Universality for the Toda algorithm to compute the eigenvalues of a random matrix

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This is joint work with

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A few years ago, Christian Pfrang, Govind Menon and PD [PDM12], initiated a statistical study of the performance of various standard algorithms to compute the eigenvalues of random real symmetric matrices H. In each case, an initial matrix H_0 is diagonalized either by

a sequence of isospectral iterates H_m

$$H_0 \to H_1 \to H_2 \to \cdots \to H_m \to \cdots$$

or by

an isospectral flow

$$t \mapsto H(t) \quad \text{with} \quad H(t=0) = H_0.$$

In the discrete case, as $m \to \infty$,

H_m converges to a diagonal matrix.

Given $\epsilon > 0$, it follows that for some (first) time m, the stopping time (or halting time), the off-diagonal entries of H_m are $O(\epsilon)$, and hence the diagonal entries of H_m give the eigenvalues of H_0 to $O(\epsilon)$. The situation is similar for continuous algorithms $t \mapsto H(t)$ as $t \to \infty$.

The main finding in [PDM12] was that, surprisingly,

$$\text{the } \underline{\text{fluctuations}} \text{ in the stopping times were } \underline{\text{universal}} \tag{1}$$

independent of the ensemble considered for the matrices H. More precisely,

- for $N \times N$ real symmetric matrices H,
- chosen from an ensemble $\mathcal{E}$, and
- for a given algorithm $\mathcal{A}$, and
- a desired accuracy ϵ,

let

$$T(H) = T_{\epsilon,N,\mathcal{A},\mathcal{E}}(H) \tag{2}$$

be the stopping time for the algorithm $\mathcal{A}$ applied to the $N \times N$ matrix H chosen from the ensemble $\mathcal{E}$, to achieve an accuracy ϵ.

Let $\tilde{T}(H) = \tilde{T}_{\epsilon,N,\mathcal{A},\mathcal{E}}(H)$ be the normalized stopping time

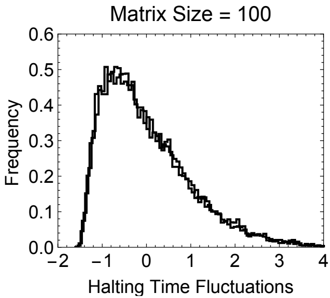
$$\tilde{T}_{\epsilon,N,\mathcal{A},\mathcal{E}}(H) = \frac{T_{\epsilon,N,\mathcal{A},\mathcal{E}}(H) - \langle T_{\epsilon,N,\mathcal{A},\mathcal{E}} \rangle}{\sigma_{\epsilon,N,\mathcal{A},\mathcal{E}}} \tag{3}$$

where $\langle T_{\epsilon,N,\mathcal{A},\mathcal{E}} \rangle$ is the sample average and $\sigma^2_{\epsilon,N,\mathcal{A},\mathcal{E}} = \langle (T_{\epsilon,N,\mathcal{A},\mathcal{E}} - \langle T_{\epsilon,N,\mathcal{A},\mathcal{E}} \rangle)^2 \rangle$ is the sample variance, taken over a large number (5,000-15,000) of samples of matrices H chosen from $\mathcal{E}$. Then for a given algorithm $\mathcal{A}$, and ϵ and N in a suitable scaling region,

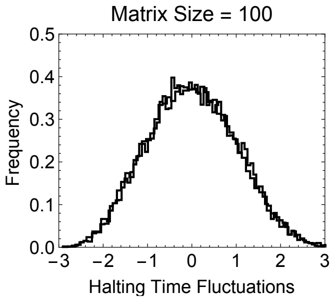
$$\text{the histogram for } \tilde{T}_{\epsilon,N,\mathcal{A},\mathcal{E}}(H) \text{ is independent of } \mathcal{E}. \tag{4}$$

In general, the histogram will depend on $\mathcal{A}$, but for a given $\mathcal{A}$ and ϵ and N in the scaling region, the histogram is independent of $\mathcal{E}$.

Here are two examples, the first is for the QR algorithm, which is one of the most successful of all numerical algorithms, and lies at the heart of most eigenvalue software packages, and the second is for the Toda algorithm.



(a)



(b)

Figure: Universality for $\tilde{T}_{\epsilon,N,\mathcal{A},\mathcal{E}}$ when (a) $\mathcal{A}$ is the QR eigenvalue algorithm and when (b) $\mathcal{A}$ is the Toda algorithm. Panel (a) displays the overlay of two histograms for $\tilde{T}_{\epsilon,N,\mathcal{A},\mathcal{E}}$ in the case of QR, one for each of the two ensembles $\mathcal{E} = \text{BE}$, consisting of iid mean-zero Bernoulli random variables and $\mathcal{E} = \text{GOE}$, consisting of iid mean-zero normal random variables. Here $\epsilon = 10^{-10}$ and $N = 100$. Panel (b) displays the overlay of two histograms for $\tilde{T}_{\epsilon,N,\mathcal{A},\mathcal{E}}$ in the case of the Toda algorithm, and again $\mathcal{E} = \text{BE}$ or GOE. And here $\epsilon = 10^{-8}$ and $N = 100$.

The stopping times, or halting times, for a given algorithm can be chosen in various ways, depending on which aspects of the given algorithm one wants to investigate. In the above figures, the stopping times takes into account the phenomenon known as deflation. In this paper, we will consider a different stopping time (see $T^{(1)}(H)$ below) which measures the time for the computation of the largest eigenvalue of a given matrix H.

