A REVIEW OF BORNEMANN'S "NUMERICAL EVALUATION OF DISTRIBUTIONS IN RMT"

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1. Introduction

Folkmar Bornemann's paper [1] on stable methods for evaluating Random Matrix Theory distributions makes the following claims: for many important distributions (Tracy-Widom, etc.) and level spacing functions in general, we are interested in numerically evaluating the distributions at certain points. In most cases, these distributions have a representation as both an integral of a special function (solution to a second order PDE) and a determinantal representation (Fredholm determinant). Bornemann challenges conventional wisdom - other authors claim that the numerical solution of a Painleve-type PDE (and subsequent numerical integration) proves more effective, efficient, stable, and flexible than numerical evaluation of a Fredholm determinant. To refute this claim, Bornemann tested several numerical approaches to solving various PDEs, and compared against a custom implementation of a Fredholm determinant approximation scheme in MATLAB. The results seem to demonstrate that the Fredholm determinant method is numerically better behaved for most distributions of interest, as well as more efficiently computable.

2. Problem Formulations

Definition 2.1 (Gaussian Ensemble Spacing Function)**.** *Let $J \subset \mathbb{R}$ be an open interval.*

$$E_\beta^{(n)}(k; J) \equiv \mathbb{P}(k \textit{ eigenvalues of the } n \times n \textit{ Gaussian } \beta\textit{-ensemble lie in } J)$$

Let $J = (0, s)$. Then $E_2(0; J) =$ probability no eigenvalues in $(0, s)$. It is a well-known result due to Gaudin that we can express $E_2(0; J)$ as a Fredholm determinant:

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Theorem 2.2 (Gaudin 1961)**.** *Given* $K_{\sin}(x,y) = sinc(\pi(x-y))$,

$$E_2(0, J) = \det\left(I - K_{\sin} \restriction_{L^2_J}\right)$$

It is important to note that we restrict the kernel to trace-class operators over the Hilbert space of square-integrable functions.

Additionally, we have

$$E_2(0; (0,s)) = \exp\left(-\int_0^{\pi s} \frac{\sigma(x)}{x} dx\right)$$

where $\sigma(x)$ solves a particular form of the Painleve V equation:

$$(x\sigma'')^2 = 4(\sigma - x\sigma')(x\sigma - \sigma - (\sigma')^2), \quad \sigma(x) \approx \frac{x}{\pi} + \frac{x^2}{\pi^2} \quad (x \to 0)$$

We're interested in evaluating $E_2(0,(0,s))$ - the probability that no eigenvalues are less than s in the GUE. In order to do this, we can either solve the differential equation for each x in some quadrature rule, then perform numerical integration to obtain the result, or approximate the Fredholm determinant. Let's look at another example, the Tracy-Widom distribution:

Definition 2.3 (Tracy-Widom Distribution)**.** *The Tracy-Widom distribution is defined by the following function* $F_2(s)$*:*

$$F_2(s) \equiv \mathbb{P}(\text{ no eigenvalues of large-matrix-limit GUE lie in } (s,\infty))$$

The Tracy-Widom distribution has a representation as a Fredholm determinant:

Theorem 2.4 (Bronk 1964)**.** *Given*

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

we have

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

Additionally, the Tracy-Widom distribution has a representation as a solution to a PDE:

Theorem 2.5 (Tracy, Widom 1993)**.**

$$F_2(s) = \exp\left(-\int_s^{\infty} (x-s)u(x)^2 dx\right)$$

where $u(x)$ is the Hastings-McLeod (1980) solution to the Painleve II equation

$$u'' = 2u^3 + xu, \quad u(x) \approx Ai(x) \quad (x \to \infty)$$

3. Problem Solutions

3.1. **Numerical Approach to PDEs.** Bornemann notes that numerically solving PDEs is a time-tested historical tradition in mathematics, and postulates that the common view (that Painleve-esque formulations are easier to approach than determinants) stems from this historical tradition. He begins by noting that we can take a straight forward approach to solving these PDEs - approach them as an initial value problem with constraints on the asymptotic form of the functions.

