Approximating Tracy–Widom distributions

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Univariate Statistics

Basic problem: testing the agreement between actual observations and an underlying probability model
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Pearson’s $\chi^2$ test (1900): sampling distribution approaches the $\chi^2$ distribution as the sample size increases.
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Pearson’s $\chi^2$ test (1900): sampling distribution approaches the $\chi^2$ distribution as the sample size increases.

Recall that if $X_j$ are independent and identically distributed standard normal random variables, $N(0, 1)$, then the distribution of

$$\chi_n^2 := X_1^2 + \cdots + X_n^2$$

has density

$$f_n(x) = \begin{cases} 
\frac{1}{2^{n/2} \Gamma(n/2)} x^{n/2-1} e^{-x/2} & \text{for } x > 0, \\
0 & \text{for } x \leq 0, 
\end{cases}$$
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Multivariate Statistics

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Suppose \( X \) is a \( p \times 1 \)-variate normal with \( \mathbb{E}(X) = \mu \) and \( p \times p \) covariance matrix \( \Sigma = \text{cov}(X) \) := \( \mathbb{E}((X - \mu) \otimes (X - \mu)) \), denoted \( N_p(\mu, \Sigma) \).
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Suppose $X$ is a $p \times 1$-variate normal with $\mathbb{E}(X) = \mu$ and $p \times p$ covariance matrix $\Sigma = \text{cov}(X) := \mathbb{E}((X - \mu) \otimes (X - \mu))$, denoted $N_p(\mu, \Sigma)$.

If $\Sigma > 0$ the density function of $X$ is

$$f_X(x) = (2\pi)^{-p/2} (\det \Sigma)^{-1/2} \exp \left[-\frac{1}{2} (x - \mu, \Sigma^{-1}(x - \mu)) \right],$$

where $x \in \mathbb{R}^p$ and $(\cdot, \cdot)$ is the standard inner product on $\mathbb{R}^p$. 
Matrix notation

Introduce a matrix notation: If $X$ is a $n \times p$ matrix (the data matrix) whose rows $X_j$ are independent $N_p(\mu, \Sigma)$ random variables,

$$X = \begin{pmatrix}
\leftarrow X_1 \rightarrow \\
\leftarrow X_2 \rightarrow \\
\vdots \\
\leftarrow X_n \rightarrow 
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\end{pmatrix},
$$

then we say $X$ is $\mathcal{N}_p(1 \otimes \mu, I_n \otimes \Sigma)$ where $1 = (1, 1, \ldots, 1)$ and $I_n$ is the $n \times n$ identity matrix.
Multivariate Gamma function

If $S^+_m$ is the space of $p \times p$ positive definite, symmetric matrices, then

$$\Gamma_p(a) := \int_{S^+_p} e^{-\text{tr}(A)} (\det A)^{a-(p+1)/2} \, dA$$

where $\text{Re}(a) > (m - 1)/2$ and $dA$ is the product Lebesgue measure of the $\frac{1}{2}p(p+1)$ distinct elements of $A$. 
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Matrix factorization $A = T^tT$ where $T$ is upper-triangular with positive diagonal elements, allows evaluation of this integral in terms of ordinary gamma functions.

$\Gamma_1(a)$ is the usual gamma function $\Gamma(a)$. 
**Definition.** If \( A = X^t X \), where the \( n \times p \) matrix \( X \) is \( N_p(0, I_n \otimes \Sigma) \), then \( A \) is said to have Wishart distribution with \( n \) degrees of freedom and covariance matrix \( \Sigma \). We write \( A \) is \( W_p(n, \Sigma) \).
Multivariate generalization

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**Theorem** (Wishart 1928). If $A$ is $W_p(n, \Sigma)$ with $n \geq p$, then the density function of $A$ is

$$
\frac{1}{2^p n^p/2 \Gamma_p(n/2) (\det \Sigma)^{n/2}} e^{-\frac{1}{2} \text{Tr}(\Sigma^{-1} A)} (\det A)^{(n-p-1)/2}.
$$
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Theorem (Wishart 1928). If $A$ is $W_p(n, \Sigma)$ with $n \geq p$, then the density function of $A$ is

$$
\frac{1}{2^{pn/2} \Gamma_p(n/2) (\det \Sigma)^{n/2}} e^{-\frac{1}{2} \text{Tr}(\Sigma^{-1} A)} (\det A)^{(n-p-1)/2}.
$$

