE

Joint pdf of extreme eigenvalues of $n \times n$ GUE

$$\mathbb{P}(x \leqslant \lambda_{\min}^{(n)} \leqslant \lambda_{\max}^{(n)} \leqslant y) = \det\left(I - \begin{pmatrix} K_n & K_n \\ K_n & K_n \end{pmatrix} \restriction_{L^2(-\infty,x)\oplus L^2(y,\infty)}\right)$$

asymptotic independence (Bianci/Debbah/Najim '10, B. '10)



correlation coefficient $\rho(\lambda_{\min}^{(n)}, \lambda_{\max}^{(n)})$

- green dots: GUE

  with asymptotics (dashed line)

  $$\rho(\lambda_{\min}^{(n)}, \lambda_{\max}^{(n)}) = \frac{n^{-2/3}}{4\sigma^2} + O(n^{-4/3})$$

  $$\sigma^2 = \text{var}(F_2) = 0.81319\,47928$$

- red squares: hermitean matrices with entries uniformly i.i.d. on $[-1, 1]$

systems of integral operators = integral operator on coproduct

$$K = \begin{pmatrix} K_{11} & \cdots & K_{1N} \\ \vdots & & \vdots \\ K_{N1} & \cdots & K_{NN} \end{pmatrix} \quad \text{on} \quad \bigoplus_{k=1}^{N} L^2(I_k) \quad \text{with matrix kernel } K_{ij}(x,y)$$

representable as a *single* integral operator on

$$L^2\left(\coprod_{k=1}^{N} I_k\right) \cong \bigoplus_{k=1}^{N} L^2(I_k), \qquad \coprod_{k=1}^{N} I_k = \bigcup_{k=1}^{N} I_k \times \{k\},$$

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

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

(Forrester/Nagao/Honner '99, Tracy/Widom '04)

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

$$S(x,y) = K_{\mathrm{Ai}}(x,y) - \tfrac{1}{2}\,\mathrm{Ai}(x)\int_y^\infty \mathrm{Ai}(\eta)\,d\eta$$

$$SD(x,y) = -\partial_y K_{\mathrm{Ai}}(x,y) - \tfrac{1}{2}\,\mathrm{Ai}(x)\,\mathrm{Ai}(y)$$

$$IS(x,y) = -\int_x^\infty K_{\mathrm{Ai}}(\xi,y)\,d\xi + \tfrac{1}{2}\int_x^\infty \mathrm{Ai}(\xi)\,d\xi \int_y^\infty \mathrm{Ai}(\eta)\,d\eta$$

$$K_{\mathrm{Ai}}(x,y) = \frac{\mathrm{Ai}(x)\,\mathrm{Ai}'(y) - \mathrm{Ai}'(x)\,\mathrm{Ai}(y)}{x-y}$$

factorization

$$K_{\mathrm{Ai}}(x,y) = \int_0^\infty K(x,\xi)K(\xi,y)\,d\xi, \qquad K(x,y) = \mathrm{Ai}(x+y),$$

yields

$$F_2(s;z) = F_+(s;z)\cdot F_-(s;z), \qquad F_\pm(s;z) = \det\left(I \mp \sqrt{z}\,K\restriction_{L^2(s/2,\infty)}\right)$$

and (Ferrari/Spohn ’05)

$$F_4(s;1) = \tfrac{1}{2}\left(F_+(s;1) + F_-(s;1)\right)$$

A new formula (B. ’10)

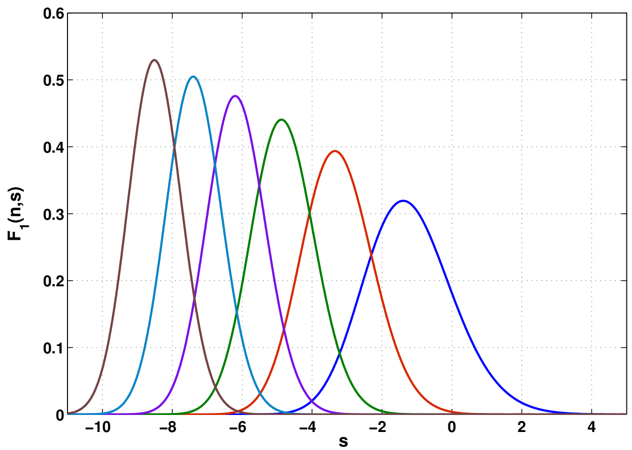
How about, in general, $\boxed{F_4(s;z) = \tfrac{1}{2}\left(F_+(s;z) + F_-(s;z)\right)}$?

- *first*, numerical tests with random s and z indicated the formula to be *true*
- *later*, proof via Painlevé II representation (B. ’10, Forrester ’06)

n-th largest level in edge scaled GOE

$$E_\pm(n;s) = \frac{(-1)^n}{n!} \frac{\partial^n}{\partial z^n} F_\pm(s;z)\Big|_{z=1}, \qquad K(x,y) = \mathrm{Ai}(x+y)$$

yields (B. '10)



Probability density of n-th largest level in edge scaled GOE

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

$$E_1(2n+1;s) = \frac{E_+(n;s) + E_-(n;s)}{2} - E_1(2n;s)$$

technique

elimination process using superposition/decimation relations (Forrester/Rains '01)

$$\mathrm{GUE}_n = \mathrm{even}(\mathrm{GOE}_n \cup \mathrm{GOE}_{n+1}), \qquad \mathrm{GSE}_n = \mathrm{even}(\mathrm{GOE}_{2n+1})$$

