Numerical Methods for Random Matrices

MIT 18.095 IAP Lecture Series

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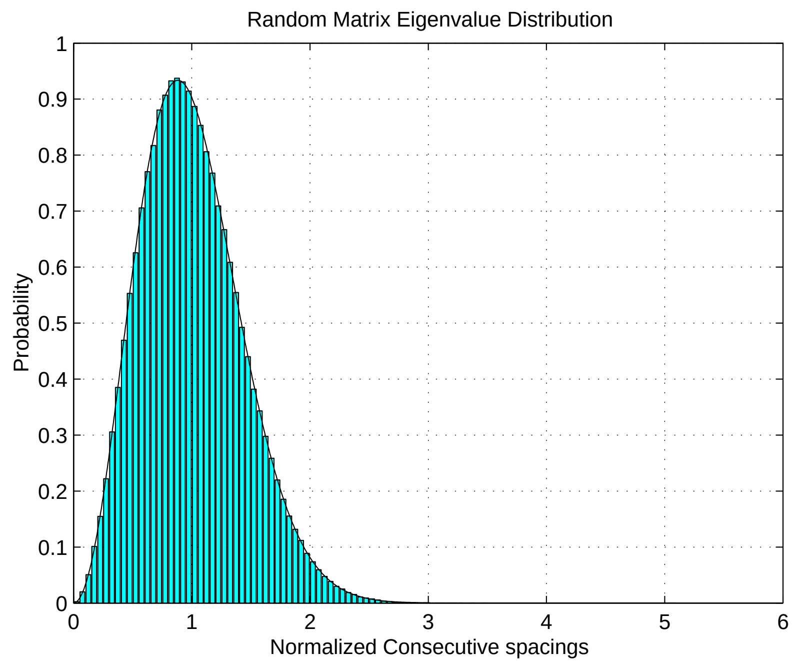
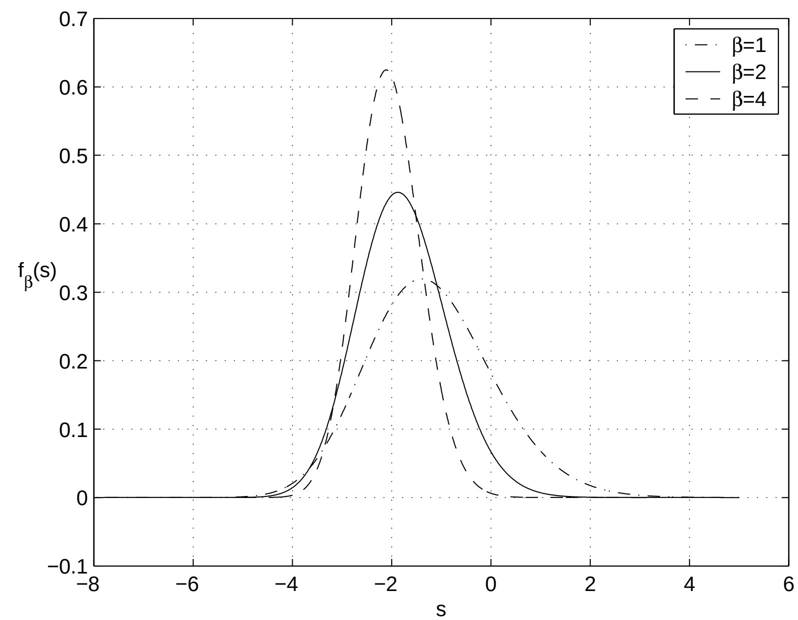




Topics

- **Histogramming random matrix eigenvalues**
  - Tridiagonal model
  - Histogramming with Sturm sequences
- Largest eigenvalue distributions
  - Simulation and approximations
  - Numerical solution of Painlevé II
  - Distributions for general β
- Eigenvalue spacing distributions
  - Numerical solution of Painlevé V
  - Eigenvalues of the Prolate matrix
  - Spacing of Riemann Zeta zeros

The Gaussian Unitary Ensemble

- The *Gaussian Unitary Ensemble*: Set of $n \times n$ random Hermitian matrices, with independent zero-mean Gaussian elements
- Diagonal elements x_{jj}, upper triangular elements $x_{jk} = u_{jk} + iv_{jk}$:

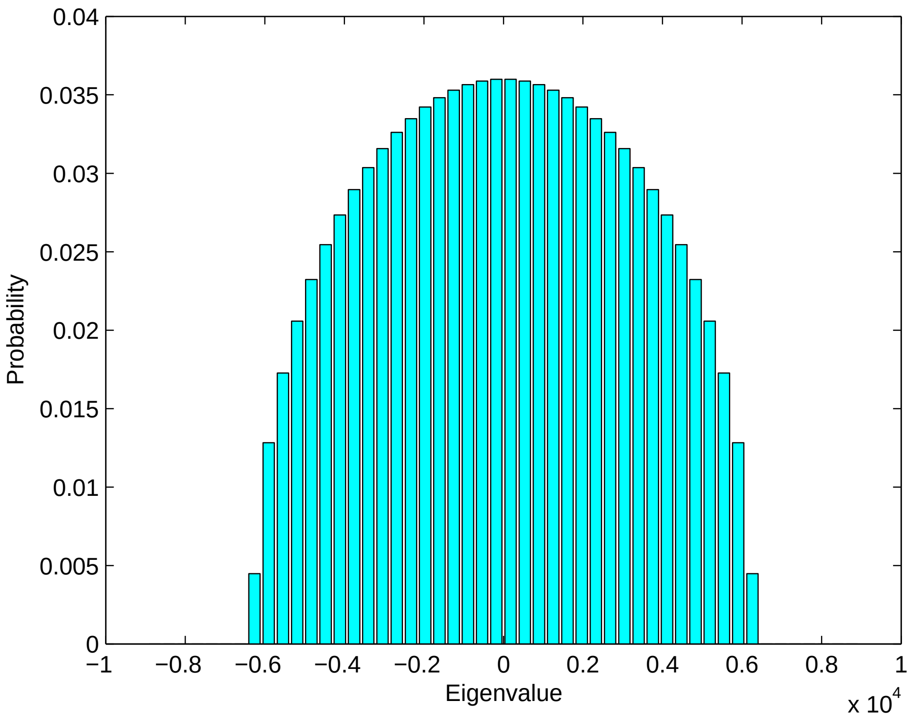
$$\begin{cases} \mathrm{Var}(x_{jj}) = 1, & 1 \le j \le n \\ \mathrm{Var}(u_{jk}) = \mathrm{Var}(v_{jk}) = \frac{1}{2}, & 1 \le j < k \le n \end{cases}$$