For $p = 1$ and $\Sigma = 1$ this reduces to the univariate Pearson $\chi^2$ density. The case $p = 2$ was obtained by Fisher in 1915 and for general $p$ by Wishart in 1928 using geometrical arguments. Most modern proofs follow James.
Importance of Wishart density

Fact: the sample covariance matrix, $S$, is $W_p(n, \frac{1}{n} \Sigma)$ where

$$S := \frac{1}{n} \sum_{j=1}^{N} (X_i - \overline{X}) \otimes (X_j - \overline{X}), \quad N = n + 1,$$

and $X_j$, $j = 1, \ldots, N$, are independent $N_p(\mu, \Sigma)$ random vectors, and $\overline{X} = \frac{1}{N} \sum_j X_j$. 
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and $X_j$, $j = 1, \ldots, N$, are independent $N_p(\mu, \Sigma)$ random vectors, and $\overline{X} = \frac{1}{N} \sum_j X_j$.

Principle component analysis, a multivariate data reduction technique, requires the eigenvalues of the sample covariance matrix; in particular, the largest eigenvalue (the largest principle component variance) is most important.
Joint pdf for Wishart matrix eigenvalues

**Theorem** (James 1964). If $A$ is $W_p (n, \Sigma)$ with $n \geq p$ the joint density function of the eigenvalues $\ell_1, \ldots, \ell_p$ of $A$ is

$$
\frac{\pi^{p^2/2} 2^{-pn/2} (\det \Sigma)^{-n/2}}{\Gamma_p(p/2)\Gamma_p(n/2)} \prod_{j=1}^{p} \ell_j^{(n-p-1)/2} \prod_{j<k} (\ell_j - \ell_k) 
\cdot \int_{\text{O}(p)} e^{-\frac{1}{2} \operatorname{Tr}(\Sigma^{-1}HLH^t)} \, dH
$$

where $\text{O}(p)$ is the orthogonal group of $p \times p$ matrices, $dH$ is normalized Haar measure and $L$ is the diagonal matrix $\text{diag}(\ell_1, \ldots, \ell_p)$. (We take $\ell_1 > \ell_2 > \cdots > \ell_p$.)
Evaluation of joint pdf

\[
\frac{\pi p^2/2^{p/2} n^{n/2}}{\Gamma_p(p/2) \Gamma_p(n/2)} \prod_{j=1}^{p} \ell_j^{(n-p-1)/2} \prod_{j<k} (\ell_j - \ell_k) \cdot \int_{\mathcal{O}(p)} e^{-\frac{1}{2} \text{Tr}(\Sigma^{-1} H LH^t)} \, dH
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Problem: the integral over the orthogonal group \( \mathbb{O}(p) \).
Evaluation of joint pdf

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Problem: the integral over the orthogonal group \( \mathbb{O}(p) \).

No known closed formula though James and Constantine developed the theory of zonal polynomials which allow one to write infinite series expansions for this integral.
\[
\frac{\pi p^2/2 \cdot 2^{-p n/2} (\det \Sigma)^{-n/2}}{\Gamma_p(p/2) \Gamma_p(n/2)} \prod_{j=1}^{p} \ell_j^{(n-p-1)/2} \prod_{j<k} (\ell_j - \ell_k) \cdot \int_{\mathbb{O}(p)} e^{-\frac{1}{2} \text{Tr}(\Sigma^{-1} H L H^t)} dH
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Expansions converge slowly and zonal polynomials themselves lack explicit formulas such as are available for Schur polynomials.
Evaluation of joint pdf 2

\[ \frac{\pi^{p^2/2}2^{-pn/2}}{\Gamma_p(p/2)\Gamma_p(n/2)} \frac{(\det \Sigma)^{-n/2}}{2} \prod_{j=1}^{p} \ell_j^{(n-p-1)/2} \prod_{j<k} (\ell_j - \ell_k) \cdot \int_{\mathbb{O}(p)} e^{-\frac{1}{2} \text{Tr}(\Sigma^{-1}HLH^t)} dH \]

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For complex Wishart matrices, the group integral is over the unitary group \( \mathbb{U}(p) \); this integral can be evaluated using the Harish-Chandra-Itzykson-Zuber integral (Zinn–Justin ’03).
Evaluation of joint pdf 3

There is one important case where the integral can be (trivially) evaluated.

**Corollary.** If $\Sigma = I_p$, then the joint density simplifies to

$$
\frac{\pi^{p^2/2} 2^{-pn/2} (\det \Sigma)^{-n/2}}{\Gamma_p(p/2) \Gamma_p(n/2)} \prod_{j=1}^{p} \ell_j^{(n-p-1)/2} \exp \left( -\frac{1}{2} \sum_j \ell_j \right) \prod_{j<k} (\ell_j - \ell_k).
$$

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Connection to RMT

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Definition.

