

18.338J/16.394J: The Mathematics of Infinite Random Matrices

Numerical Methods in Random Matrices

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1 Largest Eigenvalue Distributions

In this section, the distributions of the largest eigenvalue of matrices in the β -ensembles are studied. Histograms are created first by simulation, then by solving the Painlevé II nonlinear differential equation.

1.1 Simulation

The *Gaussian Unitary Ensemble* (GUE) is defined as the Hermitian $n \times n$ matrices A , where the diagonal elements x_{jj} and the upper triangular elements $x_{jk} = u_{jk} + iv_{jk}$ are independent Gaussians with zero-mean, and

$$\begin{cases} \text{Var}(x_{jj}) = 1, & 1 \leq j \leq n, \\ \text{Var}(u_{jk}) = \text{Var}(v_{jk}) = \frac{1}{2}, & 1 \leq j < k \leq n. \end{cases} \quad (1)$$

Since a sum of Gaussians is a new Gaussian, an instance of these matrices can be created conveniently in MATLAB:

```
A=randn(n)+i*randn(n);  
A=(A+A')/2;
```

The largest eigenvalue of this matrix is about $2\sqrt{n}$. To get a distribution that converges as $n \rightarrow \infty$, the shifted and scaled largest eigenvalue λ'_{\max} is calculated as

$$\lambda'_{\max} = n^{\frac{1}{6}} (\lambda_{\max} - 2\sqrt{n}). \quad (2)$$

It is now straight-forward to compute the distribution for λ'_{\max} by simulation:

```
for ii=1:trials  
    A=randn(n)+i*randn(n);  
    A=(A+A')/2;  
    lmax=max(eig(A));  
    lmaxscaled=n^(1/6)*(lmax-2*sqrt(n));  
    % Store lmax  
end  
  
% Create and plot histogram
```

The problem with this technique is that the computational requirements and the memory requirements grow fast with n , which should be as large as possible in order to be a good approximation of infinity. Just storing the matrix A requires n^2 double-precision numbers, so on most computers today n has to be less than 10^4 . Furthermore, computing all the eigenvalues of a full Hermitian matrix requires a computing time proportional to n^3 . This means that it will take many days to create a smooth histogram by simulation, even for relatively small values of n .

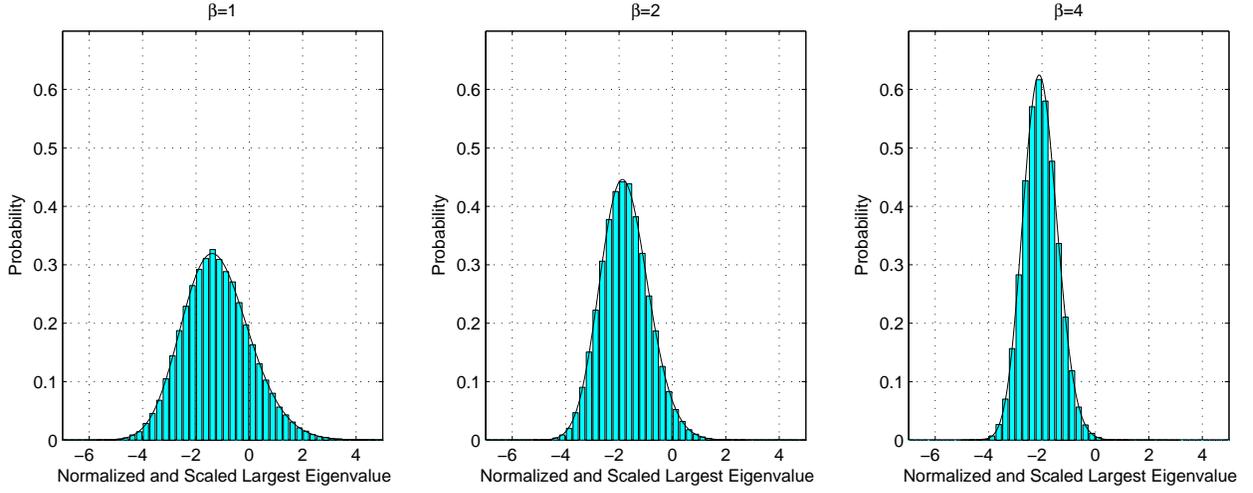


Figure 1: Probability distribution of scaled largest eigenvalue (10^5 repetitions, $n = 10^9$)

```
H=H/sum(H)/dx;
xmid=(x(1:end-1)+x(2:end))/2;

bar(xmid,H)
grid on
```

The resulting distribution is shown in Figure 1, together with distributions for $\beta = 1$ and $\beta = 4$. The plots also contain solid curves representing the “true solutions” (see next section).

