Computations of the Expected Euler Characteristic for the Largest Eigenvalue of a Real Wishart Matrix

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Largest Eigenvalue of Real Wishart Matrix

Let $\xi_i \in \mathbb{R}^m$ be distributed as $N_m(\mu_i, \Sigma)$.

The Wishart distribution $W_m(n, \Sigma; \Omega)$ is induced by the random matrix

$$W = \Xi\Xi^\top, \quad \Xi = (\xi_1, \dots, \xi_n) \in \mathbb{R}^{m \times n},$$

where $\Omega = \Sigma^{-1} \sum_{i=1}^n \mu_i \mu_i^\top$ is the parameter matrix.

We call $W_m(n, \Sigma; \Omega)$ non-central if $\Omega \neq 0$.

Let $\lambda_1(W)$ be the largest eigenvalue of W. The distribution of $\lambda_1(W)$ is of particular interest in testing hypothesis.

Motivation and Previous works

Let $W_m(n, \Sigma; \Omega)$ be non-central.

Goal: Efficient evaluation of $\Pr(\lambda_1(W) \geq x)$ for many x.

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- (James *et al.*, 1954) When $\Omega = 0$, express $\Pr(\lambda_1(W) \geq x)$ as a hypergeometric function ${}_1F_1$
- (Hashiguchi *et al.*, 2013) Efficient evaluation of ${}_1F_1$ using holonomic gradient method
- (Danufane *et al.*, 2017) In MIMO problem, evaluation of $\Pr(\lambda_1(W) \geq x)$ if W is a complex matrix and $\Omega \neq 0$.

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- (Danufane *et al.*, 2017) In MIMO problem, evaluation of $\Pr(\lambda_1(W) \geq x)$ if W is a complex matrix and $\Omega \neq 0$.

Our contribution: Efficient evaluation of $\Pr(\lambda_1(W) \geq x)$ if W is a real matrix and $\Omega \neq 0$.

Euler Characteristic Method

Let $W_m(n, \Sigma; \Omega)$ be non-central and W be a real matrix.

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Adler, Tayler and Takemura (2000, 2005), Kuriki and Takemura (2001, 2008, 2009): Use Euler characteristic heuristic to approximate probabilities of random fields.

Fact: $\lambda_1(W)^{1/2}$ is the maximum of a Gaussian field

$$\left\{ u^\top \Xi v \mid \|u\|_{\mathbb{R}^m} = \|v\|_{\mathbb{R}^n} = 1 \right\}.$$

Idea: Approximation by the expected Euler characteristic heuristic:

$$\Pr(\lambda_1(W) \geq x) \approx E\left[\chi(M_x)\right] \quad \text{when } \ x \ \text{ is large,}$$

where M_x is a manifold induced by W and x.

Outline

- Explicit formula for the expectation of th Euler characteristic number of a manifold related to a random matrix

- Numerical evaluation for the integral formula by holonomic gradient method

Manifold of a Random Matrix

Let A be a real 2×2 random matrix. Define a manifold

$$M = \{hg^T \mid g \in S, h \in S\}.$$

Set

$$f(U) = \mathrm{tr}(UA), \quad U \in M,$$

and

$$M_x = \{U \in M \mid f(U) \geq x\},$$

which is a manifold induced by A and x.

Euler Characteristic Number

Let A be a real 2×2 random matrix and M_x be the related manifold.

Recall: The Euler characteristic is defined for the surfaces of polyhedra by

$$\chi = V - E + F.$$

For convex polyhedron's surface, $\chi = 2$.

We can also define the Euler characteristic for M_x and denote it by $\chi(M_x)$.

Expectation of the Euler Characteristic Number

Let A be a real 2×2 random matrix and M_x be the related manifold.

Recall: $f(U) = \mathrm{tr}(UA), \quad U \in M_x$.

Let hg^T be a critical point of f. Take $(g, G) \in SO(2)$ and $(h, H) \in SO(2)$. Set

$$\sigma = g^T A h, \; b = G^T A H,$$

which are singular values of A.

Theorem 1: Assume $x > 0$ and $f(U)$ is a Morse function for almost all A's. Then $E[\chi(M_x)]$ is equal to

$$\frac{1}{2} \int_x^{\infty} d\sigma \int_{-\infty}^{\infty} db \int_S G^T dg \int_S H^T dh (\sigma^2 - b^2) p(A).$$

Expectation of the Euler Characteristic Number

Recall: Approximation by the expected Euler characteristic heuristic:

$$\Pr(\lambda_1(W) \geq x) \approx E\big[\chi(M_x)\big] \quad \text{when} \;\; x \;\; \text{is large,}$$

where M_x is a manifold induced by $W = \Xi\Xi^T$ and x.

Goal: Efficient evaluation of the integral in Theorem 1 when W is a non-central Wishart matrix and x is large.