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

$$\sigma_{np} = \left(\sqrt{n-1} + \sqrt{p}\right) \left(\frac{1}{\sqrt{n-1}} + \frac{1}{\sqrt{p}}\right)^{1/3}.$$
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**Theorem** (Johnstone ’01). Under the null hypothesis $\Sigma = I_p$, if $n, p \to \infty$ such that $n/p \to \gamma, 0 < \gamma < \infty$, then

$$\frac{\ell_1 - \mu_{np}}{\sigma_{np}} \xrightarrow{D} F_1(s, 1).$$
Theorem (Soshnikov, ’02). If \( n, p \to \infty \) such that \( n/p \to \gamma, 0 < \gamma < \infty \), then

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\frac{\ell_m - \mu_{np}}{\sigma_{np}} \xrightarrow{\mathcal{D}} F_1(s, m), \ m = 1, 2, \ldots.
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Important additional assumption: \( n - p = O(p^{1/3}) \).
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Generalization of Johnstone’s proof (’01) together with 
results of Dieng (’05) show this restriction can be removed.
Connection to RMT 2

**Theorem** (Soshnikov, ’02). If \( n, p \to \infty \) such that \( n/p \to \gamma, 0 < \gamma < \infty \), then

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Subsequently, El Karoui (’03) extended Soshnikov’s Theorem to \( 0 < \gamma \leq \infty \); extension to \( \gamma = \infty \) is important for modern statistics where \( p \gg n \) arises in applications.
Soshnikov lifted the Gaussian assumption, again establishing a $F_1$ universality theorem.
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Redefine the $n \times p$ matrices $X = \{x_{i,j}\}$ such that $A = X^t X$ to satisfy

1. $\mathbb{E}(x_{ij}) = 0$, $\mathbb{E}(x_{ij}^2) = 1$.

2. The random variables $x_{ij}$ have symmetric laws of distribution.

3. All even moments of $x_{ij}$ are finite, and they decay at least as fast as a Gaussian at infinity:

$$\mathbb{E}(x_{ij}^{2m}) \leq (\text{const } m)^m.$$ 

4. $n - p = O(p^{1/3})$. 

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Connection to RMT 4

With these assumptions, 

**Theorem** (Soshnikov ’02).

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It is an important open problem to remove the restriction 

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\]

It is an important open problem to remove the restriction \( n - p = O(p^{1/3}) \).

Deift and Gioev (’05), building on the work of Widom (’99), proved \( F_1 \) universality when the Gaussian weight function \( \exp(-x^2) \) is replaced by \( \exp(-V(x)) \) where \( V \) is an even degree polynomial with positive leading coefficient.
In the unitary case ($\beta = 2$), define the trace class operator $K_2$ on $L^2(s, \infty)$ with *Airy kernel*

$$K_{Ai}(x, y) := \frac{\text{Ai}(x) \text{Ai}'(y) - \text{Ai}'(x) \text{Ai}(y)}{x - y} = \int_0^\infty \text{Ai}(x+z) \text{Ai}(y+z) \, dz$$

and associated Fredholm determinant, $0 \leq \lambda \leq 1$,

$$D_2(s, \lambda) = \text{det}(I - \lambda K_2).$$
Fredholm det. representation ($\beta = 2$)

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Then

$$F_2(s, m + 1) - F_2(s, m) = \frac{(-1)^m}{m!} \frac{d^m}{d \lambda^m} D_2(s, \lambda) \bigg|_{\lambda=1}, \quad m \geq 0,$$

where $F_2(s, 0) \equiv 0$.
Fredholm det. representation ($\beta = 1, 4$)

$$K_4(x, y) := \frac{1}{2} \begin{pmatrix} S_4(x, y) & SD_4(x, y) \\ IS_4(x, y) & S_4(y, x) \end{pmatrix}$$
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where

\[ S_4(x, y) = K_{Ai}(x, y) - \frac{1}{2} \text{Ai}(x, y) \int_y^\infty \text{Ai}(z) \, dz, \]
\[ SD_4(x, y) = -\partial_y S_4(x, y) \quad \text{and} \quad IS_4(x, y) = \varepsilon S_4(x, y) \]
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and the associated Fredholm determinant, \(0 \leq \lambda \leq 1\),

\[
D_4(s, \lambda) = \det(I - \lambda K_4\chi_{(s,\infty)}).
\]
Fredholm det. representation ($\beta = 1, 4$)