- In MATLAB:

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

The Semi Circle Law

- The probability distribution of the eigenvalues of matrices in the GUE is a semi-circle as $n \to \infty$
- Create histogram for finite n by generating random matrices and solving for all eigenvalues
- Requires $O(n^2)$ memory
  $\Longrightarrow n < 10^4$ for most computers
- Requires $O(n^3)$ work per sample
  $\Longrightarrow$ Days to get a nice histogram



Faster Method – Similar Tridiagonal Matrix

- Real, symmetric, tridiagonal matrix with same eigenvalues as the GUE for $\beta = 2$ [Dumitriu, Edelman]:

$$H_\beta \sim \frac{1}{\sqrt{2}} \begin{pmatrix} N(0,2) & \chi_{(n-1)\beta} & & & \\ \chi_{(n-1)\beta} & N(0,2) & \chi_{(n-2)\beta} & & \\ & \ddots & \ddots & \ddots & \\ & & \chi_{2\beta} & N(0,2) & \chi_\beta \\ & & & \chi_\beta & N(0,2) \end{pmatrix}$$

- All eigenvalues in $O(n)$ memory and $O(n^2)$ time (e.g. the QR algorithm)
- Can easily handle $n \approx 10^6$ on a single computer

Method of Bisection

- The *Method of Bisection* finds eigenvalues in an interval $[\lambda_{\min}, \lambda_{\max})$ by considering roots of $p(x) = \det(A - xI)$
- The # of negative eigenvalues of A = The # of sign changes in the *Sturm sequence* $1,\ \det(A^{(1)}),\ \det(A^{(2)}), \ldots,\ \det(A^{(n)})$
- Shift A to get number of eigenvalues in $(-\infty, \lambda_{\max})$ and twice for $[\lambda_{\min}, \lambda_{\max})$
- Three-term recurrence for the determinants:

$$\det(A^{(k)}) = a_k \det(A^{(k-1)}) - b_{k-1}^2 \det(A^{(k-2)})$$

- With shift xI and $p^{(k)}(x) = \det(A^{(k)} - xI)$:

$$p^{(k)}(x) = (a_k - x)p^{(k-1)}(x) - b_{k-1}^2 p^{(k-2)}(x)$$

Histogramming by Bisection

- Idea [Edelman]: A histogram contains less information than all eigenvalues
- Use the method of bisection: Choose m histogram “boxes” σ_i, compute Sturm sequences to count # eigenvalues $< \sigma_i$
- Complexity:
  - Work $O(mn)$ instead of $O(n^2)$
  - Memory $O(1)$ instead of $O(n)$ (if matrix generated on-the-fly)
- Can compute histograms for $n \approx 10^{11}$ on a single computer

Topics

- Histogramming random matrix eigenvalues
  - Tridiagonal model
  - Histogramming with Sturm sequences
- **Largest eigenvalue distributions**
  - Simulation and approximations
  - Numerical solution of Painlevé II
  - Distributions for general β
- Eigenvalue spacing distributions
  - Numerical solution of Painlevé V
  - Eigenvalues of the Prolate matrix
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Largest Eigenvalue Distributions

- Consider again the GUE, but the distribution of the largest eigenvalue
- Rescale around the largest eigenvalue:

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

- Use tridiagonal matrix for $O(n)$ storage and $O(n)$ computational work for largest eigenvalue (using Arnoldi iterations or method of bisection)

