

Computing Eigenvalues of Random Matrices

Plamen Koev
Department of Mathematics
North Carolina State University

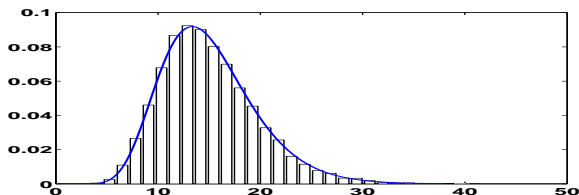
Joint work with:

Cy Chan, Vesselin Drensky, Alan Edelman, Iain Johnstone, Raymond Kan

Foundations of Computational Mathematics, Hong Kong, June 26, 2008

Goal

- ▶ Efficiently computing the distributions of
 - ▶ eigenvalues and functions thereof
 - ▶ of Wishart, Jacobi, Laguerre
 - ▶ any Σ
 - ▶ real, complex, any β ?
 - ▶ efficiently
- ▶ **Example:** λ_{\max} of 4×4 Wishart with 7 DOF



- ▶ **Exact** vs Empirical with 20,000 replications

(Central) Wishart Matrix: Real Case

► Definition:

$$A = X^T X \in \mathbb{R}^{m \times m}, \quad \text{where } X \sim \mathcal{N}(0, I_n \otimes \Sigma) \in \mathbb{R}^{n \times m}$$

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► Joint **element** density*:

$$|\Sigma|^{-\frac{n}{2}} |A|^{\frac{n-m+1}{2}-1} e^{-\text{tr}(\frac{1}{2}\Sigma^{-1}A)}$$

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► Joint **eigenvalue** density:

$$(\det \Sigma)^{-\frac{n}{2}} \prod_{i=1}^m \lambda_i^{\frac{n-m+1}{2}-1} \prod_{j < k} |\lambda_k - \lambda_j| \cdot {}_0F_0^{(1)}(-\frac{1}{2}\Lambda, \Sigma^{-1}),$$

where

$${}_0F_0^{(1)}(X, Y) = \sum_{k=0}^{\infty} \sum_{\kappa \vdash k} \frac{1}{k!} \cdot \frac{C_{\kappa}^{(1)}(X) C_{\kappa}^{(1)}(Y)}{C_{\kappa}^{(1)}(I)}$$

(Central) Wishart Matrix: Complex Case

► Definition:

$$A = X^* X \in \mathbb{C}^{m \times m}, \quad \text{where } X \sim \mathcal{CN}(0, I_n \otimes \Sigma) \in \mathbb{C}^{n \times m}$$

► Joint element density*:

$$|\Sigma|^{-\frac{n}{i}} |A|^{\frac{n-m+1}{i}-1} e^{-\text{tr}(\frac{1}{i} \Sigma^{-1} A)}$$

► Joint eigenvalue density:

$$(\det \Sigma)^{-\frac{n}{i}} \prod_{i=1}^m \lambda_i^{\frac{n-m+1}{i}-1} \prod_{j < k} |\lambda_k - \lambda_j|^2 \cdot {}_0F_0^{(2)}(-\frac{1}{i} \Lambda, \Sigma^{-1}),$$

where

$${}_0F_0^{(2)}(X, Y) = \sum_{k=0}^{\infty} \sum_{\kappa \vdash k} \frac{1}{k!} \cdot \frac{C_{\kappa}^{(2)}(X) C_{\kappa}^{(2)}(Y)}{C_{\kappa}^{(2)}(I)}$$

Wishart Matrix: Real/Complex/Quaternion ($\beta = 1, 2, 4$)

► Definition:

$$A = X^D X, \quad \text{where } X \sim \mathcal{N}^{(\beta)}(0, I_n \otimes \Sigma)$$

► Joint **element** density*:

$$|\Sigma|^{-\frac{n\beta}{2}} |A|^{\frac{(n-m+1)\beta}{2}-1} e^{-\text{tr}(\frac{\beta}{2}\Sigma^{-1}A)}$$

► Joint **eigenvalue** density:

$$(\det \Sigma)^{-\frac{n\beta}{2}} \prod_{i=1}^m \lambda_i^{\frac{(n-m+1)\beta}{2}-1} \prod_{j < k} |\lambda_k - \lambda_j|^\beta \cdot {}_0F_0^{(\beta)}\left(-\frac{\beta}{2}\Lambda, \Sigma^{-1}\right),$$

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- ▶ Joint eigenvalue density (well defined for any $\beta > 0$):

$$(\det \Sigma)^{-\frac{n\beta}{2}} \prod_{i=1}^m \lambda_i^{\frac{(n-m+1)\beta}{2}-1} \prod_{j < k} |\lambda_k - \lambda_j|^\beta \cdot {}_0F_0^{(\beta)}\left(-\frac{\beta}{2}\Lambda, \Sigma^{-1}\right),$$

where

$${}_0F_0^{(\beta)}(X, Y) = \sum_{k=0}^{\infty} \sum_{\kappa \vdash k} \frac{1}{k!} \cdot \frac{C_{\kappa}^{(\beta)}(X) C_{\kappa}^{(\beta)}(Y)}{C_{\kappa}^{(\beta)}(I)}$$