1.2 Painlevé II

Instead of using simulation to plot the distributions of the largest eigenvalues, it can be computed from the solution of the Painlevé II nonlinear differential equation [3]:

$$q'' = sq + 2q^3 \quad (5)$$

with the boundary condition

$$q(s) \sim \text{Ai}(s), \quad \text{as } s \rightarrow \infty. \quad (6)$$

The probability distribution $f_2(s)$, corresponding to $\beta = 2$, is then given by

$$f_2(s) = \frac{d}{ds} F_2(s), \quad (7)$$

where

$$F_2(s) = \exp\left(-\int_s^\infty (x-s)q(x)^2 dx\right). \quad (8)$$

The distributions for $\beta = 1$ and $\beta = 4$ are the derivatives of

$$F_1(s)^2 = F_2(s)e^{-\int_s^\infty q(x) dx} \quad (9)$$

and

$$F_4\left(\frac{s}{2^{2/3}}\right)^2 = F_2(s) \left(\frac{e^{\frac{1}{2}\int_s^\infty q(x) dx} + e^{-\frac{1}{2}\int_s^\infty q(x) dx}}{2}\right)^2. \quad (10)$$

To solve this numerically using MATLAB, first rewrite (5) as a first-order system:

$$\frac{d}{ds} \begin{pmatrix} q \\ q' \end{pmatrix} = \begin{pmatrix} q' \\ sq + 2q^3 \end{pmatrix}. \quad (11)$$

This can be solved as an initial-value problem starting at $s = s_0 =$ sufficiently large positive number, and integrating along the negative s -axis. The boundary condition (6) then becomes the initial values

$$\begin{cases} q(s_0) &= \text{Ai}(s_0) \\ q'(s_0) &= \text{Ai}'(s_0). \end{cases} \quad (12)$$

Although the distributions can be computed from $q(s)$ as a post-processing step, it is most convenient to add a few variables and equations to the ODE system. When computing $F_2(s)$, the quantity $I(s) = \int_s^\infty (x-s)q(x)^2 dx$ is required. Differentiate this twice to get

$$I'(s) = - \int_s^\infty q(x)^2 dx \quad (13)$$

and

$$I''(s) = q(s)^2. \quad (14)$$

Add these equations and the variables $I(s), I'(s)$ to the ODE system, and the solver will do the integration. This is not only easier and gives less code, it will also give a much more accurate solution since the same tolerance requirements are imposed on $I(s)$ as on the solution $q(s)$.

In a similar way, the quantity $J(s) = \int_s^\infty q(x) dx$ is needed when computing $F_1(s)$ and $F_4(s)$. This is handled by adding the variable $J(s)$ and the equation $J'(s) = -q(s)$.

The final system now has the form

$$\frac{d}{ds} \begin{pmatrix} q \\ q' \\ I \\ I' \\ J \end{pmatrix} = \begin{pmatrix} q' \\ sq + 2q^3 \\ I' \\ q^2 \\ -q \end{pmatrix} \quad (15)$$

with the initial condition

$$\begin{pmatrix} q(s_0) \\ q'(s_0) \\ I(s_0) \\ I'(s_0) \\ J(s_0) \end{pmatrix} = \begin{pmatrix} \text{Ai}(s_0) \\ \text{Ai}'(s_0) \\ \int_{s_0}^\infty (x-s_0)\text{Ai}(x)^2 dx \\ \text{Ai}(s_0)^2 \\ \int_{s_0}^\infty \text{Ai}(x) dx \end{pmatrix}. \quad (16)$$

This problem can be solved in just a few lines of MATLAB code using the built-in Runge-Kutta based ODE solver `ode45`. First define the system of equations as an inline function

```
deq=inline(' [y(2); s*y(1)+2*y(1)^3; y(4); y(1)^2; -y(1)] ','s','y');
```