Subsequent to [PDM12], Govind Menon, Sheehan Olver, Tom Trogdon and PD [DMOT14], raised the question of whether the universality results in the study [PDM12] were limited to eigenvalue algorithms, or whether they were present more generally in numerical computation. And indeed the authors in [DMOT14] found similar universality results for a wide variety of numerical algorithms, including

- more general eigenvalue algorithms such as the Jacobi eigenvalue algorithm, and also algorithms for Hermitian ensembles,
- the conjugate gradient and GMRES algorithms to solve linear $N \times N$ systems $Hx = b$,
- an iterative algorithm to solve the Dirichlet problem $\Delta u = 0$ on a random star-shaped region $\Omega \subset \mathbb{R}^2$ with random boundary data f on $\partial\Omega$, and
- a genetic algorithm to compute the equilibrium measure for orthogonal polynomials on the line.

An example from [DMOT14] is the solution of the linear system $Hx = b$ using the conjugate gradient algorithm where H is chosen randomly from an ensemble $\mathcal{E}$ of positive definite matrices, and b has iid components. The algorithm is iterative, $b \to x_0 \to x_1 \to \cdots \to x_m \to \cdots$ and halts, for a given ϵ, when

$$\|Hx_m - b\| \leq \epsilon. \tag{5}$$

The smallest value m for which (5) holds is the stopping time $h = h_{\epsilon,N,\mathcal{E}}(H, b)$ for the algorithm.

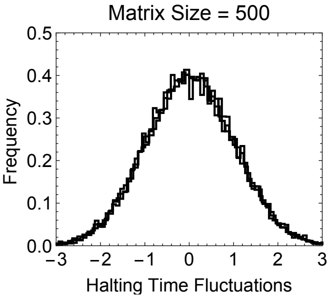


Figure: Universality in the halting time for the conjugate gradient algorithm. This plot shows three histograms of $\tilde{h}_{\epsilon,N,\mathrm{CG}}(H,b) = \dfrac{h_{\epsilon,N,\mathrm{CG}}(H,b) - \langle h_{\epsilon,N,\mathrm{CG}} \rangle}{\sigma_{\epsilon,N,\mathrm{CG}}}$ corresponding to different ensembles. Here $\epsilon = 10^{-14}$, $N = 500$, b has iid entries, uniform on $[-1,1]$, and $H = ZZ^*$ where Z is $N \times (N + \lfloor \sqrt{N} \rfloor)$ with standard normal (real and complex) or ± 1 Bernoulli entries. See [DMOT14] for more details on these computations.

The above Figure, taken from [DMOT14], displays universality in the halting time for the conjugate gradient algorithm for various ensembles for H and b.

Note that all the algorithms considered above, except for the genetic algorithm, have the character of deterministic dynamical systems with random initial data. On the other hand, for the genetic algorithm, not only is the initial data random, but the algorithm itself is stochastic.

In [DMOT14] the authors also considered recent laboratory experiments of Bakhtin and Correll [BC12] in which participants were required to make a sequence of decisions comparing geometrical properties of figures projected on a screen. Bakhtin and Correll recorded the decision times τ and the plots of the histograms for the normalized times $\tilde{\tau}$ for each participant, strongly suggest universality in the decision process. Furthermore, using a Curie–Weiss spin model, Bakhtin and Correll derive an explicit formula

$$\tilde{f}_{BC}(x) = \sqrt{\frac{2}{\pi}} \exp\left(-\frac{1}{2}\mathrm{e}^{-2x} - x\right) \tag{6}$$

for the histogram for the decision process.

It is an interesting fact, observed recently by Sagun, LeCun and Trogdon [STL15], that the fluctuations of search times on `Google` for randomly chosen English and Turkish words, in particular, also appear to follow the law f_{BC}, see Figure 3.

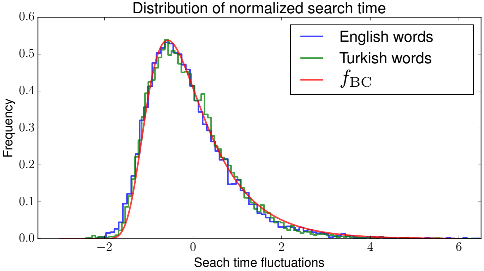


Figure: Histograms of the normalized `Google` search times obtained for English and Turkish words obtained in [STL15]. The solid curve is the normalized distribution f_{BC} of Bakhtin and Correll for the decision times in [BC12].

The above calculations and experiments suggest strongly that calculation in the presence of random data in a wide variety of situations obeys two-component universality, that is, once the mean and variance are known, the remaining statistics are universal.

So far, however, all the evidence has been numerical and experimental. As a first step towards understanding and proving universality rigorously for all the above algorithms, PD & Trogdon [DT16] have recently proved universality (rigorously) for the Toda algorithm . My goal in this talk is to describe what is involved in the proof.

The outline of the talk is as follows:

1. The Toda algorithm
2. Statement of results
3. Description of ensembles $\mathcal{E}$
4. Numerical comparisons
5. Estimates from random matrix theory
6. Sketch of the proof of Theorem 2
7. Final comment