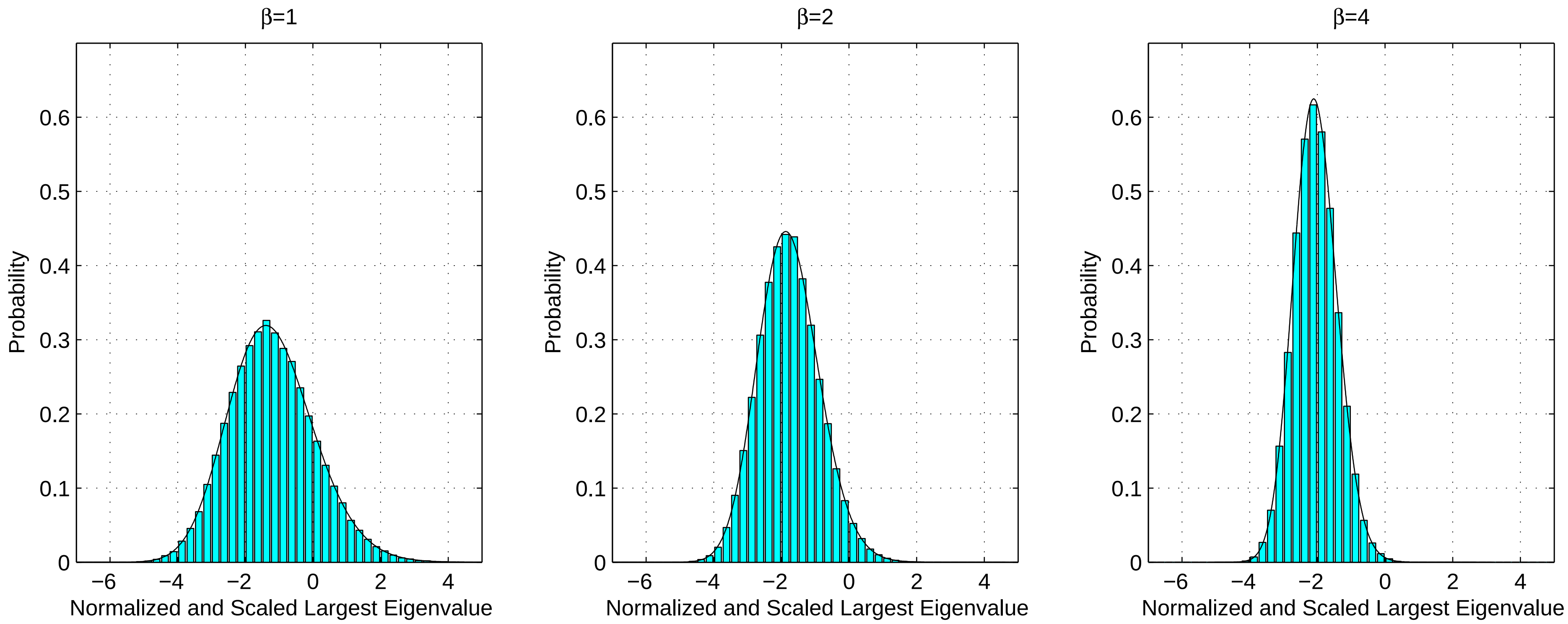
Faster Method – Sparse Eigenvector

- The eigenvector corresponding to the largest eigenvalue is very close to zero in most components
- Therefore, when computing the largest eigenvalue the matrix is well approximated by the upper-left n_{cutoff} by n_{cutoff} matrix, where

$$n_{\text{cutoff}} \approx 10n^{\frac{1}{3}}$$

- $\Longrightarrow$ very large n can be used ($> 10^{12}$)
- Also, $\chi_n^2 \approx n + \text{Gaussian}$ for large n

Largest Eigenvalue Distributions



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

Differential Equation for Distributions

- Probability distribution $f_2(s)$ is given by [Tracy, Widom]:

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

where

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

and $q(s)$ satisfies the Painlevé II differential equation:

$$q'' = sq + 2q^3$$

with the boundary condition

$$q(s) \sim \mathrm{Ai}(s), \qquad \text{as } s \to \infty$$

Distributions for $\beta = 1$ and $\beta = 4$

- The distributions for $\beta = 1$ and $\beta = 4$ can be computed from $F_2(s)$ as

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

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

Numerical Solution as Initial Value Problem

- Write as 1^{st} order system:

$$\frac{d}{ds}\begin{pmatrix} q \\ q' \end{pmatrix} = \begin{pmatrix} q' \\ sq + 2q^3 \end{pmatrix}$$

- Solve as initial-value problem starting at $s = s_0 =$ large positive number

- Initial values (boundary conditions):

$$\begin{cases} q(s_0) & = & \mathrm{Ai}(s_0) \\ q'(s_0) & = & \mathrm{Ai}'(s_0) \end{cases}$$

- Explicit ODE solver (RK4)

Post-processing to Obtain $f_\beta(s)$

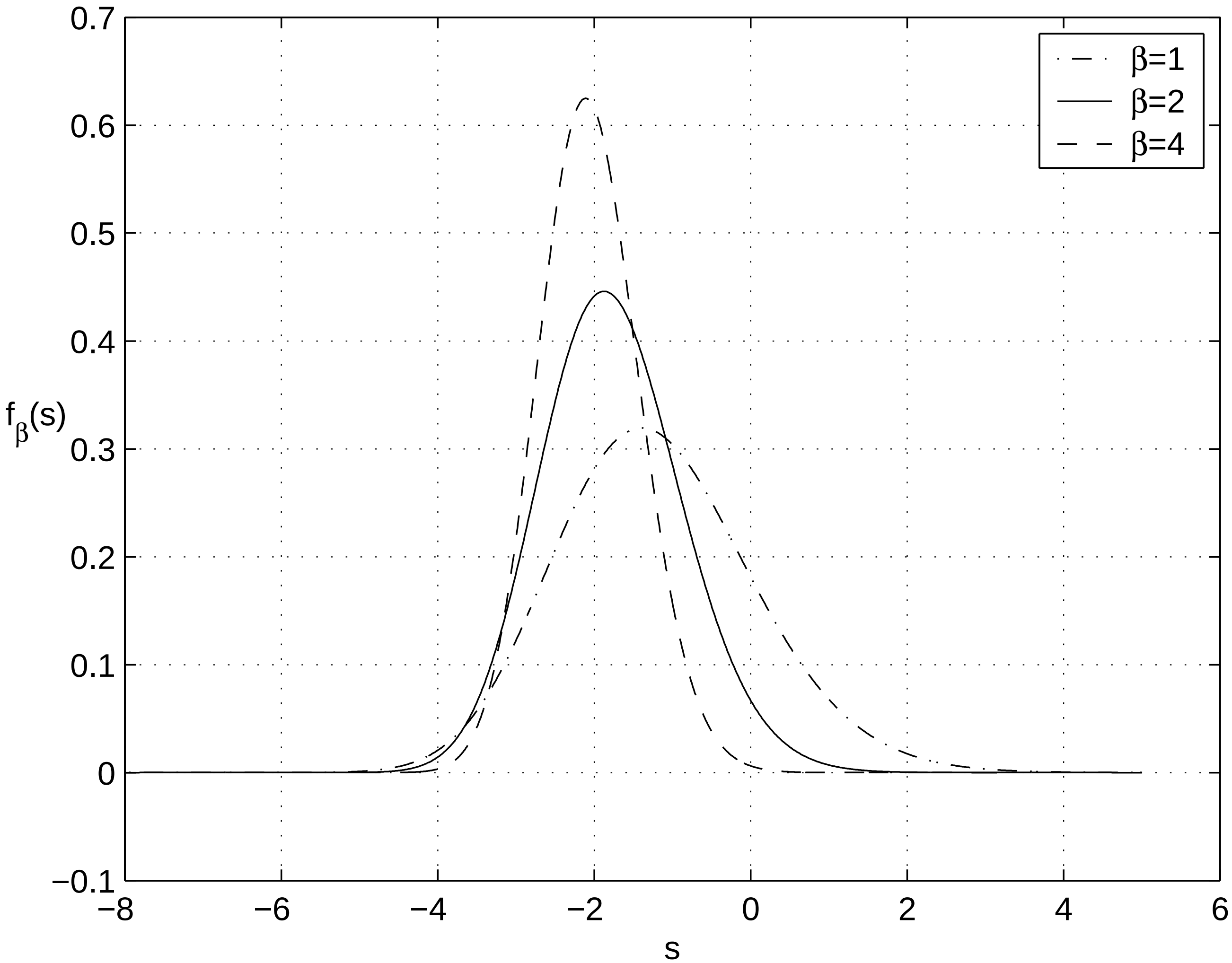
- $F_2(s) = \exp\left(-\int_s^\infty (x-s)q(x)^2\,dx\right)$ could be computed using high-order quadrature
- Convenient trick: Set $I(s) = \int_s^\infty (x-s)q(x)^2\,dx$ and differentiate:

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

  Add these equations and the variables $I(s), I'(s)$ to ODE system, and let the solver do the integration

- Also, add variable $J(s) = \int_s^\infty q(x)\,dx$ and equation $J'(s) = q(s)$ for computation of $F_1(s)$ and $F_4(s)$
- $f_\beta(s) = \frac{d}{ds}F_\beta(s)$ using numerical differentiation

Tracy-Widom Distributions using Painlevé II



The probability distributions $f_1(s)$, $f_2(s)$, and $f_4(s)$, using Painlevé II

Numerical Solution as Boundary Value Problem

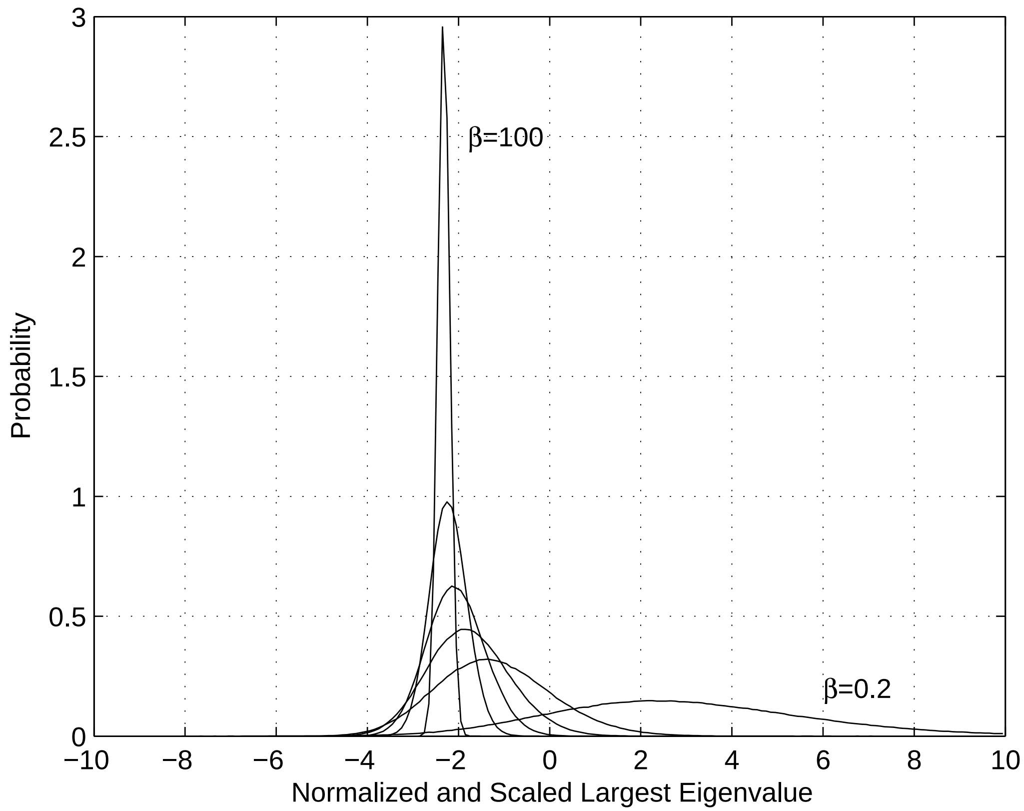
- Initial value problem sensitive to errors in $q(s_0)$ and $q'(s_0)$
- More robust and higher accuracy by solving as a BVP
- Instead of condition on $q'(s_0)$, use left end asymptotic [Dieng]:

$$q(-t/2) \approx \frac{\sqrt{t}}{2}\left(1 - \frac{1}{t^3} - \frac{73}{2t^6} - \frac{10657}{2t^9} - \frac{1391227}{8t^{12}}\right)$$

- Discretize Painlevé II $q'' = sq + 2q^3$ using centered finite differences
- Solve discrete system $R(Q) = 0$ by Newton's method (the Jacobian $\partial R/\partial Q$ is tridiagonal)
- Straight line initial guess for Newton iterations gives convergence to full accuracy in < 10 iterations