Next specify the integration interval and the desired output times.

```
s0=5;
sn=-8;
sspan=linspace(s0,sn,1000);
```

The initial values can be computed as

```
y0=[airy(s0); airy(1,s0); ...
quadl(inline('(x-s0).*airy(x).^2','x','s0'),s0,20,1e-25,0,s0); ...
airy(s0)^2; quadl(inline('airy(x)'),'s0,20,1e-18)];
```

where the `quadl` function is used to numerically approximate the integrals in (16). Now, the integration tolerances can be set and the system integrated:

```
opts=odeset('reltol',1e-13,'abstol',1e-15);
[s,y]=ode45(deq,sspan,y0,opts);
```

The five dependent variables are now in the columns of the MATLAB variable `y`. Using these, $F_2(s)$, $F_1(s)$, and $F_4(s)$ become

```
F2=exp(-y(:,3));
F1=sqrt(F2.*exp(-y(:,5)));
F4=sqrt(F2.*(exp(y(:,5)/2)+exp(-y(:,5)/2))/2);
s4=s/2^(2/3);
```

The probability distributions $f_2(s)$, $f_1(s)$, and $f_4(s)$ could be computed by numerical differentiation:

```
f2=gradient(F2,s);
f1=gradient(F1,s);
f4=gradient(F4,s4);
```

but it is more accurate to first do the differentiation symbolically:

$$f_2(s) = -I'(s)F_2(s) \quad (17)$$

$$f_1(s) = \frac{1}{2F_1(s)} (f_2(s) + q(s)F_2(s)) e^{-J(s)} \quad (18)$$

$$f_4(s) = \frac{1}{2^{\frac{1}{3}}4F_4(s)} \left(f_2(s) \left(2 + e^{J(s)} + e^{-J(s)} \right) + F_2(s)q(s) \left(e^{-J(s)} - e^{J(s)} \right) \right) \quad (19)$$

and evaluate these expressions:

```
f2=-y(:,4).*F2;
f1=1/2./F1.*(f2+y(:,1).*F2).*exp(-y(:,5));
f4=1/2^(1/3)/4./F4.*(f2.*(2+exp(y(:,5))+exp(-y(:,5)))+ ...
    F2.*y(:,1).(exp(-y(:,5))-exp(y(:,5))));
```

Finally, plot the curves:

```
plot(s,f1,s,f2,s4,f4)
legend('\beta=1', '\beta=2', '\beta=4')
xlabel('s')
ylabel('f_\beta(s)', 'rotation', 0)
grid on
```

The result can be seen in Figure 2.

