Approximating Tracy–Widom distributions

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Univariate Statistics

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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

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

Multivariate Statistics

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

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

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,

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then we say X is $N_p(\mathbf{1} \otimes \mu, I_n \otimes \Sigma)$ where $\mathbf{1} = (1, 1, \ldots, 1)$ and I_n is the $n \times n$ identity matrix.

Multivariate Gamma function

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

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

where $\mathrm{Re}(a) > (m-1)/2$ and dA is the product Lebesgue measure of the $\frac{1}{2}p(p+1)$ distinct elements of A.

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$\Gamma_1(a)$ is the usual gamma function $\Gamma(a)$.

Multivariate generalization

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* Σ*. We write* A *is* $W_p(n, \Sigma)$*.*

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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*

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

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For $p = 1$ and $\Sigma = 1$ this reduces to the univariate Pearson χ^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

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

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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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*

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

$$\cdot \int_{\mathbb{O}(p)} e^{-\frac{1}{2}\operatorname{Tr}(\Sigma^{-1} H L H^t)}\, dH$$

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

Evaluation of joint pdf

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

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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.

Evaluation of joint pdf 2

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Expansions converge slowly and zonal polynomials themselves lack explicit formulas such as are available for Schur polynomials.

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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*

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

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*

$$\frac{\ell_1 - \mu_{np}}{\sigma_{np}} \xrightarrow{\mathscr{D}} F_1(s, 1).$$

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.

Connection to RMT 3

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

Connection to RMT 4

With these assumptions,

Theorem (Soshnikov '02)**.**

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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.

Fredholm det. representation ($\beta = 2$)

In the unitary case ($\beta = 2$), define the trace class operator K_2 on $L^2(s, \infty)$ with *Airy kernel*

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

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

$$D_2(s, \lambda) = \det(I - \lambda\,K_2).$$

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Then

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

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

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

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$$\begin{aligned} S_4(x,y) &= K_{\mathsf{Ai}}(x,y) - \frac{1}{2}\,\mathsf{Ai}(x,y)\int_y^\infty \mathsf{Ai}(z)\,dz, \\ SD_4(x,y) &= -\partial_y S_4(x,y) \quad \text{and} \quad IS_4(x,y) = \varepsilon S_4(x,y) \end{aligned}$$

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

Recall that in the unitary ($\beta = 2$) case we have the recurrence

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

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

$$F_\beta(s, m+1) - F_\beta(s, m) = \frac{(-1)^m}{m\,!} \frac{d^m}{d\,\lambda^m} D_\beta^{1/2}(s, \lambda)\Big|_{\lambda=1}, \quad m \geq 0,$$

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 $q \longrightarrow \sqrt{\lambda}$ *Ai as* $x \longrightarrow \infty$ *and 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.

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

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

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Theorem (Dieng '05)**.**

$$\begin{aligned} D_1(s,\lambda) &= D_2(s,\tilde{\lambda})\, \frac{\lambda - 1 - \cosh\mu(s,\tilde{\lambda}) + \sqrt{\tilde{\lambda}}\,\sinh\mu(s,\tilde{\lambda})}{\lambda-2}, \\ D_4(s,\lambda) &= D_2(s,\lambda)\,\cosh^2\left(\frac{\mu(s,\lambda)}{2}\right). \end{aligned}$$

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Software: `http://math.arizona.edu/~momar`

Edgeworth expansions

If S_n is a sum of i.i.d. random variables X_j, each with mean μ and variance σ^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; Φ is the standard normal distribution with density ϕ, 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).

Edgeworth expansions 2

Following Tracy and Widom we define

$$\begin{aligned} u_i &:= u_i(s) = \int_s^\infty q(x) x^i \,\mathsf{Ai}(x)\, dx, \\ v_i &:= v_i(s) = \int_s^\infty q(x) x^i \,\mathsf{Ai}'(x)\, dx \end{aligned}$$

and

$$w_i := w_i(s) = \int_s^\infty q'(x) x^i \,\mathsf{Ai}'(x)\, dx \; + \; u_0(s) v_i(s)$$

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$$\begin{aligned} u_i &:= u_i(s) = \int_s^\infty q(x) x^i \, \mathsf{Ai}(x)\, dx, \\ v_i &:= v_i(s) = \int_s^\infty q(x) x^i \, \mathsf{Ai}'(x)\, dx \end{aligned}$$

and

$$w_i := w_i(s) = \int_s^\infty q'(x) x^i \, \mathsf{Ai}'(x)\, dx \; + \; u_0(s) v_i(s)$$

Let c be an arbitrary constant (tuning parameter) and

$$E(s) = 2w_1 - 3u_2 + (-20c^2 + 3)v_0 + u_1 v_0 - u_0 v_1 + u_0 v_0^2 - u_0^2 w_0,$$

Edgeworth expansions 3

Theorem (Choup '06)**.** *Setting*

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

Then as $n \to \infty$

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

uniformly in s.

Edgeworth expansions 4

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

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Then

$$\begin{aligned} R_n(x,y) \quad = \quad & R(X,Y) - c\, Q \otimes Q\, n^{-1/3} + \\ & + \frac{n^{-2/3}}{20} \left[P_1 \otimes P + P \otimes P_1 - Q_2 \otimes Q - Q_1 \otimes Q_1 \right. \\ & - Q \otimes Q_2 + \frac{3 - 20\, c^2}{2} \left(P \otimes Q + Q \otimes P \right) + \\ & \left. + 20\, c^2\, u_0(s)\, Q \otimes Q \right] + O\left(n^{-1}\right) \end{aligned}$$

Edgeworth expansions 5

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

$$
\begin{aligned}
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,
\end{aligned}
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Edgeworth expansions 5

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

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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.