Expectation of the Euler Characteristic Number

Let $M = \begin{pmatrix} m_{11} & 0 \\ m_{21} & m_{22} \end{pmatrix}$ and $\Sigma = \begin{pmatrix} 1/s_1 & 0 \\ 0 & 1/s_2 \end{pmatrix}$ such that

$$\Xi = \sqrt{\Sigma} V + M, \text{ where } V = (v_{ij}), \; v_{ij} \sim \mathcal{N}(0,1) \text{ i.i.d.}$$

Then the integral in Theorem 1 becomes

$$\int_x^\infty d\sigma \int_{-\infty}^\infty db \int_{-\infty}^\infty ds \int_{-\infty}^\infty f(\sigma, b, s, t) dt, \tag{1}$$

where

$$f = \frac{s_1 s_2 (\sigma^2 - b^2)}{(1+s^2)(1+t^2)} \exp\left\{-\frac{1}{2} R\right\}, \quad R \in \mathbb{Q}(\sigma, b, s, t)$$

We denote (1) by $F(M, \Sigma; x)$.

Challenge for Evaluation

Assume $\Xi = \sqrt{\Sigma}V + M$, where $V = (v_{ij})$, $v_{ij} \sim \mathcal{N}(0,1)$ i. i. d..

- $F(M, \Sigma; x)$ contains parameters M, Σ.
- Numerical integration for $F(M, \Sigma; x)$ is time-consuming and not reliable for many x.

Observation: the integrand of $F(M, \Sigma; x)$ is holonomic (D-finite).

Idea: Use holonomic gradient method to evaluate $F(M, \Sigma; x)$.

Holonomic Gradient Method

$f(\theta, t)$: unnormalized probability distribution function w.r.t. $t = (t_1, \ldots, t_n)$, where $\theta = (\theta_1, \ldots, \theta_m)$ is a parameter vector.

$$z(\theta) = \int_{\Omega} f(\theta, t) dt$$

is the normalizing constant. $f(t, \theta)/z(\theta)$ is a probability distribution function on Ω. Evaluation of $z(\theta)$ is a fundamental problem in statistics.

Example: $f(\theta, t) = \exp\left(\frac{-t^2}{2\theta^2}\right)$ with $\Omega = (-\infty, +\infty)$. Then

$$z(\theta) = \sqrt{2\pi\theta^2}.$$

Holonomic Gradient Method

An analytic function $f(x)$ is called holonomic or D-finite when it satisfies n linear ODE's (holonomic system)

$$\sum_{j=0}^{r_i} a_{ij} \left(\frac{\partial}{\partial x_i}\right)^j f = 0, \quad a_{ij}(x) \in \mathrm{C}[x_1, \ldots, x_n], \quad i = 1, \ldots, n.$$

Theorem (Zeilberger, 1990): If $f(x)$ is holonomic, then the integral $\int_\Omega f(x) dx_n$ is holonomic in $(x_1, \ldots, x_{n-1})$ (under some conditions on Ω).

Holonomic Gradient Method (Nakayama *et al.*, 2011): When $f(\theta, t)$ is holonomic, the normalizing constant $z(\theta)$ satisfies a system of linear PDEs, which can be constructed by Gröbner bases. Evaluate $z(\theta)$ and its derivatives by the system with methods in numerical analysis.

3 Steps of Holonomic Gradient Method

1. Construct a Pfaffian system for $z(\theta)$.
2. Evaluate numerically $z(\theta)$ and its derivatives at $\theta = \theta_0$.
3. Apply numerical analysis methods for the Pfaffian system.

Example:

$$z(\theta) = \int_\Omega \exp(\theta t) t^{1/2} (1-t)^{1/2} dt, \quad \Omega = [0, 1]$$

By creative telescoping,

$$\left(\theta \partial_\theta^2 + (3-\theta)\partial_\theta - 3/2\right) z = 0, \quad \partial_\theta = \frac{\partial}{\partial \theta}$$

Then $\frac{\partial}{\partial\theta} Z = PZ$, where

$$Z = \begin{pmatrix} z \\ \frac{\partial}{\partial \theta} z \end{pmatrix}, \quad P = \begin{pmatrix} 0 & 1 \\ \frac{3}{2\theta} & -\frac{3-\theta}{\theta} \end{pmatrix}$$

Evaluation of the Expected Euler Characteristic

Recall: $E[\chi(M_x)] = F(M, \Sigma; x)$ is equal to

$$\int_x^\infty d\sigma \int_{-\infty}^\infty db \int_{-\infty}^\infty ds \int_{-\infty}^\infty f(\sigma, b, s, t) dt,$$

where f is hyperexponential over $\mathbb{Q}(\sigma, b, s, t)$. Thus, $-F'(M, \Sigma; x)$ is equal to

$$\int_{-\infty}^\infty db \int_{-\infty}^\infty ds \int_{-\infty}^\infty f(x, b, s, t) dt,$$

Idea: Use creative telescoping method to derive an ODE for $F'(M, \Sigma; x)$

Creative Telescoping Method

Given a holonomic function $f(\theta, t)$ with annihilator

$$\mathrm{ann}(f) \subset \mathrm{C}(\theta, t)[\partial_\theta, \partial_t].$$

Find nontrivial

$$P(\theta, \partial_\theta) + \partial_t Q(\theta, t, \partial_\theta, \partial_t) \in \mathrm{ann}(f)$$

Then $z(\theta) = \int_\Omega f(\theta, t) dt$ satisfies $P(z) = 0$ (under some conditions on Ω). We call P a telescoper for $ann(f)$.