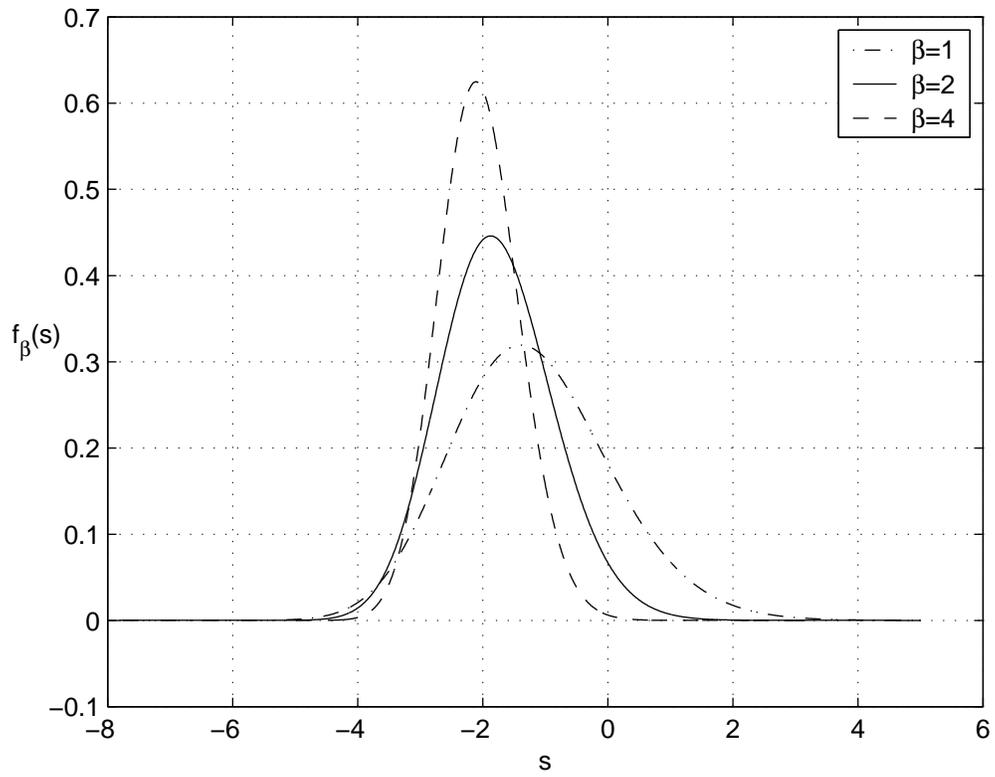


Figure 2: The probability distributions $f_1(s)$, $f_2(s)$, and $f_4(s)$, computed using the Painlevé II solution.

2 Eigenvalue Spacings Distributions

Another quantity with an interesting probability distribution is the spacings of the eigenvalues of random matrices. It turns out that the eigenvalues are almost uniformly distributed, which means that every random matrix gives a large number of spacings. The distributions can then be efficiently computed by simulation.

Two other methods are used to compute the spacings distribution – the solution of the Painlevé V nonlinear differential equation and the eigenvalues of the Prolate matrix. Finally, the results are compared with the spacings of the zeros along the critical line of the Riemann zeta function.

2.1 Simulation

As before, the simulations are made with matrices from the Gaussian Unitary Ensemble. The normalized spacings of the eigenvalues $\lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_N$ are computed according to

$$\delta'_k = \frac{\lambda_{k+1} - \lambda_k}{\pi\beta} \sqrt{2\beta n - \lambda_k^2}, \quad k \approx n/2, \quad (20)$$

where $\beta = 2$ for the GUE. The distribution of the eigenvalues is almost uniform, with a slight deviation at the two ends of the spectrum. Therefore, only half of the eigenvalues are used, and one quarter of the eigenvalues at each end is discarded.

Again, to allow for a more efficient simulation, the tridiagonal matrix (3) is used instead of the full Hermitian matrix. In this case, all the eigenvalues are computed, which can be done in a time proportional to n^2 . While this could in principle be done using the MATLAB sparse matrix structure and the `eigs` function, the more efficient `trideig` function is used below to compute all the eigenvalues of a symmetric tridiagonal matrix. It can be downloaded from <http://www.mit.edu/~persson/mltrid>.

The histogram can now be computed by simulation with the following lines of code. Note that the function `chi2rnd` from the Statistics Toolbox is required.

```
n=1000;
nrep=1000;
beta=2;

ds=zeros(1,nrep*n/2);
for ii=1:nrep
    l=trideig(randn(n,1),sqrt(chi2rnd((n-1:-1:1)*beta)/2));
    d=diff(l(n/4:3*n/4))/beta/pi.*sqrt(2*beta*n-1(n/4:3*n/4-1).^2);
    ds((ii-1)*n/2+1:ii*n/2)=d;
end

histdistr(ds,0:0.05:5);
```

The resulting histogram can be found in Figure 3. The figure also shows the expected curve as a solid line.

2.2 Painlevé V

The probability distribution $p(s)$ for the eigenvalue spacings when $\beta = 2$ can be computed with the solution to the Painlevé V nonlinear differential equation (see [4] for details):

$$(t\sigma'')^2 + 4(t\sigma' - \sigma)(t\sigma' - \sigma + (\sigma')^2) = 0 \quad (21)$$

with the boundary condition

$$\sigma(t) \approx -\frac{t}{\pi} - \left(\frac{t}{\pi}\right)^2, \quad \text{as } t \rightarrow 0^+. \quad (22)$$