Distributions for general β

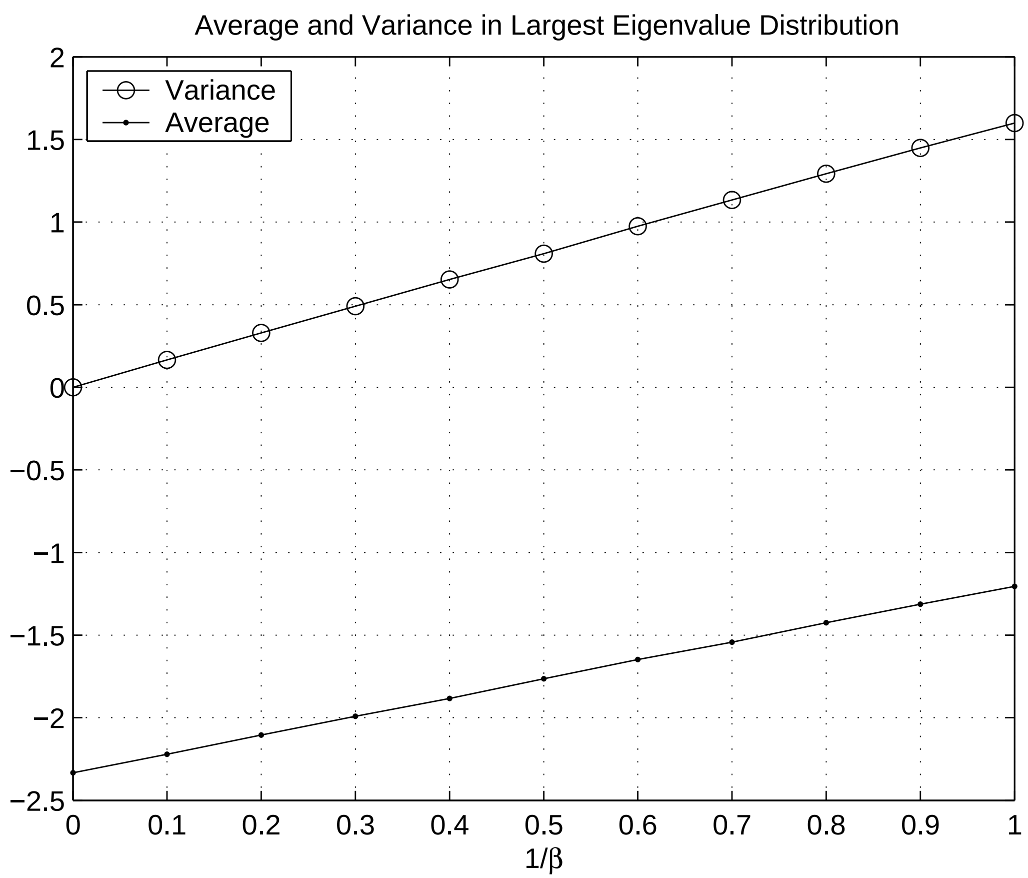
- Open question: Is there a differential equation for any β?
- Tridiagonal model allows us to experiment numerically:



Distributions of scaled largest eigenvalue, $\beta = 100, 10, 4, 2, 1, 0.2$

β-Dependence of Mean and Variance

- For large β, mean and variance are close to linear functions of $1/\beta$:



Average and variance of probability distribution as a function of $1/\beta$

Convection-Diffusion Approximation

- Average and variance linear in $t = 1/\beta$ suggest constant-coefficient convection-diffusion approximation:

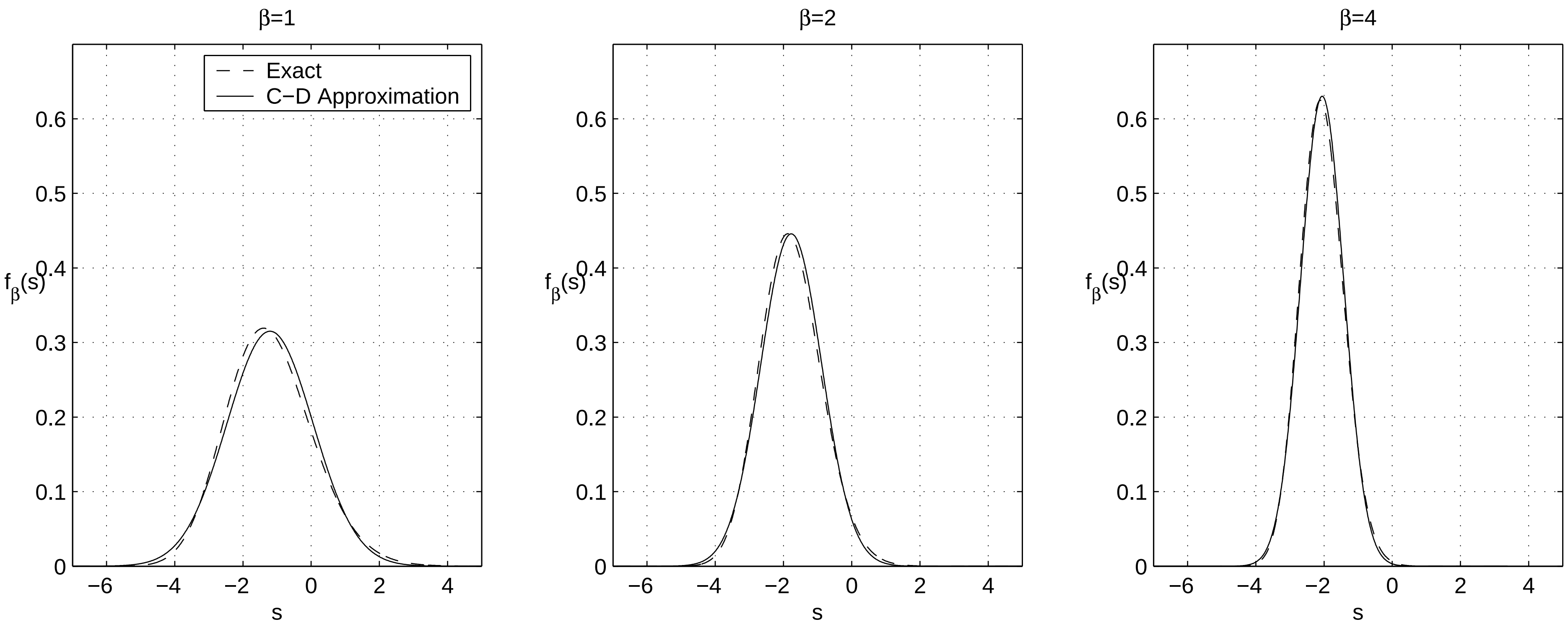
$$\frac{df}{dt} = \frac{C_2}{2}\frac{d^2 f}{ds^2} - C_1 \frac{df}{ds}$$
$$f(0, s) = \delta(s - \mathrm{AiZ}_1)$$