In the orthogonal case ($\beta = 1$)

$$K_1(x, y) := \begin{pmatrix} S_1(x, y) & SD_1(x, y) \\ IS_1(x, y) - \varepsilon(x, y) & S_1(y, x) \end{pmatrix}$$
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where

\[
\varepsilon(x - y) = \frac{1}{2} \text{sgn}(x - y).
\]

\[
S_1(x, y) = K_{\text{Ai}}(x, y) - \frac{1}{2} \text{Ai}(x) \left( 1 - \int_y^\infty \text{Ai}(z) \, dz \right),
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$$D_1(s, \lambda) = \text{det}_2(I - \lambda K_1 \chi(s, \infty))$$
Recall that in the unitary ($\beta = 2$) case we have the recurrence

$$F_2(s, m + 1) - F_2(s, m) = \frac{(-1)^m}{m!} \frac{d^m}{d \lambda^m} D_2(s, \lambda) \bigg|_{\lambda=1}, \quad m \geq 0,$$

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Fredholm det. representation \((\beta = 1, 4)\)

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where \(F_2(s, 0) \equiv 0\).

Similarly in the orthogonal and symplectic \((\beta = 1, 4)\) case

\[
F_\beta(s, m + 1) - F_\beta(s, m) = \frac{(-1)^m}{m!} \frac{d^m}{d\lambda^m} D^{1/2}_\beta(s, \lambda) \bigg|_{\lambda=1}, \quad m \geq 0,
\]

where \(\beta = 1, 4\) and \(F_\beta(s, 0) \equiv 0\).
Painlevé representations

**Theorem** (Clarkson, McLeod, ’88). There exist a unique solution $q(x, \lambda)$ to the Painlevé II equation

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

such that $q \to \sqrt{\lambda} \text{Ai}$ as $x \to \infty$ and $\text{Ai}(x)$ is the solution to the Airy equation that decays like $\frac{1}{2} \pi^{-1/2} x^{-1/4} \exp\left(-\frac{2}{3} x^{3/2}\right)$ at $+\infty$. 

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**Definition.**

$$\mu(s, \lambda) := \int_s^\infty q(x, \lambda) \, dx,$$

$$\tilde{\lambda} := 2 \lambda - \lambda^2,$$
Painlevé representations 2

We have the following (computationally useful) Painlevé representations
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**Theorem** (Tracy & Widom ’94).

\[ D_2(s, \lambda) = \exp \left[ - \int_s^\infty (x - s) q^2(x, \lambda) \, dx \right]. \]
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\]

**Theorem** (Dieng ’05).

\[
D_1(s, \lambda) = D_2(s, \tilde{\lambda}) \frac{\lambda - 1 - \cosh \mu(s, \tilde{\lambda}) + \sqrt{\lambda} \sinh \mu(s, \tilde{\lambda})}{\lambda - 2},
\]

\[
D_4(s, \lambda) = D_2(s, \lambda) \cosh^2 \left( \frac{\mu(s, \lambda)}{2} \right).
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D_1(s, \lambda) = D_2(s, \tilde{\lambda}) \frac{\lambda - 1 - \cosh \mu(s, \tilde{\lambda}) + \sqrt{\tilde{\lambda}} \sinh \mu(s, \tilde{\lambda})}{\lambda - 2},
\]

\[
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\]

**Software:** [http://math.arizona.edu/~momar](http://math.arizona.edu/~momar)
Edgeworth expansions

If $S_n$ is a sum of i.i.d. random variables $X_j$, each with mean $\mu$ and variance $\sigma^2$, the distribution $F_n$ of the normalized random variable $(S_n - n\mu)/(\sigma \sqrt{n})$ satisfies the Edgeworth expansion

$$F_n(x) - \Phi(x) = \phi(x) \sum_{j=3}^{r} n^{-\frac{1}{2}j+1} R_j(x) + o(n^{-\frac{1}{2}r+1})$$

uniformly in $x$; $\Phi$ is the standard normal distribution with density $\phi$, and $R_j$ are polynomials depending only on $\mathbb{E}(X_j^k)$ but not on $n$ and $r$ (or the underlying distribution of the $X_j$).
Following Tracy and Widom we define

\[
    u_i := u_i(s) = \int_s^{\infty} q(x)x^i \text{Ai}(x) \, dx,
\]

\[
    v_i := v_i(s) = \int_s^{\infty} q(x)x^i \text{Ai}'(x) \, dx
\]

and

\[
    w_i := w_i(s) = \int_s^{\infty} q'(x)x^i \text{Ai}'(x) \, dx + u_0(s)v_i(s)
\]
Following Tracy and Widom we define

\[ u_i := u_i(s) = \int_{s}^{\infty} q(x)x^i \text{Ai}(x) \, dx, \]

\[ v_i := v_i(s) = \int_{s}^{\infty} q(x)x^i \text{Ai}'(x) \, dx \]

and

\[ w_i := w_i(s) = \int_{s}^{\infty} q'(x)x^i \text{Ai}'(x) \, dx + u_0(s)v_i(s) \]