Then $p(s)$ is given by

$$p(s) = \frac{d^2}{ds^2} E(s) \quad (23)$$

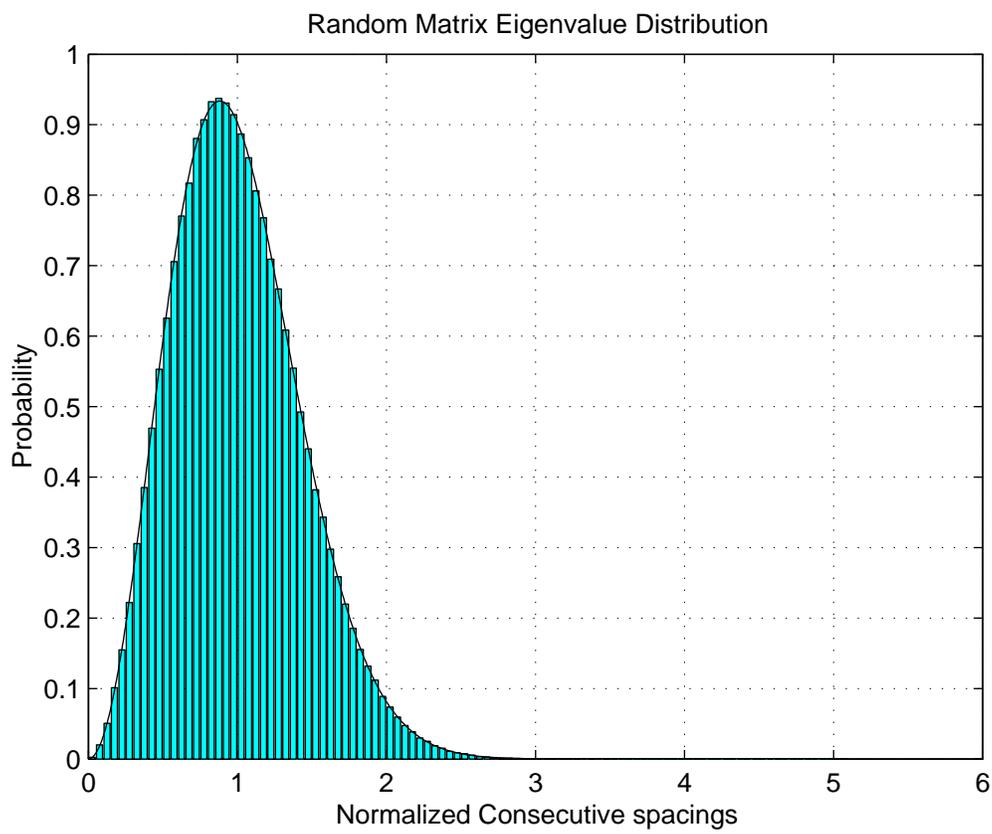


Figure 3: Probability distribution of consecutive spacings of random matrix eigenvalues (1000 repetitions, $n = 1000$)

where

$$E(s) = \exp\left(\int_0^{\pi s} \frac{\sigma(t)}{t} dt\right). \quad (24)$$

Explicit differentiation gives

$$p(s) = \frac{1}{s^2} (\pi s \sigma'(\pi s) - \sigma(\pi s) + \sigma(\pi s)^2) E(s). \quad (25)$$

The second-order differential equation (21) can be written as a first-order system of differential equations:

$$\frac{d}{dt} \begin{pmatrix} \sigma \\ \sigma' \end{pmatrix} = \begin{pmatrix} \sigma' \\ -\frac{2}{t} \sqrt{(\sigma - t\sigma')(t\sigma' - \sigma + (\sigma')^2)} \end{pmatrix}. \quad (26)$$

This is solved as an initial-value problem starting at $t = t_0 =$ very small positive number. The value $t = 0$ has to be avoided because of the division by t in the system of equations. This is not a problem, since the boundary condition (22) provides an accurate value for $\sigma(t_0)$ (as well as $E(t_0/\pi)$). The boundary conditions for the system (26) then become

$$\begin{cases} \sigma(t_0) &= -\frac{t_0}{\pi} - \left(\frac{t_0}{\pi}\right)^2 \\ \sigma'(t_0) &= -\frac{1}{\pi} - \frac{2t_0}{\pi}. \end{cases} \quad (27)$$

To be able to compute $E(s)$ using (24), the variable

$$I(t) = \int_0^t \frac{\sigma(t')}{t'} dt' \quad (28)$$

is added to the system, as well as the equation $\frac{d}{dt} I = \frac{\sigma}{t}$. The corresponding initial value is

$$I(t_0) \approx \int_0^{t_0} \left(-\frac{1}{\pi} - \frac{t}{\pi^2}\right) dt = -\frac{t_0}{\pi} - \frac{t_0^2}{2\pi^2}. \quad (29)$$