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The Toda algorithm

The Toda flow on $N \times N$ real symmetric or Hermitian matrices X is given by

$$\dot{X} = [X, B(X)], \quad B(X) = X_- - (X_-)^*, \quad X(0) = H = H^*, \tag{7}$$

where X_- is the strictly lower-triangular part of X and $[A, B]$ is the standard matrix commutator (if Y is real $Y^* = Y^T$). It is well known that this flow is (global and) isopectral

$$\operatorname{spec} X(t) = \operatorname{spec} X(0) = \operatorname{spec} H$$

and as $t \to \infty$, $X(t)$ converges to a diagonal matrix

$$X_\infty = \operatorname{diag}(\lambda_N, \ldots, \lambda_1).$$

Necessarily, the λ_i's are the eigenvalues of $X(0) = H$. Moreover, for generic H , the eigenvalues emerge ordered on the diagonal

$$\lambda_N > \lambda_{N-1} > \cdots > \lambda_1. \tag{8}$$

The Toda algorithm

The classical Toda algorithm involves running (7) with $X(0) = H$, with stopping time T such that

$$\sum_{1 \le i < j \le N} |X_{ij}(T)|^2 < \epsilon^2. \tag{9}$$

Then, as noted above, $\mathrm{diag}(X(T))$ gives the eigenvalues of H to $O(\epsilon)$. The statistical analysis of T is a very challenging problem and raises issues in random matrix theory which are still far from being resolved (see Final Comments). Here we will consider (see [DT16]) the stopping time $T^{(1)}$ for which

$$E(T^{(1)}) < \epsilon^2 \tag{10}$$

where

$$E(t) = \sum_{n=2}^{N} |X_{1n}(t)|^2. \tag{11}$$

By perturbation theory

$$|X_{11}(T^{(1)}) - \lambda_j| < \epsilon$$

for some eigenvalue λ_j of H.

Generically (compare with (8)), $\lambda_j = \lambda_N$, the largest eigenvalue of H, and so with high probability as $N \to \infty$, $T^{(1)}$ controls the computation of the largest eigenvalue of H, a problem of interest in its own right. Even though the analysis of $T^{(1)}$ is simpler than the analysis of T, it depends, as we will see, in a crucial way on recent results from random matrix theory that are at the forefront of current knowledge. As before, in order to emphasize the dependence of $T^{(1)}$ on the parameters of the problem we write

$$T^{(1)} = T^{(1)}(H) = T^{(1)}_{\epsilon,N,\mathcal{A},\mathcal{E}}(H).$$

The Toda algorithm

The history of the Toda algorithm is as follows. The Toda Lattice was introduced by M. Toda in 1967 [Tod67] and describes the motion of N classical particles x_i, $i = 1, \ldots, N$, on the line under the Hamiltonian

$$H_{\text{Toda}}(x, y) = \frac{1}{2} \sum_{i=1}^{N} y_i^2 + \frac{1}{2} \sum_{i=1}^{N} e^{x_i - x_{i+1}}.$$

In 1974, Flaschka [Fla74] (see also [Man75]) showed that Hamilton's equations

$$\dot{x} = \frac{\partial H_{\text{Toda}}}{\partial y}, \quad \dot{y} = -\frac{\partial H_{\text{Toda}}}{\partial x},$$

can be written in Lax pair form (7) where X is tridiagonal

$$X_{ii} = -y_i/2, \quad 1 \le i \le N,$$
$$X_{i,i+1} = X_{i+1,i} = \frac{1}{2} e^{\frac{1}{2}(x_i - x_{i+1})}, \quad 1 \le i \le N-1,$$

and $B(X)$ is now the tridiagonal skew-symmetric matrix $B(X) = X_- - (X_-)^T$ as in (7). As noted above, the flow $t \mapsto X(t)$ is isospectral. But more is true: The flow is completely integrable in the sense of Liouville with the eigenvalues of $X(0) = H$ providing N Poisson commuting integrals for the flow. In 1975, Moser showed that the off-diagonal elements $X_{i,i+1}(t) = X_{i+1,i}(t)$ converge to zero as $t \to \infty$ [Mos75].

The Toda algorithm

Inspired by this result, and also related work of Symes [Sym82] on the QR algorithm, the authors in [DNT83] suggested that the Toda Lattice be viewed as an eigenvalue algorithm, the Toda algorithm. The Lax equations (7) is the natural extension of the tridiagonal Toda lattice to general real symmetric matrices. It turns out that in this generality (7) is also Hamiltonian [Kos79, Adl78] and, in fact, integrable [DLNT86]. In current parlance, by the Toda algorithm one means the action of (7) on full real symmetric matrices, or by extension, on complex Hermitian matrices.

Statement of results

Our main result concerns the statistics of $T^{(1)}$ for invariant ensembles (IE) and Wigner ensembles (WE). We will describe these ensembles in detail later on. The gap $\lambda_N - \lambda_{N-1}$ between the two largest eigenvalues of a random matrix H chosen from an ensemble $\mathcal{E}$ plays a central role in describing the statistics of $T^{(1)}$. The following definition quantifies the distribution F_β^{gap} of the inverse of $\lambda_N - \lambda_{N-1}$ on the appropriate scale. In standard random matrix notation, $\beta = 1$ refers to real symmetric matrices and $\beta = 2$ refers to complex Hermitian matrices.

Definition 1

The distribution function $F_\beta^{\text{gap}}(t)$ for $\beta = 1, 2$ is given by

$$F_\beta^{\text{gap}}(t) = \lim_{N\to\infty} \mathbb{P}\left(\frac{1}{c_V^{2/3} 2^{-2/3} N^{2/3}(\lambda_N - \lambda_{N-1})} \leq t\right), \quad t \geq 0.$$

Here c_V is an explicit constant which depends only on the ensemble $\mathcal{E}$. In the case $\beta = 2$, F_β^{gap} is related to the Lax pair for the Painlevé II equation (see Perret and Schehr [PS14], see also Witte, Bornemann and Forrester [WBF13]).

