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Tracy-Widom and Painlevé II: computational aspects and realization in S-Plus

A. Iu. Bejan

Abstract. Realization of the Tracy-Widom distributions F_β ($\beta = 1, 2, 4$) in *S-Plus* is presented. These distributions appear as asymptotic laws in the spectral theory of random matrices of certain types and have comparatively short history. They are of great interest both in the theory and applications and appear to be important in modern statistical work. As the distributions are stated in terms of Painlevé II transcendent, their realization required a special approach of implementation. Performance and stability issues are also discussed.

Mathematics subject classification: Primary 65C60; Secondary 65L05, 65L07, 68W25.
Keywords and phrases: Tracy-Widom laws, Painlevé II transcendents, *S-Plus*, largest eigenvalue, sample covariance matrix..

1 Introduction

1.1 Preliminary notes

Nowadays the statistical work deals with data sets of hugeous sizes. In these circumstances it becomes more difficult to use classical, often exact, results from the fluctuation theory of the extreme eigenvalues. Thus, in some cases, asymptotic results stated in simpler forms are more preferable.

Johnstone (2001) has established that it is the Tracy-Widom law of order one that appears as the limiting distribution of the largest eigenvalue of a Wishart matrix with identity covariance in the case when the ratio of the data matrix' dimensions tends to a constant. The Tracy-Widom distribution which appears here is stated in terms of a solution to the Painlevé II differential equation – one of the six exceptional nonlinear second-order ordinary differential equations discovered by Painlevé a century ago.

The known exact distribution of the largest eigenvalue in the null case follows from a more general result of Constantine (1963) and is expressed in terms of hypergeometric function of a matrix argument. This hypergeometric function represents a zonal polynomial series. Until recently such representation was believed to be inapplicable for the efficient numerical evaluation. However, the most recent results of Koev and Edelman (2005) deliver new algorithms that allow to approximate efficiently the exact distribution. The present work is mostly devoted to the numerical study of the asymptotic results.

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Large computational work has been done for the asymptotic case and some novel programming routines for the common statistical use in the *S-Plus* package are presented. This work required a whole bag of tricks, mostly related to peculiarities of the forms in which the discussed distributions are usually presented. Section 2 contains the corresponding treatment to assure the efficient computations. Special effort was put to provide statistical tools for using in *S-Plus*. The codes are publicly downloadable from `www.vitrum.md/andrew/MScWrwck/codes.txt`. Refer further to this document as *Listing*.

The computational work allowed to tabulate the Tracy-Widom distributions (of order 1, 2, and 4). Particularly, a table containing standard tail p-values for the Tracy-Widom distribution is given. It is ready for the usual statistical look-up use.

The final section concludes the paper with a discussion on some open problems and suggestions on the further work seeming to be worth of doing.

For the extended version of this paper, applications and more thorough discussions appeal to Bejan (2005).

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1.2 Asymptotic distribution function for the largest eigenvalue in the white Wishart case

The asymptotic distribution for the largest eigenvalue in Wishart sample covariance matrices was found by Johstone (2001). He also reported that the approximation is satisfactory for n and p as small as 10. The main result from his work can be formulated as follows.

Theorem 1. *Let $\mathcal{W}$ be a white Wishart matrix and l_1 be its largest eigenvalue. Then*

$$\frac{l_1 - \mu_{np}}{\sigma_{np}} \xrightarrow{\text{dist}} F_1,$$

where the center and scaling constants are

$$\mu_{np} = (\sqrt{n-1} + \sqrt{p})^2,\ \sigma_{np} = \mu_{np}\left((n-1)^{-\frac{1}{2}} + p^{-\frac{1}{2}}\right)^{1/3},$$

and F_1 stands for the distribution function of the Tracy-Widom law of order 1.

The limiting distribution function F_1 is a particular distribution from a family of distributions F_β. For $\beta = 1,\ 2,\ 4$ functions F_β appear as the limiting distributions for the largest eigenvalues in the *Gaussian Orthogonal* (GOE), *Gaussian Unitary* (GUE) and *Gaussian Symplectic ensembles* (GSE), correspondingly. This was shown by Tracy and Widom (1993, 1994, 1996). Their results state that for the largest eigenvalue $l_{\max}(\mathcal{A})$ of the random matrix $\mathcal{A}$ (whenever this comes from GOE ($\beta = 1$), GUE ($\beta = 2$) or GSE ($\beta = 4$)) its distribution function $F_{N,\beta}(s) \stackrel{\partial ef}{=} \mathbb{P}(l_{\max}(A) < s),\ \beta = 1, 2, 4$ satisfies the following limit law:

$$F_\beta(s) = \lim_{N\to\infty} F_{N,\beta}(2\sigma\sqrt{N} + \sigma N^{-1/6}s),$$

where F_β are given explicitly by

$$F_2(s) = \exp\left(-\int_s^\infty (x-s)q^2(x)dx\right), \tag{1}$$

$$F_1(s) = \exp\left(-\frac{1}{2}\int_s^\infty q(x)dx\right)[F_2(s)]^{1/2}, \tag{2}$$

$$F_4(2^{-2/3}s) = \cosh\left(-\frac{1}{2}\int_s^\infty q(x)dx\right)[F_2(s)]^{1/2}. \tag{3}$$