Introducing the Beta-Wishart Matrix

- ▶ Def. (for any $\beta > 0$): A matrix with joint eigenvalue density

$$(\det \Sigma)^{-\frac{n\beta}{2}} \prod_{i=1}^m \lambda_i^{\frac{(n-m+1)\beta}{2}-1} \prod_{j < k} |\lambda_k - \lambda_j|^\beta \cdot {}_0F_0^{(\beta)}\left(-\frac{\beta}{2}\Lambda, \Sigma^{-1}\right)$$

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- ▶ Extends the Beta-Laguerre model (Dumitriu/Edelman)
- ▶ Extends the Beta-Jacobi model (Dumitriu/K)
- ▶ All one needs to derive distributions of λ_j 's, det, tr, etc.

λ_{\max} of a Beta-Wishart Matrix

- ▶ Joint eigenvalue density

$$(\det \Sigma)^{-\frac{n\beta}{2}} \prod_{i=1}^m \lambda_i^{\frac{(n-m+1)\beta}{2}-1} \prod_{j < k} |\lambda_k - \lambda_j|^{\beta} \cdot {}_0F_0^{(\beta)}\left(-\frac{\beta}{2}\Lambda, \Sigma^{-1}\right)$$

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- ▶ Distribution of λ_{\max}

$$P(\lambda_{\max} < x) = c \int_{[0,x]^m} \prod_{i=1}^m \lambda_i^{\frac{(n-m+1)\beta}{2}-1} \prod_{j < k} |\lambda_k - \lambda_j|^\beta {}_0F_0^{(\beta)}\left(-\frac{\beta}{2}\Lambda, \Sigma^{-1}\right) d\Lambda$$

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- ▶ Distribution of λ_{\max}

$$\begin{aligned} P(\lambda_{\max} < x) &= \mathbf{c} \int_{[0,x]^m} \prod_{i=1}^m \lambda_i^{\frac{(n-m+1)\beta}{2}-1} \prod_{j < k} |\lambda_k - \lambda_j|^\beta {}_0F_0^{(\beta)}\left(-\frac{\beta}{2}\Lambda, \Sigma^{-1}\right) d\Lambda \\ &= \mathbf{c} x^{\frac{mn\beta}{2}} \int_{[0,1]^m} \prod_{i=1}^m \lambda_i^{\frac{(n-m+1)\beta}{2}-1} \prod_{j < k} |\lambda_k - \lambda_j|^\beta {}_0F_0^{(\beta)}\left(\Lambda, -\frac{x\beta}{2}\Sigma^{-1}\right) d\Lambda \end{aligned}$$

λ_{\max} of a Beta-Wishart Matrix

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It all comes down to computing ${}_pF_q^{(\beta)}$

$${}_pF_q^{(\beta)}(a; b; X, Y) = \sum_{k=0}^{\infty} \sum_{\kappa \vdash k} c_{\kappa}(a, b) \frac{c_{\kappa}^{(\beta)}(X) c_{\kappa}^{(\beta)}(Y)}{c_{\kappa}^{(\beta)}(I)}$$

- ▶ No alternative expressions known, except for $\beta = 2$
- ▶ Approximate by truncating for $k \leq M$; still very hard

Previous Best Algorithm for ${}_pF_q$ on a 5×5 matrix

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ETNA
Kent State University
etna@mcs.kent.edu

APPROXIMATION OF HYPERGEOMETRIC FUNCTIONS WITH MATRICIAL ARGUMENT THROUGH THEIR DEVELOPMENT IN SERIES OF ZONAL POLYNOMIALS*

R. GUTIÉRREZ[†], J. RODRIGUEZ[‡], AND A. J. SÁEZ[§]

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► New result (2.33 GHz Pentium):

```
>> tic; mhg(20, 2, [], [], [1 : 5]/15), toc  
ans = 2.71828182845905  
elapsed_time = 0.031000000000000
```

Computing ${}_pF_q$ efficiently

$${}_pF_q^{(\beta)}(\cdot; \cdot; X) = \sum_{k=0}^{\infty} \sum_{\kappa \vdash k} a_{\kappa} \cdot C_{\kappa}^{(\beta)}(x_1, \dots, x_n)$$