Statement of results

Our main results are the following:

Theorem 2 (Universality for the Toda algorithm)

Let $0 < \sigma < 1$ *be fixed and let* (ϵ, N) *be in the scaling region* $\frac{\log \epsilon^{-1}}{\log N} \geq \frac{5}{3} + \frac{\sigma}{2}$. *Then if* H *is distributed according to any real (*$\beta = 1$*) or complex (*$\beta = 2$*) invariant or Wigner ensemble*

$$\lim_{N\to\infty} \mathbb{P}\left(\frac{T^{(1)}}{c_V^{2/3} 2^{-2/3} N^{2/3} (\log \epsilon^{-1} - 2/3 \log N)} \leq t \right) = F_\beta^{\mathrm{gap}}(t). \qquad (12)$$

Statement of results

The relation of this theorem to universality for the normalized stopping time is the following. Let $\xi = \xi_\beta$ be the random variable with distribution $F_\beta^{\text{gap}}(t)$, $\beta = 1$ or 2. For $\beta = 2$ IEs one can (using results from [BEY14]) prove that

$$\mathbb{E}[T^{(1)}] = c_V^{2/3} 2^{-2/3} N^{2/3} (\log \epsilon^{-1} - 2/3 \log N) \mathbb{E}[\xi](1 + o(1)), \tag{13}$$

$$\sqrt{\text{Var}(T^{(1)})} = c_V^{2/3} 2^{-2/3} N^{2/3} (\log \epsilon^{-1} - 2/3 \log N) \sqrt{\text{Var}(\xi)}(1 + o(1)). \tag{14}$$

For such ensembles, we can restate Theorem 2 as

$$\lim_{N\to\infty} \mathbb{P}\left(\frac{T^{(1)} - \mathbb{E}[T^{(1)}]}{\sqrt{\text{Var}(T^{(1)})}} \leq t \right) = F_\beta^{\text{gap}}(\sqrt{\text{Var}(\xi)}t + \mathbb{E}[\xi]).$$

Of course, by the Law of Large Numbers, for a sufficiently large number of samples

$$\langle T^{(1)} \rangle \to \mathbb{E}[T^{(1)}], \quad \sigma^2_{T^{(1)}} \to \text{Var}(T^{(1)}).$$

The proof of the analogs of (13) and (14) for non-IEs and $\beta = 1$ requires information from random matrix theory that has yet to be established. On the other hand, numerical evidence strongly suggests that these analogs are indeed correct.

P Bourgade, L Erdős, and H-T Yau. Edge Universality of Beta Ensembles. *Commun. Math. Phys.*, 332(1):261–353, nov 2014

Statement of results

To see that the algorithm computes the top eigenvalue to an accuracy beyond its fluctuations, we have the following proposition.

Proposition 0.1 (Computing the largest eigenvalue)

Let (ϵ, N) be in the scaling region. Then if H is distributed according to any real or complex invariant or Wigner ensemble

$$\epsilon^{-1}|\lambda_N - X_{11}(T^{(1)})|$$

converges to zero in probability as $N \to \infty$. Furthermore, both

$$\epsilon^{-1}|b_V - X_{11}(T^{(1)})|, \quad \epsilon^{-1}|\lambda_j - X_{11}(T^{(1)})|$$

converge to ∞ in probability for any $j = j(N) < N$ as $N \to \infty$.

Here b_V is the top edge of the equilibrium measure for the ensemble in question.

Description of ensembles

Theorem 2 and Proposition 0.1 concern the following ensembles. Let H be an $N \times N$ Hermitian (or just real symmetric) matrix with eigenvalues $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_N$ and let $\beta_1, \beta_2, \ldots, \beta_N$ denote the absolute values of the first components of the corresponding normalized eigenvectors. The following definitions are taken from [BY13, Dei00].

Description of ensembles

Definition 3 (Generalized Wigner Ensemble (WE))

A generalized Wigner matrix (ensemble) is a real symmetric ($\beta = 1$) or Hermitian ($\beta = 2$) matrix $H = (H_{ij})_{i,j=1}^{N}$ such that H_{ij} are independent random variables for $i \leq j$ given by a probability measure ν_{ij} with

$$\mathbb{E}H_{ij} = 0, \quad \sigma_{ij}^2 := \mathbb{E}H_{ij}^2.$$

Next, assume there is a fixed constant v (independent of N, i, j) such that

$$\mathbb{P}(|H_{ij}| > x\sigma_{ij}) \leq v^{-1}\exp(-x^{v}), \quad x > 0.$$

Finally, assume there exists $C_1, C_2 > 0$ such that for all i, j

$$\sum_{i=1}^{N} \sigma_{ij}^2 = 1, \quad \frac{C_1}{N} \leq \sigma_{ij}^2 \leq \frac{C_2}{N},$$

and for $\beta = 2$ the matrix

$$\Sigma_{ij} = \begin{bmatrix} \mathbb{E}(\mathrm{Re}\, H_{ij})^2 & \mathbb{E}(\mathrm{Re}\, H_{ij})(\mathrm{Im}\, H_{ij}) \\ \mathbb{E}(\mathrm{Re}\, H_{ij})(\mathrm{Im}\, H_{ij}) & \mathbb{E}(\mathrm{Im}\, H_{ij})^2 \end{bmatrix}$$

has its smallest eigenvalue $\lambda_{\min}$ satisfy $\lambda_{\min} \geq C_1 N^{-1}$.

Description of ensembles

Definition 4 (Invariant Ensemble (IE))

Let $V : \mathbb{R} \to \mathbb{R}$ satisfy $V \in C^4(\mathbb{R})$, $\inf_{x\in\mathbb{R}} V''(x) > 0$ and $V(x) > (2+\delta)\log(1+|x|)$ for sufficiently large x and some fixed $\delta > 0$. Then we define an invariant ensemble[3] to be the set of all $N \times N$ symmetric ($\beta = 1$) or Hermitian ($\beta = 2$) matrices $H = (H_{ij})_{i,j=1}^N$ with probability density

$$\frac{1}{Z_N} \mathrm{e}^{-N\frac{\beta}{2}\operatorname{tr}V(H)} \mathrm{d}H$$

Here $\mathrm{d}H = \prod_{i\le j} \mathrm{d}H_{ij}$ if $\beta = 1$ and $\mathrm{d}H = \prod_{i=1}^N \mathrm{d}H_{ii} \prod_{i<j} \mathrm{d}\,\mathrm{Re}\,H_{ij} \mathrm{d}\,\mathrm{Im}\,H_{ij}$ if $\beta = 2$.