Putting it all together, the final system is

$$\frac{d}{dt} \begin{pmatrix} \sigma \\ \sigma' \\ I \end{pmatrix} = \begin{pmatrix} \sigma' \\ -\frac{2}{t} \sqrt{(\sigma - t\sigma')(t\sigma' - \sigma + (\sigma')^2)} \\ \frac{\sigma}{t} \end{pmatrix} \quad (30)$$

with boundary condition

$$\begin{pmatrix} \sigma(t_0) \\ \sigma'(t_0) \\ I(t_0) \end{pmatrix} = \begin{pmatrix} -\frac{t_0}{\pi} - \left(\frac{t_0}{\pi}\right)^2 \\ -\frac{1}{\pi} - \frac{2t_0}{\pi} \\ -\frac{t_0}{\pi} - \frac{t_0^2}{2\pi^2} \end{pmatrix}. \quad (31)$$

This system is defined as an inline function in MATLAB:

```
desig=inline([' [y(2); -2/t*sqrt((y(1)-t*y(2))*' ...
              '(t*y(2)-y(1)+y(2)^2)); y(1)/t] ', 't', 'y');
```

Specify the integration interval and the desired output times:

```
t0=1e-12;
tn=16;
tspan=linspace(t0,tn,1000);
```

Set the initial condition:

```
y0=[-t0/pi-(t0/pi)^2; -1/pi-2*t0/pi; -t0/pi-t0^2/2/pi^2];
```

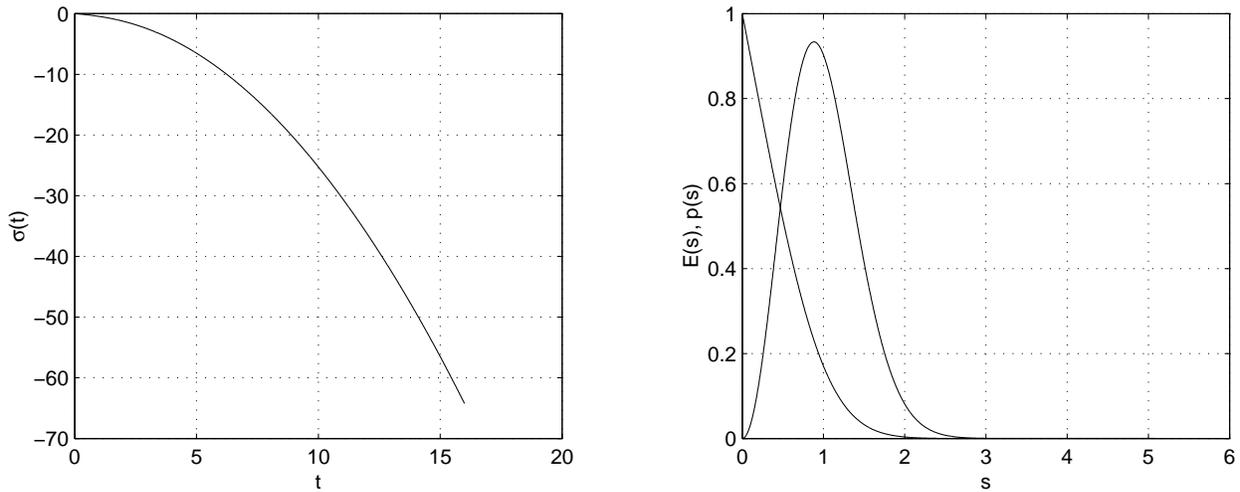


Figure 4: Painlevé V (left), $E(s)$ and $p(s)$ (right).

Finally, set the integration tolerances and call the solver:

```
opts=odeset('reltol',1e-13,'abstol',1e-14);
[t,y]=ode45(desig,tspan,y0,opts);
```

The solution components are now in the columns of y . Use these to evaluate $E(s)$ and $p(s)$:

```
s=t/pi;
E=exp(y(:,3));
p=1./s.^2.*E.*(t.*y(:,2)-y(:,1)+y(:,1).^2);
p(1)=2*s(1); % Fix due to cancellation
```

A plot of $p(s)$ can be made with the command

```
plot(s,p)
grid on
```

and it can be seen in Figure 4. Plots are also shown of $E(s)$ and $\sigma(t)$.