Here $q(s)$ is the unique solution to the Painléve II equation [1]

$$q'' = sq + 2q^3 + \alpha \text{ with } \alpha = 0, \tag{4}$$

satisfying the boundary condition

$$q(s) \sim \mathrm{Ai}(s),\ \ s \to +\infty, \tag{5}$$

where $\mathrm{Ai}(s)$ denotes the Airy function – a participant of one of the pairs of linearly independent solutions to the following differential equation:

$$w'' - sw = 0.$$

The boundary condition (5) means that

$$\lim_{s\to+\infty} \frac{q(s)}{\mathrm{Ai}(s)} = 1. \tag{6}$$

The Painlev'e II (4) is one of the six exceptional second-order ordinary differential equations of the form

$$\frac{d^2w}{ds^2} = F(s, w, dw/ds), \tag{7}$$

where F is locally analytic in s, algebraic in w, and rational in dw/ds. Painlevé (1902a,b) and Gambier (1909) studied the equations of the form (7) and identified all the solutions to such equations which have no movable points, i.e. the branch points or singularities whose locations do not depend on the constant of integration of (7). From the fifty canonical types of such solutions, forty four are either integrable in terms of previously known functions, or can be reduced to one of the rest six new nonlinear ordinary differential equations known nowadays as the *Painlevé equations*, whose solutions became to be called the *Painlevé transcendents*. The Painlevé II is *irreducible* – it cannot be reduced to a simpler ordinary differential equation or combinations thereof, see Ablowitz and Segur (1977).

Hastings and McLeod (1980) proved that there is a unique solution to (4) satisfying the boundary conditions:

$$q(s) \sim \begin{cases} \mathrm{Ai}(s), & s \to +\infty \\ \sqrt{-\frac{1}{2}s}, & s \to -\infty \end{cases}.$$

Moreover, these conditions are independent of each other and correspond to the same solution.

For the mathematics beyond the connection between the Tracy-Widom laws and the Painlevé II see the work of Tracy and Widom (2000).

[1] referred further to simply as the Painlevé II.

2 Tracy-Widom and Painlevé II: computational aspects of realization in *S-Plus*

A description of the numerical work on the Tracy-Widom distributions and Painlevé II equation is given in this section.

2.1 Painlevé II and Tracy-Widom laws

An approach of the representation of the Painlevé II equation (4) by a system of ODE's is discussed. We describe an approximation algorithm of its solving in *S-Plus*, supporting it by all analytic and algebraic manipulations needed for this purpose. The motivation is to evaluate numerically the Tracy-Widom distribution and to provide appropriate statistical tools for using in *S-Plus*.

2.1.1 From ordinary differential equation to a system of equations

To solve numerically the Painlevé II and evaluate the Tracy-Widom distributions we exploit heavily the idea of Per-Olof Persson (2002) [see also Edelman and Per-Olof Persson (2005)]. His approach for implementation in *MATLAB* is adapted for a numerical work in *S-Plus*.

Since the Tracy–Widom distributions F_β ($\beta = 1, 2, 4$) are expressible in terms of the Painlev'e II whose solutions are transcendent, consider the problem of numerical evaluation of the particular solution to the Painleve II satisfying (5):

$$q'' = sq + 2q^3 \tag{8}$$

$$q(s) \sim \mathrm{Ai}(s), s \to \infty. \tag{9}$$

To obtain a numeric solution to this problem in *S-Plus*, first rewrite (8) as a system of the first order differential equations (in the vector form):

$$\frac{d}{ds}\begin{pmatrix} q \\ q' \end{pmatrix} = \begin{pmatrix} q' \\ sq' + 2q^3 \end{pmatrix}, \tag{10}$$

and by virtue of (6) substitute the condition (9) by the condition $q(s_0) = \mathrm{Ai}(s_0)$, where s_0 is a "sufficiently large" positive number. This condition, being added to the system (10), has the form

$$\left.\begin{pmatrix} q(s) \\ q'(s) \end{pmatrix}\right|_{s=s_0} = \begin{pmatrix} \mathrm{Ai}(s_0) \\ \mathrm{Ai}'(s_0) \end{pmatrix}. \tag{11}$$

Now, the problem (10)+(11) can be solved in *S-Plus* as initial-value problem using the function `ivp.ab` – the initial value solver for systems of ODE's, which finds the solution of a system of ordinary differential equations by an adaptive Adams-Bashforth predictor-corrector method at a point, given solution values at another point. However, before applying this, notice that for the evaluation of the Tracy-Widom functions $F_1(s)$, $F_2(s)$ and $F_4(s)$ some integrals of $q(s)$ should be found, in our situation – numerically estimated. This can be done using the tools for numerical integration, but this would lead to very slow calculations since such numerical integration would require a huge number of calls of the function `ivp.ab`, which is inadmissible for efficient calculations. Instead, represent F_1, F_2 and F_4 in the following form

$$F_2(s) = e^{-I(s;\,q(s))}, \tag{12}$$

$$F_1(s) = e^{-\frac{1}{2}J(s;\,q(s))}[F_2(s)]^{1/2}, \tag{13}$$

$$F_4(2^{-2/3}s) = \cosh(-\frac{1}{2}J(s))[F_2(s)]^{1/2}, \tag{14}$$

introducing the following notation

$$I(s;\, h(s)) \stackrel{\partial ef}{=} \int\limits_s^\infty (x-s)h(x)^2 dx, \tag{15}$$

$$J(s;\, h(s)) \stackrel{\partial ef}{=} \int\limits_s^\infty h(x) dx, \tag{16}$$

for some function $h(s)$.