- ▶ $C_{\kappa}^{(\beta)}(X) = C_{\kappa}^{(\beta)}(x_1, \dots, x_n) =$ **Jack function**
- ▶ orthogonal basis of $\Pi(x_1, \dots, x_n)$
- ▶ Indexed by **partitions** κ :
Leading terms: $x_1, x_1^2, x_1 x_2, x_1^3, x_1^2 x_2, x_1 x_2 x_3, \dots$
- ▶ Even a single $C_{\kappa}^{(\alpha)}$ very hard—sum of exp many terms

Naive Cost of Jacks ($\beta = 2$; $C_{\kappa}^{(1)} = s_{\kappa}$)

Degree	Partition κ	s_{κ}	Number of terms
1	(1)	$x_1 + \cdots + x_n$	$\mathcal{O}(n)$
2	(2)	$\sum_{i < j} x_i x_j$	$\mathcal{O}(n^2)$
2	(1, 1)	$\sum_{i < j} x_i x_j$	$\mathcal{O}(n^2)$
3	(1, 1, 1)	$\sum_{i < j < k} x_i x_j x_k$	$\mathcal{O}(n^3)$
$ \kappa $	κ	$\sum x_1^{\kappa_1} \cdots x_n^{\kappa_n}$	$\mathcal{O}(n^{ \kappa })$

► New result: $\mathcal{O}(n)$ each

Computing the Schur Polynomial “Cleverly” ($\beta = 2$)

- ▶ s_{κ} of higher degree “contain” s_{λ} of lower degree.
Redundancy.

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Redundancy.
- ▶ E.g.:

$$\begin{aligned} s_{(1,1)}(x_1, \dots, x_n) &= \sum_{i < j} x_i x_j \\ &= x_1 x_2 + (x_1 + x_2) x_3 + \dots + (x_1 + \dots + x_{n-1}) x_n \end{aligned}$$

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- ▶ In general:

$$s_\kappa(x_1, x_2, \dots, x_n) = \sum_{\lambda < \kappa} s_\lambda(x_1, x_2, \dots, x_{n-1}) \cdot x_n^{|\kappa| - |\lambda|}$$

- ▶ Connection with representation theory:
 - ▶ s_κ are the irreducible characters of $\mathrm{GL}_n(\mathbb{C})$
 - ▶ the characters of $\mathrm{GL}_{n-1}(\mathbb{C})$ induce those of $\mathrm{GL}_n(\mathbb{C})$
- ▶ Result long known (Macdonald), but missed for 40 years

Computing the Schur Polynomial “Cleverly”

► Example: $s_{(1,1)}(x_1, \dots, x_n)$

$$= \sum_{i < j} x_i x_j \quad (\sim n^2 \text{ operations})$$

$$= \underbrace{x_1}_{s_1} x_2 + \underbrace{(x_1 + x_2)}_{s_2} x_3 + \underbrace{(x_1 + x_2 + x_3)}_{s_3} x_4 + \cdots + \underbrace{(x_1 + \cdots + x_{n-1})}_{s_{n-1}} x_n$$

Computing the Schur Polynomial “Cleverly”

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- ▶ New cost: $3n - 2$ instead of n^2
- ▶ Generalizes to all κ :
Cost of $s_\kappa(x_1, \dots, x_n)$ goes down from $\mathcal{O}(n^{|\kappa|})$ to $\mathcal{O}(N_\kappa n)$
- ▶ This trick made all the difference and works for all $\beta > 0$
- ▶ For $\beta = 2$ it gets better:
We can get rid of $N_\kappa \equiv \{ \#\lambda \mid \lambda < \kappa \}$

Analogy with the FFT

- ▶ Idea: $(\text{DFT})_{ij}$ —char. of $\mathbb{Z}/n\mathbb{Z}$ \longleftrightarrow s_λ —char. of $\text{GL}_n(\mathbb{C})$
- ▶ Our main identity

$$s_\kappa(x_1, x_2, \dots, x_n) = \sum_{\lambda < \kappa} s_\lambda(x_1, x_2, \dots, x_{n-1}) \cdot x_n^{|\kappa| - |\lambda|}$$

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in matrix form is $S_n = S_{n-1} \cdot Y_n(x_n)$, where

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in matrix form is $S_n = S_{n-1} \cdot Y_n(x_n)$, where

$$Y = \left[\begin{array}{cccc|cccc|cccc|cccc} 1 & x & x^2 & x^3 & x & x^2 & x^3 & x^4 & x^2 & x^3 & x^4 & x^5 & x^3 & x^4 & x^5 & x^6 \\ & 1 & x & x^2 & & x & x^2 & x^3 & & x & x^2 & x^3 & & x^3 & x^4 & x^5 & x^6 \\ & & 1 & x & & & x & x^2 & & & x & x^2 & & & x^3 & x^4 & x^5 & x^6 \\ & & & 1 & & & & x & & & & x & & & & x^3 & x^4 & x^5 & x^6 \end{array} \right]$$

$$\left[\begin{array}{cccc} 1 & x & x^2 & x^3 \\ & 1 & x & x^2 \\ & & 1 & x \\ & & & 1 \end{array} \right]^{-1} = \left[\begin{array}{cccc} 1 & -x & & \\ & 1 & -x & \\ & & 1 & -x \\ & & & 1 \end{array} \right]$$