[3] This is not the most general class of V but these assumptions simplify the analysis.

Numerical comparisons

We demonstrate Theorem 2 numerically using the following WEs defined by letting X_{ij} for $i \leq j$ be iid with distributions:

GUE Mean zero standard complex normal.

BUE $X + \mathrm{i}Y$ where X and Y are each the sum of independent mean zero Bernoulli random variables, *i.e.* binomial random variables.

GOE Mean zero standard (real) normal.

BOE Mean zero Bernoulli random variable

Define

$$\tau^{(1)} = \frac{T^{(1)}}{c_V^{2/3} 2^{-2/3} N^{2/3} (\log \epsilon^{-1} - 2/3 \log N + \gamma)},$$

where γ is a constant chosen to increase the convergence rate of this random variable as $N \to \infty$. Note that as $N \to \infty$ the limiting distribution of $\tau^{(1)}$ is independent of γ.

Numerical comparisons

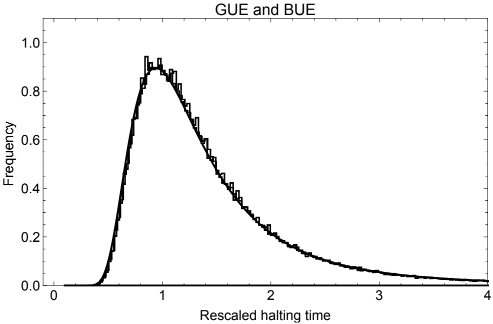

Figure: The simulated rescaled histogram for $\tau^{(1)}$ for both BUE and GUE. Here $\epsilon = 10^{-14}$ and $N = 500$ with 250,000 samples. The solid curve is the rescaled density $f_2^{\text{gap}}(t) = \mathrm{d}/\mathrm{d}t F_2^{\text{gap}}(t)$. The density $f_2^{\text{gap}}(t) = \frac{1}{\sigma t^2} A^{\text{soft}}\left(\frac{1}{\sigma t}\right)$, where $A^{\text{soft}}(s)$ is shown in [WBF13, Figure 1]: In order to match the scale in [WBF13] our choice of distributions (BUE and GUE) we must take $\sigma = 2^{-7/6}$. This is a numerical demonstration of Theorem 2.

Numerical comparisons

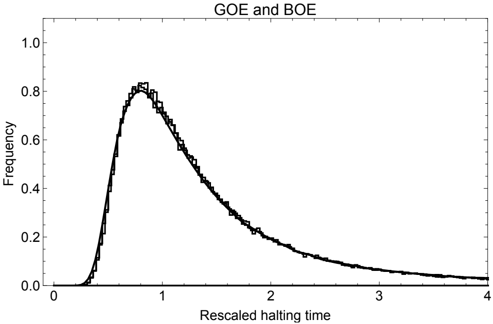

Figure: The simulated rescaled histogram for $\tau^{(1)}$ for both BOE and GOE demonstrating Theorem 2. Here $\epsilon = 10^{-14}$ and $N = 500$ with 250,000 samples. The solid curve is an approximation to the density $f_1^{\text{gap}}(t) = \mathrm{d}/\mathrm{d}t F_1^{\text{gap}}(t)$. We compute $f_1^{\text{gap}}(t)$ by smoothing the histogram for $c_V^{-2/3} 2^{-2/3} N^{-2/3} (\lambda_N - \lambda_{N-1})$ when $N = 800$ with 500,000 samples.

Estimates from random matrix theory

The proofs of Theorem 2 and Proposition 0.1 rely on the following facts from random matrix theory.

Define the averaged empirical spectral measure

$$\mu_N(z) = \mathbb{E}\frac{1}{N}\sum_{i=1}^{N}\delta(\lambda_i - z),$$

where the expectation is taken with respect to the given ensemble.

Theorem 5 (Equilibrium measure, [BEY14])

For any WE or IE the measure μ_N converges weakly to a measure μ, called the equilibrium measure, which has support on a single interval $[a_V, b_V]$ and has a density ρ that satisfies $\rho(x) \leq C_\mu\sqrt{b_V - x}\chi_{(-\infty,b_V]}(x)$ and $\rho(x) = \frac{2^{3/4}c_V}{\pi}\sqrt{b_V - x}(1 + \mathcal{O}(b_V - x))$ as $x \to b_V$.

Estimates from random matrix theory

With the chosen normalization for WEs, $\sum_{i=1}^{N} \sigma_{ij}^2 = 1$, $[a_v, b_V] = [-2, 2]$ and $c_V = 1$ [BEY14]. One can vary the support as desired by shifting and scaling, $H \to aH + bI$: the constant c_V then changes accordingly. When the entries of H are distributed according to a WE or an IE with high probability (see Theorem 8) the top three eigenvalues are distinct and $\beta_j \neq 0$ for $j = N, N-1, N-2$. Next, let $d\mu$ denote the limiting spectral density or equilibrium measure for the ensemble as $N \to \infty$. Then define γ_n to be the smallest value of t such that

$$\frac{n}{N} = \int_{-\infty}^{t} \mathrm{d}\mu.$$

Thus $\{\gamma_n\}$ represent the quantiles of the equilibrium measure.