Proposition 2. *The following holds*

$$\frac{d^2}{ds^2} I(s;\, q(s)) = q(s)^2 \tag{17}$$

$$\frac{d}{ds} J(s; q(s)) = -q(s) \tag{18}$$

Proof. First, consider the function

$$W(s) = \int\limits_s^\infty R(x,s)dx,\ s \in \mathbb{R},$$

where $R(x,s)$ is some function.

Recall [e.g. Korn and Korn (1968, pp. 114-115)] that the *Leibnitz rule* of the differentiation under the sign of integral can be applied in the following two cases as follows:

$$\frac{d}{ds}\int\limits_a^b f(x,s)dx = \int\limits_a^b \frac{\partial}{\partial s} f(x,s)dx, \tag{19}$$

$$\frac{d}{ds}\int\limits_{\alpha(s)}^{\beta(s)} f(x,s)dx = \int\limits_{\alpha(s)}^{\beta(s)} \frac{\partial}{\partial s} f(x,s)dx + f(\alpha(s),s)\frac{d\alpha}{ds} - f(\beta(s),s)\frac{d\beta}{ds}, \tag{20}$$

under conditions that the function $f(x,s)$ and its partial derivative $\frac{\partial}{\partial s}f(x,s)$ are continuous in some rectangular $[a,b]\times[s_1,s_2]$ and the functions $\alpha(s)$ and $\beta(s)$ are differentiable on $[s_1,s_2]$ and are bounded on this segment. Furthermore, the formula (19) is also true for improper integrals under condition that the integral $\int\limits_a^b f(x,s)dx$ converges, and the integral $\int\limits_a^b \frac{\partial}{\partial s}f(x,s)$ converges uniformly on the segment $[s_1,s_2]$. In this case the function $f(x,s)$ and its partial derivative $\frac{\partial}{\partial s}f(x,s)$ are only supposed to be continuous on the set $[a,b)\times[s_1,s_2]$, or $(a,b]\times[s_1,s_2]$, depending on which point makes the integral improper.

Now represent $W(s)$ as follows

$$W(s)=\int\limits_s^b R(x,s)dx+\int\limits_b^\infty R(x,s)dx,\ \text{for some } b\in[s,\infty),$$

and apply the Leibnitz rule for each of the summands under the suitable conditions imposed on $R(x,s)$:

$$\begin{aligned}\frac{d}{ds}\int\limits_s^b R(x,s)dx&=\int\limits_s^b \frac{\partial}{\partial s}R(x,s)dx+R(b,s)\frac{db}{ds}-R(s,s)\frac{ds}{ds}\\&=\int\limits_s^b \frac{\partial}{\partial s}R(x,s)dx-R(s,s),\ \text{and}\end{aligned}$$

$$\frac{d}{ds}\int\limits_b^\infty R(x,s)dx=\int\limits_b^\infty \frac{\partial}{\partial s}R(x,s)dx,$$

where for the second differentiation we have used the rule (20) for improper integrals as exposed above.

Finally, derive that

$$W'(s)=\frac{d}{ds}\int\limits_s^\infty R(x,s)dx=\int\limits_s^\infty \frac{\partial}{\partial s}R(x,s)dx-R(s,s). \tag{21}$$

This particularly gives for $R(x,s)\equiv I(s;q(s))$ the expression

$$\frac{d}{ds}I(s;q(s))=-\int\limits_s^\infty q(x)^2dx,$$

which after the repeated differentiation using the same rule becomes

$$\frac{d^2}{ds^2}I(s;q(s))=q(s)^2.$$

Similarly, for $J(s;q(s))$ one gets

$$\frac{d}{ds}J(s;q(s))=-q(s).$$

The conditions under which the differentiation takes place can be easily verified knowing the properties of the Painlevé II transcendent $q(s)$ and its asymptotic behaviour at $+\infty$. □

Write further $[\cdot]$ for a vector and $[\cdot]^T$ for a vector transpose.

Define the following vector function

$$\mathbf{V}(s) \overset{\partial ef}{=} \left[\, q(s), q'(s), I(s;\, q(s)), I'(s;\, q(s)), J(s; q(s))\,\right]^T . \tag{22}$$

The results of the Proposition 2 can be used together with the idea of artificial representation of an ODE with a system of ODE's. Namely, the following system with the initial condition is a base of using the solver `ivp.ab`, which will perform the numerical integration automatically:

$$\mathbf{V}'(s) = \left[\, q'(s), sq + 2q^3(s), I'(s; q(s)), q^2(s), -q(s)\,\right]^T , \tag{23}$$

$$\mathbf{V}(s_0) = \left[\, \mathrm{Ai}(s_0), \mathrm{Ai}'(s_0),\, I(s_0;\, \mathrm{Ai}(s_0)), \mathrm{Ai}(s_0)^2, J(s_0;\, \mathrm{Ai}(s_0))\right]^T . \tag{24}$$