- ▶ Matrix-vector multipl. now costs $\mathcal{O}(n)$ instead of $\mathcal{O}(nN_\kappa)$

Our New Fast Algorithm

- ▶ $A \equiv$ lower shift matrix ($a_{i+1,i} = 1$); $B = A^T$
- ▶ Structure of Y_n :

$$\begin{aligned}U_n(x_n) &= I_{(N+1)^{n-1}} + x_n(A \otimes B_{n-1}) + \cdots + x_n^N(A^N \otimes B_{n-1}^N) \\ &= \left(I_{(N+1)^{n-1}} - x_n(A \otimes B_{n-1}) \right)^{-1}, \\ C_n(x_n) &= U_n(x_n)K_{n-1}(x_n), \\ K_n(x_n) &= I_{N+1} \otimes C_n(x_n), \\ B_n &= B_{n-1} \otimes I_{N+1} = B \otimes I_{(N+1)^{n-2}}, \\ Q_n(x_n) &= \left(I_{(N+1)^{n-1}} \mid x_n B_n \mid \cdots \mid x_n^N B_n^N \right) \\ Y_n &= Q_n(x_n)K_n(x_n)\end{aligned}$$

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- ▶ New algorithm:

```
for i=n:-1:1
    for all  $\lambda, |\lambda| \leq M$ , in reverse lex. order
         $s_\lambda = s_\lambda + s_{\lambda^{(i)}} x_n$ 
```

(where $\lambda^{(i)} \equiv (\lambda_1, \dots, \lambda_i - 1, \dots, \lambda_n)$)

- ▶ Final cost: $\mathcal{O}(n)$ per each s_λ , optimal

Open Problem: Can we extend the FFT idea to $\beta \neq 1$?

- ▶ How does one multiply quickly by the matrix ($\alpha \equiv 2/\beta$):

$$A = \begin{bmatrix} 1 & 1 & \frac{\alpha+1}{2} & \frac{(\alpha+1)(2\alpha+1)}{6} \\ & 1 & 1 & \frac{\alpha+1}{2} \\ & & 1 & 1 \\ & & & 1 \end{bmatrix}$$
$$= \begin{bmatrix} 1 & -\alpha & & \\ & 1 & -\alpha & \\ & & 1 & -\alpha \\ & & & 1 \end{bmatrix}^{-1/\alpha}$$

Open Problem: Beta-Wishart Matrix Model?

- ▶ A Beta-Wishart, $A = X^*X$, $X \sim N^{(\beta)}(0, I_n \otimes \Sigma)$
- ▶ To get $\lambda_i(X^*X)$ right suffices to get $\sigma_i(X)$ right

$$\begin{bmatrix} G & G & G & G \\ G & G & G & G \\ G & G & G & G \\ G & G & G & G \end{bmatrix} \times \Sigma^{1/2}$$

Open Problem: Beta-Wishart Matrix Model 2?

- ▶ A Beta-Wishart, $A = X^*X$, $X \sim N^{(\beta)}(0, I_n \otimes \Sigma)$
- ▶ To get $\lambda_i(X^*X)$ right suffices to get $\sigma_i(X)$ right

$$H \times \begin{bmatrix} \chi_{4\beta} & G & G & G \\ 0 & G & G & G \\ 0 & G & G & G \\ 0 & G & G & G \end{bmatrix} \times \Sigma^{1/2}$$

Open Problem: Beta-Wishart Matrix Model 3?

- ▶ A Beta-Wishart, $A = X^*X$, $X \sim N^{(\beta)}(0, I_n \otimes \Sigma)$
- ▶ To get $\lambda_i(X^*X)$ right suffices to get $\sigma_i(X)$ right

$$Q_4^{(\beta)} \begin{bmatrix} \chi_{4\beta} & \chi_{3\beta} & 0 & 0 \\ 0 & \chi_{3\beta} & \chi_{2\beta} & 0 \\ 0 & 0 & \chi_{2\beta} & \chi_\beta \\ 0 & 0 & 0 & \chi_\beta \end{bmatrix} \times Q_3^{(\beta)} \times \Sigma^{1/2}$$

Conclusions

- ▶ For small matrices takes less than a second to get the distributions
- ▶ Papers and software at: <http://www4.ncsu.edu/~pskoev>
- ▶ Impact on important applications:
 - ▶ 3D target classification
 - ▶ Genomics
 - ▶ Wireless communications

Future work

- ▶ New algorithms based on saddle point approximations
- ▶ Automatic convergence detection
- ▶ FFT generalization to zonal polynomials
- ▶ Tracy–Widom finite inference