2.3 The Prolate Matrix

Another method to calculate the distribution of the eigenvalue spacings is to compute the eigenvalues λ_i of the operator

$$f(y) \rightarrow \int_{-1}^1 Q(x,y)f(y) dy, \quad Q(x,y) = \frac{\sin((x-y)\pi t)}{(x-y)\pi}. \quad (32)$$

Then $E(2t) = \prod_i (1 - \lambda_i)$, and $p(s)$ can be computed as before. To do this, first define the infinite symmetric Prolate matrix:

$$A_\infty = \begin{pmatrix} a_0 & a_1 & \dots \\ a_1 & a_0 & \dots \\ \vdots & \vdots & \ddots \end{pmatrix} \quad (33)$$

with $a_0 = 2w$, $a_k = (\sin 2\pi wk)/\pi k$ for $k = 1, 2, \dots$, and $0 < w < \frac{1}{2}$. A discretization of $Q(x,y)$ is achieved by setting $w = t/n$ and extracting the upper-left $n \times n$ submatrix A_n of A_∞ .

Below, the full matrix A_n is used, and all the eigenvalues are computed in n^3 time using the `eig` function. However, A_n commutes with the following symmetric tridiagonal matrix [5], and therefore has the same eigenvectors:

$$T_n = \begin{pmatrix} \alpha_1 & \beta_1 & & & & \\ \beta_1 & \alpha_2 & \beta_2 & & & \\ & \ddots & \ddots & \ddots & & \\ & & \beta_{n-2} & \alpha_{n-1} & \beta_{n-1} & \\ & & & \beta_{n-1} & \alpha_n & \end{pmatrix} \quad (34)$$

where

$$\begin{cases} \alpha_k &= \left(\frac{n+1}{2} - k\right)^2 \cos 2\pi w \\ \beta_k &= \frac{1}{2}k(n-k). \end{cases} \quad (35)$$

It is then in principle possible to use the new techniques described in [6] to compute all the eigenvalues and eigenvectors of T_n in n^2 time, and then get the eigenvalues of A_n by dot products. This is not done in this example.

The code for computing $E(s)$ is shown below. This time, $p(s)$ is evaluated by numerical differentiation since no information about the derivative of $E(s)$ is available.

```
s=0:0.01:5;
n=100;
E0=zeros(size(s));
for ii=1:length(s)
    Q=gallery('prolate',n,s(ii)/2/n);
    E0(ii)=prod(1-eig(Q));
end
p0=gradient(gradient(E0,s),s);
```

To improve the accuracy in $E(s)$, Richardson extrapolation can be used. This is done as follows, where the values are assumed to converge as $1/n^2$:

```
% ... Compute s and E using Painleve V in previous section

Es=zeros(length(t),0);
E1=zeros(size(s));
for n=20*2.^(0:3)
    for ii=1:length(s)
        Q=gallery('prolate',n,s(ii)/2/n);
        E1(ii)=prod(1-eig(Q));
    end
    Es=[Es,E1];
end

for ii=1:3
    max(abs(Es-E(:,ones(1,size(Es,2))))))
    Es=Es(:,2:end)+diff(Es,1,2)/(2^(ii+1)-1);
end
max(abs(Es-E))
```

The errors $\max_{0 \leq s \leq 5} |E_1(s) - E(s)|$ are shown in Table 1, for $n = 20, 40, 80$, and 160. The error after all extrapolations is of the same order as the “exact solution” using Painlevé V.

2.4 Riemann Zeta Zeros

It has been observed that the zeros of the Riemann zeta function along the critical line $\text{Re}(z) = \frac{1}{2}$ behave similar to the eigenvalues of random matrices in the GUE. Here, the distribution of the scaled spacings of the

N	Error 0	Error 1	Error 2	Error 3
20	0.2244			
40	0.0561	0.7701		
80	0.0140	0.0483	0.5486	
160	0.0035	0.0032	0.0323	2.2673
	$\cdot 10^{-3}$	$\cdot 10^{-7}$	$\cdot 10^{-8}$	$\cdot 10^{-11}$

Table 1: Difference between Prolate solution $E_1(s)$ and Painlevé V solution $E(s)$ after 0, 1, 2, and 3 Richardson extrapolations.

zeros is compared to the corresponding distribution for eigenvalues computed using the Painlevé V equation from the previous chapters.