The initial values in (24) should be computed to be passed to the function `ivp.ab`. The Airy function $\mathrm{Ai}(s)$ can be represented in terms of other common special functions, such as the Bessel function of a fractional order, for instance. However, there is no default support neither for the Airy function, nor for the Bessel functions in *S-Plus*. Therefore, the values from (24) at some "large enough" point s_0 can, again, be approximated using the asymptotics of the Airy function ($s \to \infty$). The general asymptotic expansions for large complex s of the Airy function $\mathrm{Ai}(s)$ and its derivative $\mathrm{Ai}'(s)$ are as follows [see, e.g., Antosiewitcz (1972)]:

$$\mathrm{Ai}(s) \sim \frac{1}{2}\pi^{-1/2}s^{-1/4}e^{-\zeta}\sum_{k=0}^{\infty}(-1)^k c_k \zeta^{-k},\ |\arg s| < \pi, \tag{25}$$

where

$$c_0 = 1,\ c_k = \frac{\Gamma(3k+\frac{1}{2})}{54^k k!\Gamma(k+\frac{1}{2})} = \frac{(2k+1)(2k+3)\dots(6k-1)}{216^k k!},\ \zeta = \frac{2}{3}s^{3/2}; \tag{26}$$

and

$$\mathrm{Ai}'(s) \sim -\frac{1}{2}\pi^{-1/2}s^{1/4}e^{-\zeta}\sum_{k=0}^{\infty}(-1)^k d_k \zeta^{-k},\ |\arg s| < \pi, \tag{27}$$

where

$$d_0 = 1,\ d_k = -\frac{6k+1}{6k-1}c_k,\ \zeta = \frac{2}{3}s^{3/2}. \tag{28}$$

Setting

$$\tilde{c}_k \overset{\partial ef}{=} \ln c_k = \ln(2k+1) + \ln(2k+3) + \ldots + \ln(6k-1) - k\ln 216 - \sum_{i=1}^{k}\ln i,\ \text{and}$$

$$\tilde{d}_k \stackrel{\partial ef}{=} \ln(-d_k) = \ln \frac{6k+1}{6k-1} + \tilde{c}_k,$$

one gets the following recurrences:

$$\tilde{c}_k = \tilde{c}_{k-1} + \ln(3 - (k - 1/2)^{-1}),$$
$$\tilde{d}_k = \tilde{c}_{k-1} + \ln(3 + (k/2 - 1/4)^{-1}),$$

which can be efficiently used for the calculations of the asymptotics (26) and (27) in the following form:

$$\mathrm{Ai}(s) \sim \frac{1}{2}\pi^{-1/2} s^{-1/4} e^{-\zeta} \sum_{k=0}^{\infty} (-1)^k e^{\tilde{c}_k} \zeta^{-k}, \tag{29}$$

$$\mathrm{Ai}'(s) \sim \frac{1}{2}\pi^{-1/2} s^{1/4} e^{-\zeta} \sum_{k=0}^{\infty} (-1)^{k+1} e^{\tilde{d}_k} \zeta^{-k}. \tag{30}$$

The function `AiryAsymptotic` can be found in *Listing*. For example, its calls with 200 terms of the expansion at the points 4.5, 5 and 6 return:

```
> AiryAsymptotic(c(4.5,5,6),200)
[1] 3.324132e-004 1.089590e-004 9.991516e-006
```

which is precise up to a sixth digit (compare with the example in Antosiewitcz (1972, p. 454) and with MATLAB's output).

However, if the value for s_0 is set to be fixed appropriately, there is no need in asymptotic expansions of $\mathrm{Ai}(s)$ and $\mathrm{Ai}'(s)$ for solving the problem[2] (23)+(24). From the experimental work it has been found that the value $s_0 = 5$ would be an enough "good" to perform the calculations. The initial values are as follows:

$$\mathbf{V}(5) = [1.0834\times 10^{-4}, -2.4741\times 10^{-4}, 5.3178\times 10^{-10}, 1.1739\times 10^{-8}, 4.5743\times 10^{-5}]^T.$$

From now on let $I(s) \equiv I(s; q(s))$ and $J(s) \equiv J(s; q(s))$. Further we show how to express F_β, f_β in terms of $I(s)$ and $J(s)$ and their derivatives. This will permit to evaluate approximately the Tracy-Widom distribution for $\beta = 1, 2, 4$ by solving the initial value problem (23)+(24).

From (12)-(14) the expressions for F_1 and F_4 follow immediately:

$$F_1(s) = e^{-\frac{1}{2}[I(s)+J(s)]} \tag{31}$$

$$F_4(s) = \cosh(-\frac{1}{2}J(\gamma s))e^{-I(\gamma s)}, \tag{32}$$

where $\gamma = 2^{2/3}$.

Next, find expressions for f_β. From (12) it follows that

$$f_2(s) = -I'(s)e^{-I(s)}. \tag{33}$$

[2]Note also that the using of (26) and (27) would add an additional error while solving the Painlevé II with the initial boundary condition (5), and, thus, while evaluating F_β.

$\beta \setminus p$-points	0.995	0.975	0.95	0.05	0.025	0.01	0.005	0.001
1	-4.1505	-3.5166	-3.1808	0.9793	1.4538	2.0234	2.4224	3.2724
2	-3.9139	-3.4428	-3.1945	-0.2325	0.0915	0.4776	0.7462	1.3141
4	-4.0531	-3.6608	-3.4556	-1.0904	-0.8405	-0.5447	-0.3400	0.0906

Table 1. Values of the Tracy-Widom distributions (β=1, 2, 4) exceeded with probability p.

The expressions for f_1, f_4 follow from (31) and (32):

$$f_1(s) = -\frac{1}{2}[I'(s) - q(s)]e^{-\frac{1}{2}[I(s)+J(s)]}, \tag{34}$$

and

$$f_4(s) = -\frac{\gamma}{2}e^{-\frac{I(\gamma s)}{2}} \left[\sinh\left(\frac{J(\gamma s)}{2}\right) q(\gamma s) + I'(\gamma s)\cosh\left(\frac{J(\gamma s)}{2}\right)\right]. \tag{35}$$

Note that $J'(s) = -q(s)$ as shown in the Proposition 2.