Estimates from random matrix theory

There are four fundamental parameters involved in our calculations, σ, p, s and c, which are utilized in the proof in the following order. First we fix $0 < \sigma < 1$ once and for all, then we fix $0 < p < 1/3$, then we choose $0 < s < \min\{\sigma/44, p/8\}$ and then finally $0 < c \leq 10/\sigma$ will be a constant that will allow us to estimate the size of various sums.

Definition 6 (Scaling region)

Fix $0 < \sigma < 1$. The scaling region for ϵ is given by $\dfrac{\log \epsilon^{-1}}{\log N} \geq 5/3 + \sigma/2$.

For convenience in what follows we use the notation $\epsilon = N^{-\alpha/2}$, so

$$(\epsilon, N) \text{ are in the scaling region if and only if } \alpha - 10/3 \geq \sigma > 0$$

and $\alpha = \alpha_N$ is allowed to vary with N.

Estimates from random matrix theory

Condition 0.1

For $0 < p < 1/3$,

- $\lambda_{N-1} - \lambda_{N-2} \geq p(\lambda_N - \lambda_{N-1})$.

Let $G_{N,p}$ *denote the set of matrices that satisfy this condition.*

Condition 0.2

For any fixed $0 < s < \min\{\sigma/44, p/8\}$

1. $\beta_n \leq N^{-1/2+s/2}$ *for all* n
2. $N^{-1/2-s/2} \leq \beta_n$ *for* $n = N, N-1$,
3. $N^{-2/3-s} \leq \lambda_N - \lambda_{n-1} \leq N^{-2/3+s}$, *for* $n = N, N-1$, *and*
4. $|\lambda_n - \gamma_n| \leq N^{-2/3+s}(\min\{n, N-n+1\})^{-1/3}$ *for all* n.

Let $R_{N,s}$ *denote the set of matrices that satisfy these conditions.*

Estimates from random matrix theory

The following theorem has it roots in the pursuit of proving universality in random matrix theory. See [TW94] for the seminal result when $V(x) = x^2$ and $\beta = 2$. Further extensions include the works of Soshnikov [Sos99] and Tao and Vu [TV10] for Wigner ensembles and [DG07] for invariant ensembles.

Theorem 7

For both IEs and WEs

$$N^{1/2}(|\beta_N|, |\beta_{N-1}|, |\beta_{N-2}|)$$

converges jointly in distribution to $(|X_1|, |X_2|, |X_3|)$ *where* $\{X_1, X_2, X_3\}$ *are iid real (*$\beta = 1$*) or complex (*$\beta = 2$*) standard normal random variables. Additionally, for IEs and WEs*

$$2^{-2/3}N^{2/3}(b_V - \lambda_N, b_V - \lambda_{N-1}, b_V - \lambda_{N-2})$$

converges jointly in distribution to random variables $(\Lambda_{1,\beta}, \Lambda_{2,\beta}, \Lambda_{3,\beta})$ *which are the smallest three eigenvalues of the so-called stochastic Airy operator. Furthermore,* $(\Lambda_{1,\beta}, \Lambda_{2,\beta}, \Lambda_{3,\beta})$ *are distinct with probability one.*

The proof relies on results from Bourgade et al. [BY13, BEY14] and Ramírez, Rider and Virag [RRV11].

Estimates from random matrix theory

The remaining theorems in this section are compiled from results that have been obtained recently in the literature by Erdős et al. [EY12, Erd12] and Bourgade and Yau [BY13].

Theorem 8

For WEs or IEs Condition 0.2 holds with high probability as $N \to \infty$, that is, for any $s > 0$

$$\mathbb{P}(R_{N,s}) = 1 + o(1),$$

as $N \to \infty$.

Theorem 9

For both WEs and IEs

$$\lim_{p \downarrow 0} \limsup_{N \to \infty} \mathbb{P}(G_{N,p}^c) = 0.$$

Sketch of the proof of Theorem 2

Let $H = H^*$ have eigenvalues $\lambda_N \geq \lambda_{N-1} \geq \cdots \geq \lambda_1$ with associated normalized eigenvectors $u_j = [u_{1j}, \ldots, u_{Nj}]^T$, $\|u_j\|^2 = \sum_i |u_{ij}|^2 = 1$. Following Moser, a straightforward calculation shows that if $X(t)$ solves the Toda equations (7) with $X(0) = H$ then $\lambda_j(t) = \lambda_j(0)$ (*i.e.* the flow is isospectral) and

$$u_{1j}(t) = \frac{u_{1j}(0)\mathrm{e}^{\lambda_j t}}{\left(\sum_i |u_{ij}(0)|^2 \mathrm{e}^{2\lambda_i t}\right)}, \tag{15}$$

where $u_j(t) = [u_{1j}(t), \ldots, u_{Nj}(t)]^T$ are the normalized eigenvectors for $H(t)$.

The key point is that

$$E(t) = \sum_{i=2}^{N} |X_{1i}(t)|^2$$

and $X_{11}(t)$ can expressed in terms of $\{\lambda_k, u_{1j}(t)\}$ alone.

Sketch of the proof of Theorem 2

We have

$$X_{11}(t) = \sum_i \lambda_i |u_{1i}(t)|^2, \tag{16}$$

and

$$E(t) = \sum_i (\lambda_i - X_{11}(t))^2 |u_{1i}(t)|^2. \tag{17}$$

It follows that the dynamics of the algorithm, and hence the statistics of the stopping time $T^{(1)}$ (when $E(T^{(1)}) < \epsilon^2$) , is completely determined by the explicit solution formula (15). This formula reflects the complete integrability of the Toda lattice.