Compare with matrix kernel determinant for edge scaled GOE

$$E_1(n;s) = \frac{(-1)^n}{n!}\,\frac{\partial^n}{\partial z^n} F_1(s;z)\Big|_{z=1}$$

(Tracy/Widom '04)

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

$$S(x,y) = K_{\mathrm{Ai}}(x,y) + \tfrac{1}{2}\left(1 - \tfrac{1}{2}\,\mathrm{Ai}(x)\int_y^\infty \mathrm{Ai}(\eta)\,d\eta\right)$$

$$SD(x,y) = -\partial_y K_{\mathrm{Ai}}(x,y) - \tfrac{1}{2}\,\mathrm{Ai}(x)\,\mathrm{Ai}(y)$$

$$IS(x,y) = -\tfrac{1}{2}\mathrm{sgn}(x-y) - \int_x^\infty K_{\mathrm{Ai}}(\xi,y)\,d\xi + \tfrac{1}{2}\left(\int_y^x \mathrm{Ai}(\xi)\,d\xi + \int_x^\infty \mathrm{Ai}(\xi)\,d\xi \int_y^\infty \mathrm{Ai}(\eta)\,d\eta\right)$$

$$K_{\mathrm{Ai}}(x,y) = \frac{\mathrm{Ai}(x)\,\mathrm{Ai}'(y) - \mathrm{Ai}'(x)\,\mathrm{Ai}(y)}{x-y}$$

Hilbert–Schmidt operator with trace class diagonal

$\leadsto$ *determinant to be understood as Hilbert–Carleman regularized determinant*

A reformulation of the GOE recursion

(B. '10, Forrester '06)

$$F_1(s;z) = \frac{1}{2}\sum_{\pm}\left(1 \pm \sqrt{\frac{z}{2-z}}\right)\det\left(I \mp \sqrt{z(2-z)}\,K\restriction_{L^2(s/2,\infty)}\right)$$

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

amenable to exponential convergence in the quadrature method

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similar structure for

- bulk scaling limits
- hard-edge scaling limits (LOE/LUE/LSE)

RMFredholmToolbox for Matlab (B. '10)

function	command
$E_2^{(n)}(k;J)$	`E(2,k,J,n)`
$E_2^{(n)}((k,0);J_1,J_2)$	`E(2,[k,0],{J1,J2},n)`
$E_2^{(\text{bulk})}(k;J)$	`E(2,k,J,'bulk')`
$E_2^{(\text{bulk})}((k,0);J_1,J_2)$	`E(2,[k,0],{J1,J2},'bulk')`
$E_2^{(\text{soft})}(k;J)$	`E(2,k,J,'soft')`
$E_2^{(\text{soft})}((k,0);J_1,J_2)$	`E(2,[k,0],{J1,J2},'soft')`
$F(x,y)$	`F2Joint(x,y)`
$E_4^{(\text{soft})}(k;J)$	`E(4,k,J,'soft','MatrixKernel')`
$E_{\text{LUE}}^{(n)}(k;J,\alpha)$	`E('LUE',k,J,n,alpha)`
$E_{\text{LUE}}^{(n)}((k,0);J_1,J_2,\alpha)$	`E('LUE',[k,0],{J1,J2},n,alpha)`
$E_2^{(\text{hard})}(k;J,\alpha)$	`E(2,k,J,'hard',alpha)`
$E_2^{(\text{hard})}((k,0);J_1,J_2,\alpha)$	`E(2,[k,0],{J1,J2},'hard',alpha)`

function	command
$E_2^{(\text{hard})}((k,0);J_1,J_2,\alpha)$	`E(2,[k,0],{J1,J2},'hard',alpha)`
$E_+(k;s)$	`E('+',k,s)`
$E_-(k;s)$	`E('-',k,s)`
$E_\beta(k;s)$	`E(beta,k,s)`
$\tilde{E}_+(k;s)$	`E('+',k,s,'soft')`
$\tilde{E}_-(k;s)$	`E('-',k,s,'soft')`
$\tilde{E}_\beta(k;s)$	`E(beta,k,s,'soft')`
$F_\beta(k;s)$	`F(beta,k,s)`
$F_\beta(s)$	`F(beta,s)`
$E_{+,\alpha}(k;s)$	`E('+',k,s,'hard',alpha)`
$E_{-,\alpha}(k;s)$	`E('-',k,s,'hard',alpha)`
$E_{\beta,\alpha}(k;s)$	`E(beta,k,s,'hard',alpha)`
$F_{\beta,\alpha}(k;s)$	`F(beta,k,s,alpha)`

send e-mail to: `bornemann@ma.tum.de`

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 F1(k,s) for as large k as is practical. I'd certainly like to get this for k = 1, ..., 50.

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a next day delivery: mean and variance of the k-largest level in edge-scaled GOE

1	-1.2065335745	1.6077810345
2	-3.2624279028	1.0354474415
3	-4.8216302757	0.8223901151
4	-6.1620399636	0.7031581054
5	-7.3701147042	0.6242523679
6	-8.4862183723	0.5670071487
7	-9.5331810321	0.5229902526
.	.	.
.	.	.
.	.	.
38	-31.3497235299	0.2159078706
39	-31.9083474476	0.2129575824
40	-32.4621235403	0.2101204063
41	-33.011211545_	0.207380416_
42	-33.5557807___	0.2047596___
43	-34.09586_____	0.20201_____
44	-34.631_______	0.198_______
45	-35.14________	0.18________
46	-35.5_________	0.1_________
47	-3_.__________	0.__________

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