Implementation notes. As already mentioned, the problem (23)+(24) can be solved in *S-plus* using the initial value solver `ivp.ab`.

For instance, the call

```
> out <- ivp.ab(fin=s,init=c(5,c(1.0834e-4,-2.4741e-4, 5.3178e-10,
1.1739e-8,4.5743e-5)), deriv=fun,tolerance=1e-11) ,
```

where the function `fun` is defined as follows

```
> fun <- function(s,y) c(y[2],s*y[1]+2*y[1]^3,y[4],y[1]^2,-y[1]) ,
```

evaluates the vector $\mathbf{V}$, defined in (22), at some point `s`, and, hence, evaluates the functions $q(s)$, $I(s)$ and $J(s)$. Further, F_β, f_β can be evaluated using (12), (31), (32), (34)-(35). The corresponding functions are `FTWb(s,beta)` and `fTWb(s,beta)`, and these can be found in *Listing*.

The Tracy-Widom quantile function `qTWb(p,beta)` uses the dichotomy method applied for the cdf of the corresponding Tracy-Widom distribution. Alternatively, the Newton-Raphson method can be used, since we know how to evaluate the derivative of the distribution function of the Tracy-Widom law, i.e. how to calculate the Tracy-Widom density.

Finally, given a quantile returning function it is easy now to generate Tracy-Widom random variables using the *Inverse Transformation Method* (e.g. see Ross (1997)). The corresponding function `rTWb(beta)` can be found in *Listing*.

Using the written *S-Plus* functions which are mentioned above, the statistical tables of the Tracy-Widom distributions ($\beta = 1, 2, 4$) have been constructed. These can be found in Bejan (2005). Table 1 comprises some standard tail p-values of the Tracy-Widom laws.

Some examples of using the described functions follow:

0.05% p-value of TW_2 is

```
> qTWb(1-0.95,2)
[1] -3.194467
```

Conversely, check the 0.005% **tail** p-value of TW_1:

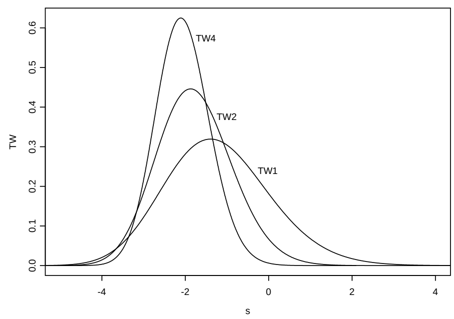

Figure 1. Tracy-Widom density plots, corresponding to the values of β: 1, 2 and 4.

```
> 1-FTWb(2.4224,1)
val 5
0.004999185
```

(compare with the corresponding entries of Table 1)

Next, evaluate the density of TW_4 at the point $s = -1$:

```
> fTWb(-1,4)
val 3
0.1576701
```

Generate a realization of a random variable distributed as TW_1:

```
> rTWb(1)
[1] -1.47115
```

Finally, for the density plots of the Tracy-Widom distributions ($\beta = 1, 2, 4$) appeal to Figure 1.

Performance and stability issues. There are two important questions: how fast the routines evaluating the Tracy-Widom distributions are, and whether the calculations provided by these routines are enough accurate to use them in statistical practice.

The answer to the former question is hardly not to be expected – the "Tracy-Widom" routines in the form as they are presented above exhibit an extremely slow performance. This reflects dramatically on the quantile returning functions which use the dichotomy method and therefore need several calls of corresponding cumulative functions. The slow performance can be well explained by a necessity to solve a system of ordinary differential equations given an initial boundary condition. However, if the calculations provided by these routines are "enough" precise we could tabulate the Tracy-Widom distributions on a certain grid of points and then proceed with an approximation of these distributions using, for instance, *smoothing* or *interpolating splines*.

Unfortunately, there is not much to say on the former question, although some insight can be gained. The main difficulty here is the evaluation of the error appearing while substituting the Painlevé II problem with a boundary condition at

$+\infty$ by a problem with an initial value at some finite point, i.e., while substituting (8)+(9) by the problem (10)+(11). However, it would be really good to have any idea about how sensible such substitution is. For this, appeal to Figure 2, where the plots of three different Painlevé II transcendents evaluated on a uniform grid from the segment $[-15, 5]$ using the calls of `ivp.ab` with different initial values are given, such that these transcendents "correspond" to the following boundary conditions: $q(s) \sim k\,\mathrm{Ai}(s),\ k = 1 - 10^{-4}, 1, 1 + 10^{4}$. The plots were produced by evaluating the transcendents using the substitution (11) of the initial boundary condition. The value for s_0 has been chosen the same as in the calculations for the Tracy-Widom distribution: $s_0 = 5$. The question is how the output obtained with the help of `ivp.ab` after a substitution of the boundary condition at $+\infty$ with the local one agrees with the theory?