where C_1, C_2 are the slopes of the average and the variance.

- Solution:

$$f(t, s) = \frac{1}{\sqrt{2\pi C_2 t}} \exp\left(-\frac{(x - \mathrm{AiZ}_1 - C_1 t)^2}{2C_2 t}\right)$$

Convection-Diffusion Approximation



Approximate distributions for $\beta = 1, 2, 4$ using the convection-diffusion model.

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- **Eigenvalue spacing distributions**
  - Numerical solution of Painlevé V
  - Eigenvalues of the Prolate matrix
  - Spacing of Riemann Zeta zeros

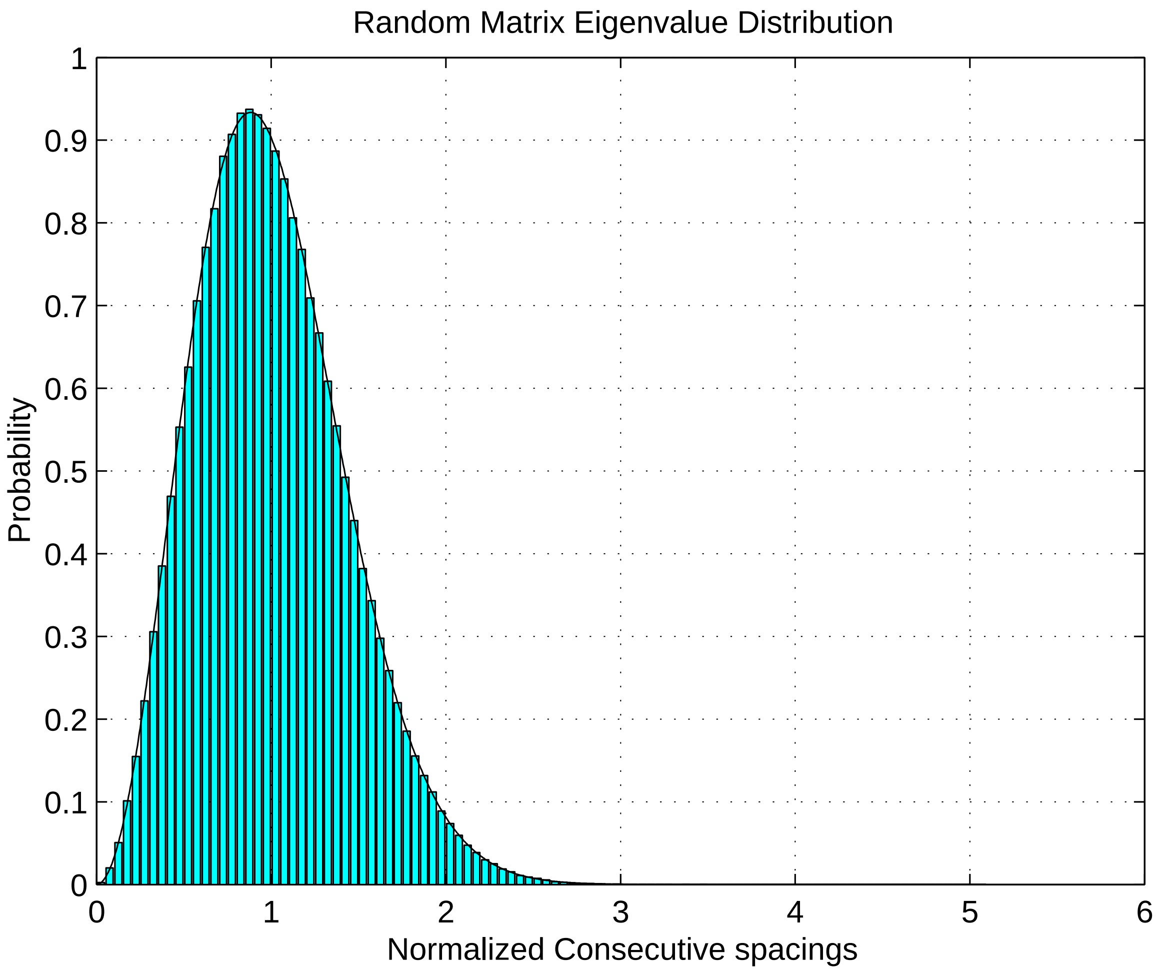
Eigenvalue Spacing Distribution

- Consider again the GUE, but the spacing of consecutive eigenvalues
- Normalized spacing of eigenvalues $\lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_n$:

$$\delta'_k = \frac{\lambda_{k+1} - \lambda_k}{4\pi} \sqrt{8n - \lambda_k^2}, \qquad k \approx n/2$$

- Need to compute all eigenvalues – use tridiagonal model for $O(n)$ storage but $O(n^2)$ work