Specifically, given an interval (a, b), we seek $u(x)$ that solves

$$u''(x) = f(x, u(x), u'(x))$$

subject to either of the asymptotic one-sided conditions

$$u(x) \approx u_a(x) \quad (x \to a)$$

or

$$u(x) \approx u_b(x) \quad (x \to b)$$

Given a taylor series expansion for $u(x)$ at the specified boundary points, we need to choose an initial point and an asymptotic order of approximation:

choose $a_+ > a$ (or $b_- < b$) close to boundary and compute solution to the (standard) IVP problem

$$v''(x) = f(x, v(x), v'(x))$$
$$v(a_+) = u_a(a_+), \quad v'(a_+) = u_a'(a_+)$$

or

$$v(b_-) = u_b(b_-), \quad v'(b_-) = u_b'(b_-)$$

However, as noted by Bornemann, this method (solving an IVP) demonstrates unacceptable numerical instability, even when using an intelligent numerical integrator with adaptive error control (Runge-Kutta 4/5 method).

Another approach to solving this PDE is to constrain the value of the function at both endpoints, rather than constrain the value of the function and its first derivative at a single endpoint. This formulation is known as a Boundary Value Problem (BVP).

Additionally, we must use an asymptotic expression $u_a(x)$ at $(x \to a)$ to infer asymptotic expression $u_b(x)$ at $(x \to b)$, or vice versa.

We approximate $u(x)$ by solving the BVP:

$$v''(x) = f(x, v(x), v'(x)), \quad v(a_+) = u_a(a_+), \quad v(b_-) = u_b(b_-)$$

An example of this is the Tracy-Widom Distribution.

Computing $F_2(s)$ via computation of $u(x)$ via BVP methods:

By definition, $u(x) \approx \mathrm{Ai}(x) \quad (x \to \infty)$ so we take $u_b(x) = \mathrm{Ai}(x)$. Choose $a_+ = -10$, $b_- = 6$ (Dieng, 2005).

We need to choose a sufficiently accurate asymptotic expansion for $u_a(x)$. Tracy and Widom show

$$u(x) = \sqrt{-\frac{x}{2}}\left(1 + \frac{1}{8}x^{-3} - \frac{73}{128}x^{-6} + \frac{10657}{1024}x^{-9} + O(x^{-12})\right), \quad (x \to -\infty)$$

so we'll use that for $u_a(x)$.

Unfortuantely, the BVP approach also has numerical issues (although they are less severe than the IVP problem by several orders of magnitude). Additionally, the BVP approach requires the evaluator to have an excellent ability to make informed choices about asymptotic expansions, initial values, boundary values, and PDE discretization step size. In short, Bornemann finds the method to be too involved to be used as a black-box evaluation procedure.

3.2. **Numerical Approach to Fredholm Determinant.** A better approach to this problem exists: Bornemann approximates the Fredholm determinant in the following manner.

The Fredholm determinant

$$d(z) = \det\left(I - zK \restriction_{L^2_{(a,b)}}\right)$$

has the approximation

$$A_m = K(x_i, y_j)_{i,j=1}^m$$

$$d_m(z) = \det\left(\delta_{ij} - z \cdot w_i^{1/2} A_m w_j^{1/2}\right)$$

, given quadrature weights w_j and nodes x_i.

If we want the value of the determinant We can evaluate this determinant in MATLAB fairly easily: we can compute LU of $(I - zA_m)$, and get the determinant from $\prod_{j=1}^m U_{jj}$

Computing $d_m(z)$ for a single z takes $O(m^3)$ time, but we can do better (though not asymptotically better) via a QR decomposition if we care about evaluating at multiple z. We compute eigenvalues λ_j of A_m via QR (one-time cost of $O(m^3)$ time, but has worse constant factor than LU in practice), then form

$$d_m(z) = \prod_{j=1}^{m}(1 - z\lambda_j)$$

Computing $d_m(z)$ now takes $O(m)$ time.

The numerics of this approach are much better - we see full convergence to double numerical precision in 1/10th the time.

References

[1] Bornemann, Folkmar. "The Numerical Evaluation of Distributions in Random Matrix Theory: A Review." Markov Processes and Related Fields. Accessed electronically at http://arxiv.org/pdf/0904.1581.pdf