Consider the null parameter Painlevé II equation

$$q'' = sq + 2q^3, \tag{36}$$

and a boundary condition

$$q(s) \sim k\,\mathrm{Ai}(s),\ \ s \to +\infty. \tag{37}$$

The asymptotic behaviour on the negative axis of the solutions to (36) satisfying the condition (37) is as follows [Clarkson and McLeod (1988), Ablowitz and Segur (1977)]:

- if $|k| < 1$, then as $z \to -\infty$

$$q(s) \sim d(-s)^{-1/4} \sin\left(\frac{2}{3}(-s)^{3/2} - \frac{3}{4}d^2 \ln(-s) - \theta\right), \tag{38}$$

  where the so called *connection formulae* for d and θ are

$$\begin{aligned} d^2(k) &= -\pi^{-1} \ln(1 - k^2), \\ \theta(k) &= \frac{3}{2}d^2 \ln 2 + \arg\left(\Gamma(1 - \frac{1}{2}id^2)\right); \end{aligned}$$

- if $|k| = 1$, then as $z \to -\infty$

$$q(s) \sim \mathrm{sign}(k)\sqrt{-\frac{1}{2}s}; \tag{39}$$

- if $|k| > 1$, then $q(s)$ blows up at a finite s^*:

$$q(s) \sim \mathrm{sign}(k)\frac{1}{s - s^*}. \tag{40}$$

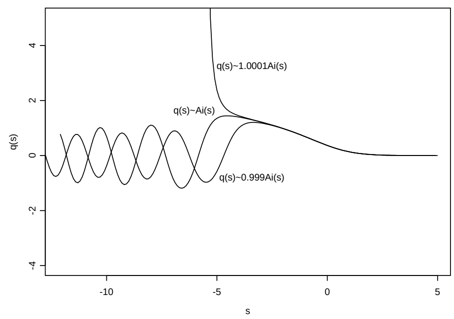

Figure 2. Comparison of the evaluated Painlevé II transcendents $q(s) \sim k\,\mathrm{Ai}(s)$, $s \to \infty$, corresponding to the different values of k: $1 - 10^{-4},\ 1,\ 1 + 10^{-4}$, as they were passed to `ivp.ab`. Practically, the solutions are hardly distinguished to the right from $s = -2.5$.

From Figure 2 one can see that the cases when $k < 1$ and $k > 1$ are sensitively different, whereas the case with $k = 1$ appeared to have the asymptotics of the solutions with $k < 1$. However, all the three solutions are hardly distinguished to the right from $s = -2.5$.

Next, compare the plot of the solution corresponding to the case $k = 1$ with the curve corresponding to the theoretical asymptotic behaviour given by (39). The plot is presented in Figure 3. Here we see that the plot of our solution congruently follows the asymptotic curve up to the point $s \approx -4$. In this connection an important observation should be made – to the left from this point the Tracy-Widom densities' values ($\beta = 1, 2, 4$) become smaller and smaller, starting with $\max\limits_{\beta=1,2,4} f_\beta(-4) = f_1(-4) \approx 0.0076$.

Finally, Figure 4 represents a graphical comparison of the evaluated Painlevé II transcendent, for which k is less but close to one, with the predicted theoretical behaviour of the decay oscillations type, given by (38).

All these graphical comparisons permit us to conclude that the using of the function `ivp.ab` for solving the initial value problem for a system of ordinary differential equations, which was a result of some artificial transformations, delivers quite sensible calculations, according with the theoretical prediction based on the asymptotic behaviour of the desired objects. Unfortunately, there is not much information on the numerical estimation of the accuracy of the computations presented here.

It is believed by the author that the values of the Tracy-Widom distributions tabulated in this way are precise up to the fourth digit.

The problem is now to struggle with the speed of performance. We move to the spline approximation.

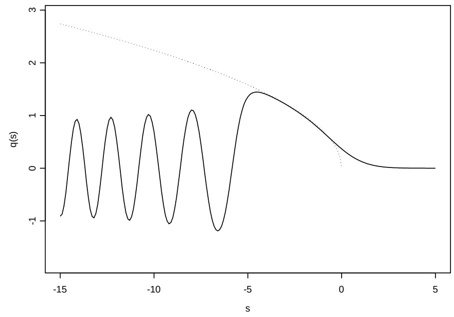

Figure 3. The evaluated Painlevé II transcendent $q(s) \sim \mathrm{Ai}(s)$, $s \to \infty$, and the parabola $\sqrt{-\frac{1}{2}s}$.

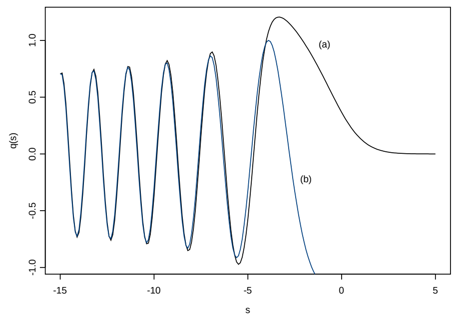

Figure 4. (a) The evaluated Painlevé II transcendent $q(s) \sim 0.999\,\mathrm{Ai}(s)$, $s \to +\infty$, and (b) the asymptotic ($s \to -\infty$) curve (38), corresponding to $k = 1 - 10^{-4}$.

2.1.2 Spline approximation

As we found, the functions calculating the Tracy-Widom distributions, described above, have a very slow performance, which makes their use almost ineffective in applications. On the other hand, our *heuristical* analysis has shown that the accuracy of those functions is relatively high. How to use this latter property and make away with the former one?

We use the cubic spline interpolation for representing the functions related with the Tracy-Widom (cumulative distribution functions, density functions and quantile functions).