Sketch of the proof of Theorem 2

Let

$$\delta_n = 2(\lambda_N - \lambda_n), \quad 1 \le n \le N-1, \tag{18}$$

$$\nu_n = \frac{\beta_n^2}{\beta_N^2} = \left|\frac{u_{1n}(0)}{u_{1N}(0)}\right|^2. \tag{19}$$

Then a simple calculation shows that

$$E(t) = E_0(t) + E_1(t)$$

where

$$E_0(t) = \frac{1}{4}\frac{\sum_{n=1}^{N-1}\delta_n^2\nu_n e^{-\delta_n t}}{\left(1+\sum_{n=1}^{N-1}\nu_n e^{-\delta_n t}\right)^2},$$

$$E_1(t) = \frac{\left(\sum_{n=1}^{N-1}\lambda_n^2\nu_n e^{-\delta_n t}\right)\left(\sum_{n=1}^{N-1}\nu_n e^{-\delta_n t}\right) - \left(\sum_{n=1}^{N-1}\lambda_n\nu_n e^{-\delta_n t}\right)^2}{\left(1+\sum_{n=1}^{N-1}\nu_n e^{-\delta_n t}\right)^2}.$$

Sketch of the proof of Theorem 2

Note that, by the Cauchy–Schwarz inequality, both $E_0(t)$ and $E_1(t)$ are positive. This gives an essential simplification in the proof as $E(t)$ is small if and only if $E_0(t)$ and $E_1(t)$ are small.

- First technical lemma: Given Condition 0.2, the stopping time $T^{(1)}$ satisfies

  $$(\alpha - 4/3 - 5s)\log N/\delta_{N-1} \leq T^{(1)} \leq (\alpha - 4/3 + 7s)\log N/\delta_{N-1},$$

  for sufficiently large N.
- Second technical lemma: Consider the interval

  $$I_\alpha = [(\alpha - 4/3 - 5s)\log N/\delta_{N-1}, (\alpha - 4/3 + 7s)\log N/\delta_{N-1}] = [t_0, t_1].$$

  The given Condition 0.2 and $t \in I_\alpha$

  $$-E_0'(t) \geq CN^{-12s-\alpha-2/3},$$

  for sufficiently large N and some $C > 0$, *i.e* $E_0(t)$ is strictly monotone decreasing in I_α.

Sketch of the proof of Theorem 2

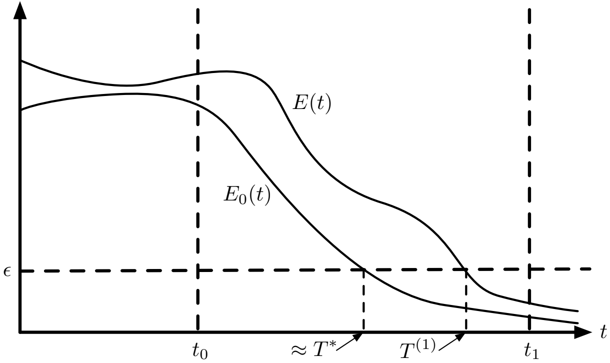

Figure: A schematic for the relationship between the functions $E_0(t)$, $E(t)$ and the times $T^{(1)}$ and T^*. Here $t_0 = (\alpha - 4/3 - 5s)\log N/\delta_{N-1}$ and $t_1 = (\alpha - 4/3 + 7s)\log N/\delta_{N-1}$. Note that E_0 is monotone on $[t_0, t_1]$.

In this figure, T^* is given by

$$T^* = \frac{\alpha \log N + 2\log \delta_{N-1} + \log \nu_{N-1} - 2\log 2}{\delta_{N-1}}. \tag{20}$$

Sketch of the proof of Theorem 2

In terms δ_n and ν_n, E_0 has the form

$$E_0(t) = \frac{1}{4}\delta_{N-1}^2 \nu_{N-1} \mathrm{e}^{-\delta_{N-1}t} \frac{1 + \sum_{n=1}^{N-2} \frac{\delta_n^2}{\delta_{N-1}^2} \frac{\nu_n}{\nu_{N-1}} \mathrm{e}^{-(\delta_n - \delta_{N-1})t}}{\left(1 + \sum_{n=1}^{N-1} \nu_n \mathrm{e}^{-\delta_n t}\right)^2}.$$

- <u>Third technical lemma:</u> Given Conditions 0.1 and 0.2, we have

  $$T^* \in I_\alpha$$

  and

  $$|E_0(T^*) - N^{-\alpha}| \leq C N^{-\alpha - 2p + 4s} \tag{21}$$

  and

  $$\max_{\eta \in I_\alpha} |E_1(\eta)| \leq N^{-2\alpha + 8/3}. \tag{22}$$

Sketch of the proof of Theorem 2

We have

$$E_0(T^{(1)}) - E_0(T^*) = E_0'(\eta)(T^{(1)} - T^*), \tag{23}$$

for some $\eta \in I_\alpha$. Also

$$E_0(T^{(1)}) = E(T^{(1)}) - E_1(T^{(1)}) = N^{-\alpha} - E_1(T^{(1)}) \tag{24}$$

and so, using the second technical lemma, we obtain (22) from (21) and (24) from (23), under Conditions 0.1 and 0.2 with σ and p fixed and $s < \min\{\sigma/44, p/8\}$. Thus

$$|T^{(1)} - T^*| \leq \frac{|N^{-\alpha} - E_0(T^*) - E_1(T^{(1)})|}{\min\limits_{\eta \in I_\alpha} |E_0'(\eta)|} \leq \frac{|N^{-\alpha} - E_0(T^*)| + \max_{\eta \in I_\alpha} |E_1(\eta)|}{\min\limits_{\eta \in I_\alpha} |E_0'(\eta)|}. \tag{25}$$

This yields

$$|T^{(1)} - T^*| \leq CN^{\alpha+12s+2/3}(N^{-\alpha-2p+4s} + N^{-2\alpha+8/3}), \tag{26}$$

and our fourth technical lemma.