Let \( c \) be an arbitrary constant (tuning parameter) and

\[ E(s) = 2w_1 - 3u_2 + (-20c^2 + 3)v_0 + u_1v_0 - u_0v_1 + u_0v_0^2 - u_0^2w_0, \]
Theorem (Choup ’06). Setting

\[ t = (2(n + c))^{\frac{1}{2}} + 2^{-\frac{1}{2}} n^{-\frac{1}{6}} s \]

Then as \( n \to \infty \)

\[ F_{n,2}(t) = F_2(s) \left\{ 1 + c u_0(s) n^{-\frac{1}{3}} - \frac{1}{20} E(s) n^{-\frac{2}{3}} \right\} + O(n^{-1}) \]

uniformly in \( s \).
One key consequence of Choup’s work is the expansion for
\[ R_n(x, y) = (I - K_{n,2} \chi_{(s,\infty)}) \].
One key consequence of Choup’s work is the expansion for $R_n(x, y) = (I - K_{n,2} \chi_{(s,\infty)})$. Let

$$x = (2(n + c))^{\frac{1}{2}} + 2^{-\frac{1}{2}} n^{-\frac{1}{6}} X, \quad y = (2(n + c))^{\frac{1}{2}} + 2^{-\frac{1}{2}} n^{-\frac{1}{6}} Y$$

$$Q_i(s) := (I - K_{Ai}) X^i \text{Ai}(X) \quad \text{and} \quad P_i(s) := (I - K_{Ai}) X^i \text{Ai}'(X)$$
One key consequence of Choup’s work is the expansion for
\( R_n(x, y) = (I - K_{n,2} \chi_{(s,\infty)}) \). Let

\[
x = (2(n + c))^{\frac{1}{2}} + 2^{-\frac{1}{2}} n^{-\frac{1}{6}} X, \quad y = (2(n + c))^{\frac{1}{2}} + 2^{-\frac{1}{2}} n^{-\frac{1}{6}} Y
\]

\( Q_i(s) := (I - K_{Ai}) X^i \text{Ai}(X) \) and \( P_i(s) := (I - K_{Ai}) X^i \text{Ai}'(X) \)

Then

\[
R_n(x, y) = R(X, Y) - c Q \otimes Q n^{-1/3} + \\
+ \frac{n^{-2/3}}{20} \left[ P_1 \otimes P + P \otimes P_1 - Q_2 \otimes Q - Q_1 \otimes Q_1 \\
- Q \otimes Q_2 + \frac{3 - 20 c^2}{2} (P \otimes Q + Q \otimes P) + \\
+ 20 c^2 u_0(s) Q \otimes Q \right] + O \left( n^{-1} \right)
\]
In the $\beta = 1, 4$ cases we have the formulas (Tracy and Widom)

\[
F_{n,1}(t) = (1 - \tilde{v}_\epsilon) \left( 1 - \frac{1}{2} R_1 \right) - \frac{1}{2} (q_\epsilon - c_\varphi) P_1,
\]

\[
F_{n,4}(t/\sqrt{2}) = (1 - \tilde{v}_\epsilon) \left( 1 + \frac{1}{2} R_4 \right) + \frac{1}{2} q_\epsilon P_4,
\]
Edgeworth expansions 5

In the $\beta = 1, 4$ cases we have the formulas (Tracy and Widom)

$$F_{n,1}(t) = (1 - \tilde{v}_\varepsilon)(1 - \frac{1}{2}\mathcal{R}_1) - \frac{1}{2}(q_\varepsilon - c_\varphi)\mathcal{P}_1,$$

$$F_{n,4}(t/\sqrt{2}) = (1 - \tilde{v}_\varepsilon)(1 + \frac{1}{2}\mathcal{R}_4) + \frac{1}{2}q_\varepsilon\mathcal{P}_4,$$

All quantities are expressible in terms of $R_n(x, y)$ and other quantities whose known expansions can be used in the above formulas. Details are rather messy, so we leave them for private discussions.