The main idea is in the following: the Tracy-Widom distributions are tabulated on a uniform one-dimensional grid from the segment of the maximal concentration of a respective distribution ($\beta = 1, 2, 4$) using "precise" functions from *Listing* and described in § 2.1.1. Then, this data set is used for interpolating by using the cubic splines.

The *S-Plus* function `spline`, which interpolates through data points by means of a cubic spline, can be used rather for visualizing purposes, since this function can only interpolate the initial data set at evenly situated new points. The function `bs` can be used for a generation of a basis matrix for polynomial splines and can be used together with linear model fitting functions. Its use is rather tricky and, again, inappropriate in our situation. What we want is the function which would permit us to interpolate through a given set of tabulated points of a desired distribution. Preferably, it should be a vector-supporting function.

Such functions have been written for using in *S-Plus*: the function `my.spline.eval` is designed for the coefficients' calculation of a cubic spline given a data set, and the function `my.spline` returns a value of the spline with the coefficients passed to this function. Practically, the both functions can be used efficiently together. See their description and body texts in *Listing*.

The following examples are to demonstrate the use of the functions `my.spline.eval` and `my.spline`, as well as some peculiarities of the spline interpolation depending on the data set's features and character.

Figures 5(a) and 5(b) contain the graphical outputs of the following two *S-Plus* sessions:

```
> x<-runif(20,0,1);y<-runif(20,0,1);x<-sort(x);reg<-seq(0,10,0.01)
> plot(x,y,xlim=c(-1,11),ylim=c(-10,21))
> lines(reg,my.spline.eval(reg,x,y,my.spline(x,y)))
> x<-seq(0,10,0.5);y<-sqrt(x)+rnorm(21,0,0.1);reg<-seq(0,10,0.01)
> plot(x,y);lines(reg,my.spline.eval(reg,x,y,my.spline(x,y)))
```

Listing contains the text bodies of the functions `dtw`, `ptw` and `qtw` which implement the evaluation of the Tracy-Widom density, cumulative distribution and quantile, correspondingly, using the cubic spline interpolation. The use of these functions is standard, e.g.

```
> dtw(runif(4,-6,7),1)
[1] 0.0002247643 0.2891297912 0.0918758337 0.2393426156
```

(a) first example: phenomenon of a sudden oscillation in spline interpolation of data

(b) second example: no sudden oscillations

Figure 5. Characteristic example of using the functions `my.spline` and `my.spline.eval` in *S-Plus*.

Interestingly, it has been found that the *S-Plus* function `smooth.spline` provides even faster calculations, though relatively as good as the functions based on `my.spline` and `my.spline.eval`. Analogs of `dtw`, `ptw` and `qtw` based on the using of `smooth.spline` can be found in Listing 5b.

```
> reg<-runif(4,-6,7); dtw(reg,1);dtwsmooth1(reg)
> [1] 0.00738347825 0.06450056711 0.00009679960 0.00004254274
> 0.007383475 0.06450054 0.00009685025 0.00004254317
```

3 Summary and conclusions

3.1 Conclusions

The asymptotic result of Johnstone (§ 1.2) in the real white Wishart case followed the work of Johansson (2000) for the complex case, and established the convergence of the properly rescaled largest eigenvalue to the Tracy-Widom distribution TW_1 – one of the three limiting distributions for the largest eigenvalues in the Gaussian Orthogonal, Unitary and Symplectic Ensembles, found by Tracy and Widom just some ten years ago. These distributions have seen great generalizations, both theoretical and practical in the consecutive works of many authors.

The Johnstone's asymptotic result gives a good approximation for the data matrices' sizes as small as 10×10. This is especially important for the today applications where one deals with data matrices of great, sometimes huge sizes. However, the main difficulty in using of the results of Johnstone, as well as similar and earlier results of Johansson, Tracy and Widom, is due to the fact that the limiting distributions, – the Tracy-Widom distributions – are stated in terms of the particular solution to the second order differential equation Painlevé II. This particular solution is specified with the boundary condition.

To evaluate the functions related to the Tracy-Widom distributions in *S-Plus* (density, cumulative distribution, quantile, random number generation functions), the boundary condition which specifies the solution to Painlevé II has been substituted by a local initial value condition. This permitted to reduce a set of ordinary differential equations to a system of ODE's and use the initial value solver for such systems in *S-Plus*.

Using these, relatively precise calculations, the Tracy-Widom distributions ($\beta = 1, 2, 4$) have been tabulated on the intervals of the most concentration. The table of standard p-values was presented in this paper. It is useful for the inferential statistical work involving these distributions.

However, the use of the written *S-Plus* functions for evaluating the Tracy-Widom distributions using the described above conception of solving the Painlevé II practically is hardly possible, since the performance of those functions is extremely slow. The cubic spline interpolation has been used therefore to "recover" the distribution values from the set of pre-tabulated points. As a result, fast performance functions evaluating the Tracy-Widom distributions have been presented for the statistical work in *S-Plus*.

Interestingly, both the Tracy-Widom distribution as the limiting law and the exact largest eigenvalue distribution law required quite sophisticated computational algorithms to be efficiently evaluated using the standard mathematical software packages. We saw it for the asymptotic case, and the problem of the evaluation of the exact distribution was studied in the work of Koev and Edelman (2005), from which I draw the same conclusion.