- <u>Fourth technical lemma:</u> For σ and $p < 1/3$ fixed and $s < \min\{\sigma/44, p/8\}$

$$N^{-2/3}|T^{(1)} - T^*| \leq CN^{-2p+16s} \to 0 \tag{27}$$

as $N \to \infty$ provided $s < p/8$.

Sketch of the proof of Theorem 2

We now add in the probability.

- Probability Lemma One: For $\alpha \geq 10/3 + \sigma$, and $\sigma > 0$

$$\frac{|T^{(1)} - T^*|}{N^{2/3}} \to 0$$

in probability as $N \to \infty$.

Proof.
For $\eta > 0$,

$$\mathbb{P}\left(\frac{|T^{(1)} - T^*|}{N^{2/3}} > \eta\right) = \mathbb{P}\left(\frac{|T^{(1)} - T^*|}{N^{2/3}} > \eta, G_{N,p} \cap R_{N,s}\right) + \mathbb{P}\left(\frac{|T^{(1)} - T^*|}{N^{2/3}} > \eta, G^c_{N,p} \cup R^c_{N,s}\right).$$

For $s < \min\{\sigma/44, p/8\}$, on the set $G_{N,p} \cap R_{N,s}$, $\frac{|T^{(1)} - T^*|}{N^{2/3}} < \eta$ for sufficiently large N by the fourth technical lemma.

Sketch of the proof of Theorem 2

On the other hand, using Theorem 8,

$$\limsup_N \mathbb{P}\left(\frac{|T^{(1)} - T^*|}{N^{2/3}} > \eta, G^c_{N,p} \cup R^c_{N,s}\right) \leq \limsup_N \mathbb{P}\left(G^c_{N,p}\right) + \limsup_N \mathbb{P}\left(R^c_{N,s}\right)$$
$$= \limsup_N \mathbb{P}(G^c_{N,p}).$$

Thus

$$\limsup_N \mathbb{P}\left(\frac{|T^{(1)} - T^*|}{N^{2/3}} > \eta\right) \leq \limsup_N \mathbb{P}(G^c_{N,p}),$$

but the LHS is independent of p. Letting $p \downarrow 0$, Probability Lemma One now follows by Theorem 9.

■

Sketch of the proof of Theorem 2

We now compare T^* which solves

$$N^{-\alpha} e^{-\delta_{N-1} T^*} = \frac{1}{4} \delta_{N-1}^2 \nu_{N-1},$$

to $\hat{T}$ which is given by

$$\hat{T} = \frac{(\alpha - 4/3) \log N}{\delta_{N-1}} = \frac{(\alpha - 4/3) \log N}{2(\lambda_N - \lambda_{N-1})}, \tag{28}$$

i.e.

$$N^{-\alpha} e^{\delta_{N-1} \hat{T}} = N^{-4/3}. \tag{29}$$

But from Condition 0.2, $\delta_{N-1}^2 \sim 2^2 N^{-4/3-2s}$. And $\nu_{N-1} = \beta_{N-1}^2 / \beta_N^2$, which on the appropriate scale is $O(1)$ by results from Bourgade, Erdős and Yau [BEY14]. So we expect

$$T^* \sim \hat{T}.$$

More precisely, we have

- Probability Lemma Two: For $\alpha \geq 10/3 + \sigma$

$$\frac{T^* - \hat{T}}{N^{2/3} \log N} \to 0 \tag{30}$$

in probability as $N \to \infty$.

Sketch of the proof of Theorem 2

Comparing $T^{(1)} \to T^* \to \hat{T}$, this finally yields our Theorem 2,

$$\begin{aligned}
&\lim_{N\to\infty} \mathbb{P}\left(\frac{T^{(1)}}{c_V^{2/3} 2^{-2/3} N^{2/3} (\log \epsilon^{-1} - 2/3 \log N)} \leq t \right) \\
&= \lim_{N\to\infty} \mathbb{P}\left(\frac{T^{*}}{c_V^{2/3} 2^{-2/3} N^{2/3} (\log \epsilon^{-1} - 2/3 \log N)} \leq t \right) \\
&= \lim_{N\to\infty} \mathbb{P}\left(\frac{\hat{T}}{c_V^{2/3} 2^{-2/3} N^{2/3} (\log \epsilon^{-1} - 2/3 \log N)} \leq t \right) \\
&= \lim_{N\to\infty} \mathbb{P}\left(\frac{1}{c_V^{2/3} 2^{-5/3} N^{2/3} \delta_{N-1}} \leq t \right) \\
&= \lim_{N\to\infty} \mathbb{P}\left(\frac{1}{c_V^{2/3} 2^{-2/3} N^{2/3} (\lambda_N - \lambda_{N-1})} \leq t \right) = F_\beta^{\mathrm{gap}}(t).
\end{aligned}$$

■

Similar arguments yield the proof of Proposition 0.1.

Final comment

Our final comment is an invitation to the random matrix community. Numerical algorithms provide a natural arena for a new, wide and challenging set of questions in random matrix theory. For example, the proof of universality for the classical Toda algorithm with stopping time T requires detailed knowledge of the joint distribution of all the eigenvalues and all the components of all the eigenvectors. In another direction, the proof of universality for the QR algorithm requires detailed statistical information about eigenvalues λ_j in the bulk around $\lambda_j \approx 0$. And so on...

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