Eigenvalue Spacing Distribution



Probability distribution of consecutive spacings of random matrix eigenvalues

(1000 repetitions, $n = 1000$)

Differential Equation for Distributions

- Probability distribution $p(s)$ is given by

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

where

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

and $\sigma(t)$ satisfies the Painlevé V differential equation:

$$(t\sigma'')^2 + 4(t\sigma' - \sigma)\left(t\sigma' - \sigma + (\sigma')^2\right) = 0$$

with the boundary condition

$$\sigma(t) \approx -\frac{t}{\pi} - \left(\frac{t}{\pi}\right)^2, \qquad \text{as } t \to 0^+$$

Numerical Solution as Initial Value Problem

- Write as 1^{st} order system:

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

- Solve as initial-value problem starting at $t = t_0 =$ small positive number
- Initial values (boundary conditions):

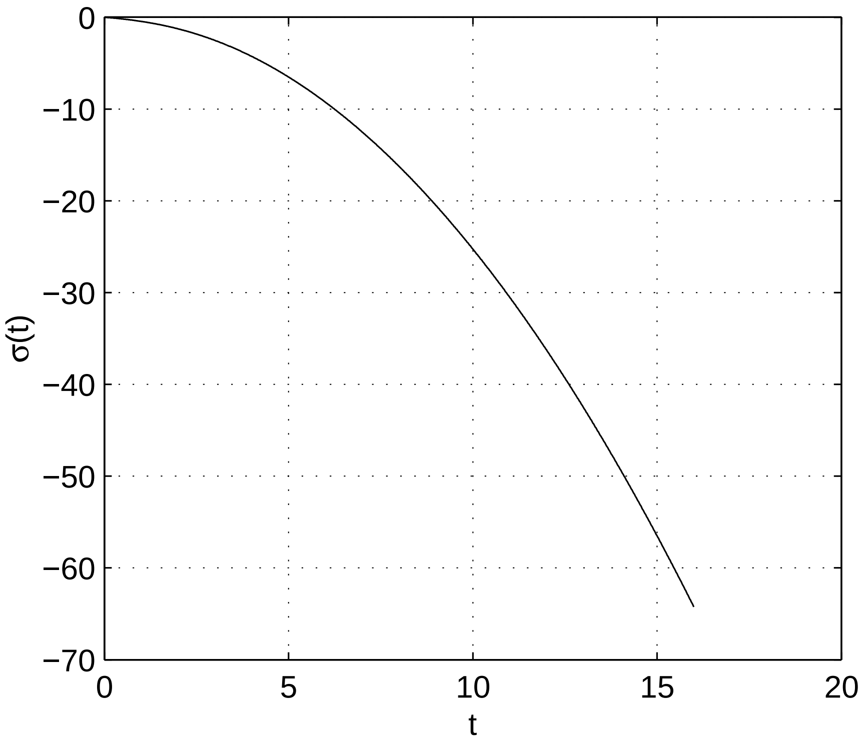
$$\begin{cases} \sigma(t_0) & = & -\frac{t_0}{\pi} - \left(\frac{t_0}{\pi}\right)^2 \\ \sigma'(t_0) & = & -\frac{1}{\pi} - \frac{2t_0}{\pi} \end{cases}$$

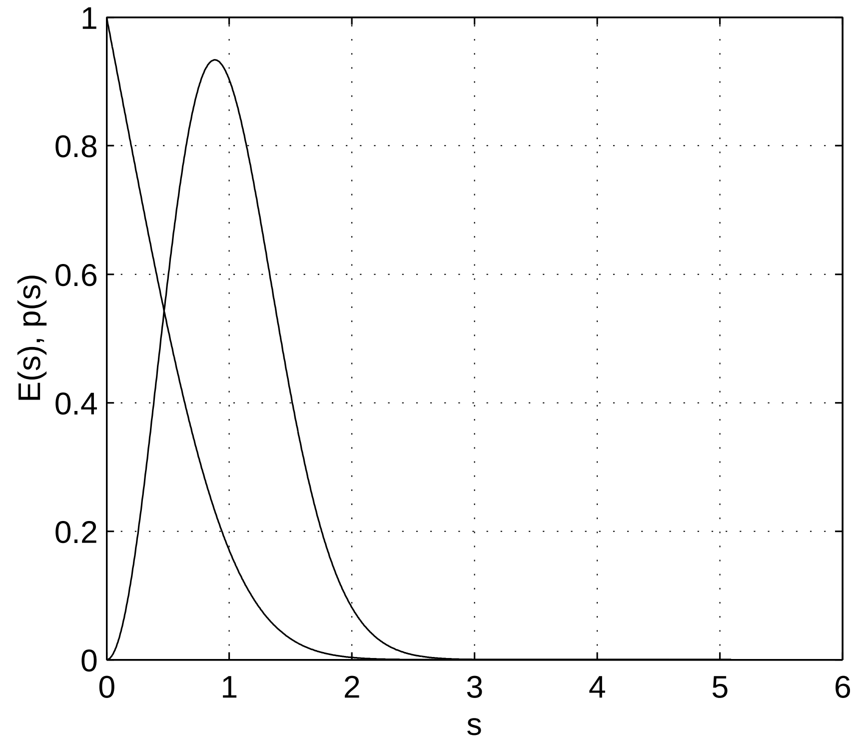
- Explicit ODE solver (RK4)

Post-processing to Obtain $p(s)$

- $E(s) = \exp\left(\int_0^{\pi s} \frac{\sigma(t)}{t} dt\right)$ could be computed using high-order quadrature
- Convenient trick: Add variable $I(t)$ and equation $\frac{d}{dt}I = \frac{\sigma}{t}$ to ODE system, and let the solver do the integration
- $p(s) = \frac{d^2}{ds^2}E(s)$ using numerical differentiation

Spacing Distributions using Painlevé V





Painlevé V (left), $E(s)$ and $p(s)$ (right)

The Prolate Matrix

- $E(2t) = \prod_i (1 - \lambda_i)$ where λ_i are eigenvalues of the operator

$$f(y) \to \int_{-1}^{1} Q(x,y) f(y)\, dy, \qquad Q(x,y) = \frac{\sin((x-y)\pi t)}{(x-y)\pi}$$

- Infinite symmetric Prolate matrix:

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

with $a_0 = 2w$, $a_k = (\sin 2\pi wk)/\pi k$ for $k = 1, 2, \ldots$, and $0 < w < \frac{1}{2}$.