To summarize, the work related to the numerical evaluation of the Tracy-Widom density, cumulative distribution functions as well as quantile and random number generation functions for the using in *S-Plus* was described in this chapter. The approach based on the representation of an ordinary differential equation of the order higher than one with the system of ordinary differential equations led to extremely slow, though "sensible" computations. Therefore, the method of spline approximation on a uniform one-dimensional grid has been used. The implementation of this method provided significantly faster calculations which permit an efficient statistical work, although there are some principal difficulties with the estimation of the accuracy of the calculations.

3.2 Open problems and further work

In this paper many interesting problems from the area of the study have not been touched.

We did not study the recent developments related to the efficient evaluation of the hypergeometric function of a matrix argument. This refers to the problem of the evaluation of the largest eigenvalue's exact distribution. The most recent results in this area are reported by Koev and Edelman (2005). A comparative analysis of the two different ways: the use of asymptotic distributions and evaluation of the exact ones, – could be done in perspective.

However, both approaches require methods of estimation of an error of approximation appearing therein. In our study it is the error appearing while substituting of the Painlevé II with a boundary condition with the Painlevé II with a local initial value condition. Although, it was shown on examples that the methods we implement by the means of *S-Plus* to solve the Painlevé II and evaluate the Tracy-Widom distributions are enough "sensible" to distinguish between what is predicted by theory even when we make such substitution of initial value problems. However, more rigorous justification should be found to use the methods we follow and to estimate the approximation error we make by using these methods. The use of splines and general theory of spline approximation could permit then to estimate the error appearing while recovering the Tracy-Widom distributions from the tabulated set of points, by considering these distributions as functions-members of a certain class of functions, and thus to estimate the final approximation error. Currently, the author cannot estimate exactly the accuracy of the numerical evaluation of the Tracy-Widom distributions using the described approach and proposed routines. It is only believed from the experimental work the approximation is precise up to a fourth digit.

A general suggestion can be given to increase the performance of the written *S-Plus* routines: the calculation code should be written in C++ where possible and then compiled into *.dll file to be used in *S-Plus*.

References

[1] Ablowitz, M.J., Segur, H. (1977) Exact linearization of a Painlevé transcendent. *Phys. Rev. Lett.* **38**(20), 1103–1106.

[2] Antosiewitcz, H.A. (1972) Bessel functions of fractional order. In *Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables.* Abramowitz, M., Stegun, I. (eds.), 10th printing, 435–456.

[3] Bejan, A. (2005) Largest eigenvalues and sample covariance matrices. Tracy-Widom and Painlevé II: computational aspects and realization in S-Plus with applications. *Preprint.* `http://www.vitrum.md/andrew/MScWrwck/TWinSplus.pdf`

[4] Clarkson, P.A., McLeod, J.B. (1988) A connection formula for the second Painlevé transcendent. *Archive for Rational Mechanics and Analysis*, **103**, 97–138.

[5] Constantine, A.G. (1963) Some noncentral distribution problems in multivariate analysis. *Ann. Math. Statist.*, **34**, 1270–1285.

[6] Edelman, A., Persson, Per-Olof (2005) Numerical methods for eigenvalue distributions of random matrices. *Preprint.*
`http://arxiv.org/pdf/math-ph/0501068`

[7] Gambier, B. (1909) Sur les équations différentielles du second ordre et du premier degré dont l'intégrale générale est à points critiques fixes. *Acta Math.* **33**, 1–55.

[8] Hastings, S.P., McLeod, J.B. (1980) A boundary value problem associated with the second Painlevé transcendent and the Korteweg-de Vries equation. *Arch. Rational Mech. Anal.* **73**, 31–51.

[9] Johansson, K. (2000) Shape fluctuations and random matrices. *Comm. Math. Phys.*, **209**, 437–476.

[10] Johnstone, I.M. (2001) On the distribution of the largest eigenvalue in principal component analysis. *Ann. of Stat.*, **29**(2), 295–327.

[11] Koev, P., Edelman A. (2005) The efficient evaluation of the hypergeometric function of a matrix argument. *Preprint.*
`http://arxiv.org/pdf/math.PR/0505344`

[12] Korn, G.A., Korn, T.M. (1968) *Mathematical Handbook for Scientists and Engineers. Definitions, Theorems and Formulas for Reference and review.* McGraw-Hill, New-York.

[13] Painlevé, P. (1902a) Mémoires sur les équations différentielles dont l'intégrale générale est uniforme. *Bull. Soc. Math.*, **28**, 201–261.

[14] Painlevé, P. (1902b) Sur les équations différentielles du second ordre supérieur dont l'intégrale générale est uniforme. *Acta Math.*, **25**, 1–85.

[15] Persson, Per-Olof (2002) Random matrices. Numerical methods for random matrices. `http://www.mit.edu/~persson/numrand_report.pdf`

[16] Ross, S.M. (1997) *Simulation.* Academic Press.

[17] Tracy, C.A., Widom, H. (1993) Level-spacing distribution and Airy kernel. *Phys. Letts. B* **305**, 115–118.

[18] Tracy, C.A., Widom, H. (1994) Level-spacing distribution and Airy kernel. *Comm. Math. Phys.* **159**, 151–174.

[19] Tracy, C.A., Widom, H. (1996) On orthogonal and symplectic matrix ensambles. *Comm. Math. Phys.* **177**, 727–754.

[20] Tracy, C.A., Widom, H. (2000) Airy Kernel and Painlevé II. `arXiv:solv-int/9901004`

A. Bejan,
Heriot-Watt University,
School of Mathematics and Actuarial Science,
Edinburgh, EH14 4AS, UK.
E-mail:*A.I.Bejan@ma.hw.ac.uk*

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