Define the n th zero $\gamma_n = n^{\text{th}}$ as

$$\zeta\left(\frac{1}{2} + i\gamma_n\right) = 0, \quad 0 < \gamma_1 < \gamma_2 < \dots \quad (36)$$

Compute a normalized spacing:

$$\tilde{\gamma}_n = \frac{\gamma_n}{\text{av spacing near } \gamma_n} = \gamma_n \cdot \left[\frac{\log \gamma_n / 2\pi}{2\pi} \right]. \quad (37)$$

Zeros of the Riemann zeta function can be downloaded from [7]. Assuming that the MATLAB variable `gamma` contains the zeros, and the variable `offset` the offset, these two lines compute the consecutive spacings $\tilde{\gamma}_{n+1} - \tilde{\gamma}_n$ and plot the histogram:

```
delta=diff(gamma)/2/pi.*log((gamma(1:end-1)+offset)/2/pi);
histdistr(delta,0:0.05:5.0);
```

The result can be found in Figure 5, along with the Painlevé V distribution. The curves are indeed in good agreement, although the number of samples here is a little to low to get a perfect match.

References

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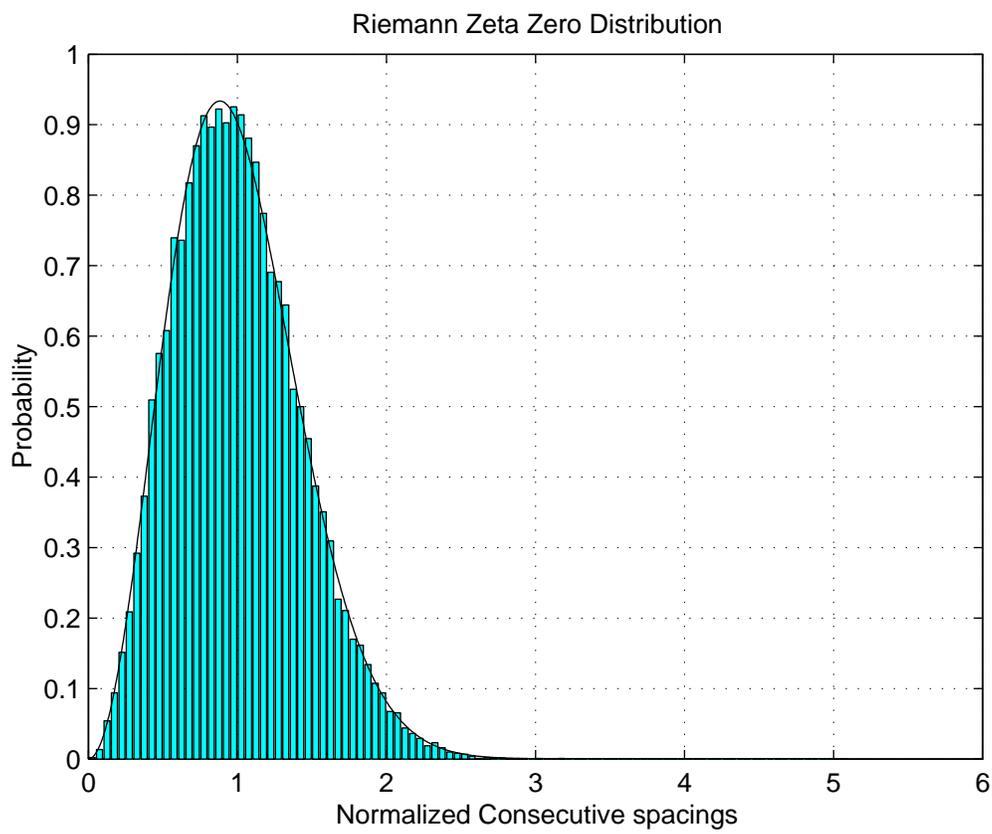


Figure 5: Probability distribution of consecutive spacings of Riemann zeta zeros (30,000 zeros, $n \approx 10^{12}, 10^{21}, 10^{22}$)