- Set $w = t/n$. The upper-left $n \times n$ submatrix A_n is then a discretization of $Q(x,y)$.

Improving Accuracy by Richardson Extrapolation

- Difference between Prolate solution $E(s)$ and Painlevé V solution $E_0(s)$:

$$\max_{0 \leq s \leq 5} |E(s) - E_0(s)|$$

after 0, 1, 2, and 3 Richardson extrapolations:

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	2.2619
	$\cdot 10^{-3}$	$\cdot 10^{-7}$	$\cdot 10^{-8}$	$\cdot 10^{-11}$

Riemann Zeta Zeros

- Consider the zeros of the Riemann Zeta function along the *critical line*

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

where $\gamma_n = n^{\text{th}}$ zero on the line

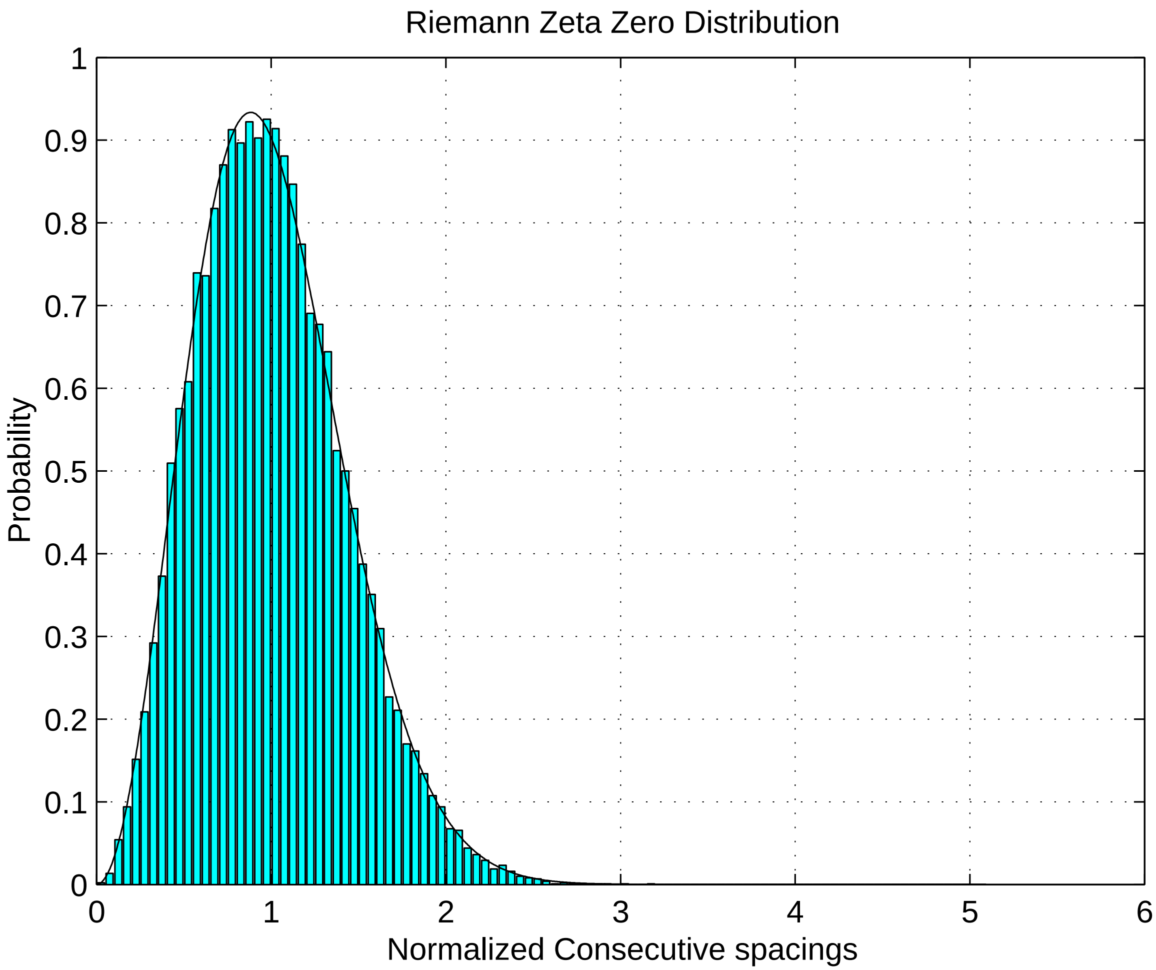
- Numerical values available for γ_{N+n}, $N = 0, 10^6, 10^{12}, 10^{18}$, $n = 1, 2, \dots, 10^5$ [Odlyzko]

- Normalize the zeros:

$$\tilde{\gamma}_n = \frac{\gamma_n}{\text{avg spacing near } \gamma_n} = \gamma_n \cdot \left[\frac{\log \gamma_n / 2\pi}{2\pi}\right]$$

- Histogram consecutive spacings $\tilde{\gamma}_{n+1} - \tilde{\gamma}_n$ and compare with eigenvalue spacing for the GUE

Riemann Zeta Zeros and Eigenvalue Spacings



Probability distribution of consecutive spacings of Riemann Zeta zeros

($30,000$ zeros, $n \approx 10^{12}, 10^{21}, 10^{22}$)