Creative Telescoping Method

- (Zeilberger, 1990): Sylvester's dialytic elimination for multiple integrals
- (Takayama, 1992; Oaku, 1997): D-module theoretical algorithms for multiple integrals
- (Chyzak, 2000): a generalization of Gosper's algorithm for single integrals of multivariate holonomic functions
- (Koutschan, 2010): rational ansatz approach for multiple integrals
- (Bostan *et al.*, 2010, 2013; Chen *et al.*, 2015, 2016): reduction-based algorithms for single integrals of bivariate holonomic functions

Chyzak's algorithm

Given a holonomic function $f(\theta, t)$ with annihilator

$$\text{ann}(f) \subset R = \mathsf{C}(\theta, t)[\partial_\theta, \partial_t].$$

We call $\dim_{\mathsf{C}}(R/\text{ann}(f))$ the (holonomic) rank of $\text{ann}(f)$.

Goal: Drive an ODE for

$$G(M, \Sigma; x) = \int_{-\infty}^{\infty} db \int_{-\infty}^{\infty} ds \int_{-\infty}^{\infty} f(x, b, s, t) dt,$$

where f is hyperexponential over $\mathbb{Q}(\sigma, b, s, t)$.

Using Chyzak's algorithm, find a holonomic system of rank 2 for

$$f_1(x, b, s) = \int_{-\infty}^{\infty} f(x, b, s, t) dt$$

in 5 seconds using a Linux computer with 15.10 GB RAM.

Chyzak's algorithm

Goal: Drive an ODE for

$$G(M,\Sigma;x) = \int_{-\infty}^{\infty} db \int_{-\infty}^{\infty} f_1(x,b,x)ds,$$

where $\mathrm{ann}(f_1)$ has holonomic rank 2.

Using Chyzak's algorithm, find a holonomic system of rank 6 for

$$f_2(x,b) = \int_{-\infty}^{\infty} f_1(x,b,s)ds$$

in 16 mins by specifying M and Σ.

Question: Is it possible to compute a holonomic system for f_2 without specifying M and Σ?

Stafford Heuristic

Consider

$$R_n = \mathbb{K}(x_1, \ldots, x_n)[\partial_1, \ldots, \partial_n],$$
$$T_n = \{\partial_1^{i_1} \cdots \partial_n^{i_n} \mid (i_1, \ldots, i_n) \in \mathbb{N}^n\}.$$

Heuristic: Given a holonomic system H in R_n, compute new holonomic system H_1 in R_{n-1} s.t. $H_1 \subset (R_n \cdot H + \partial_n R_n) \cap R_{n-1}$.

1. Pick $S_1, S_2 \in T_{n-1}$.

2. Using rational ansatz method, check existence of telescoper P_i of H with support S_i, $i = 1, 2$. If P_i exists, go to step 3. Otherwise, go to step 1.

3. Compute Gröbner basis H_1 of $\{P_1, P_2\}$. If H_1 is holonomic, then output G_1. Otherwise, go to step 1.

Stafford Theorem: Every left ideal in R_n can be generated by 2 elements.

Stafford Heuristic

Goal: Drive an ODE for

$$G(M, \Sigma; x) = \int_{-\infty}^{\infty} db \int_{-\infty}^{\infty} f_1(x, b, x) ds,$$

where $\mathrm{ann}(f_1) = \langle H \rangle$ has holonomic rank 2.

1. Pick

$$S_1 = \{1, \partial_b, \partial_x, \partial_b^2, \partial_b\partial_x, \partial_x^2, \partial_x^3\},$$
$$S_2 = S_1 \cup \{\partial_b^2\partial_x, \partial_b\partial_x^2, \partial_b^3\}.$$

2. Using rational ansatz method, find telescoper P_i of H with support S_i, $i = 1, 2$.

3. Compute Gröbner basis H_1 of $\{P_1, P_2\}$. We find that H_1 has holonomic rank 6.

Chyzak's algorithm vs Stafford Heuristic

Goal: Drive an ODE for

$$G(M, \Sigma; x) = \int_{-\infty}^{\infty} db \int_{-\infty}^{\infty} f_1(x, b, x) ds,$$

where $\mathrm{ann}(f_1)$ has holonomic rank 2.

Below is a table of time (seconds) for deriving holonomic systems of

$$f_2(x, b) = \int_{-\infty}^{\infty} f_1(x, b, s) ds.$$

# pars	0	1	2	3	4	5
Chyzak	976	9.8×10^4	-	-	-	-
Heuristic	43.49	394.4	8527	4.3957×10^5	-	1.5×10^6

Evaluation of the Expected Euler Characteristic

Goal: Drive an ODE for

$$G(M,\Sigma;x) = \int_{-\infty}^{\infty} f_2(x,b)db,$$

where $\mathrm{ann}(f_2)$ has rank 6 (Recall: $G(M,\Sigma;x) = -F'(M,\Sigma;x)$).

Example 1: Set

$$\Sigma^{-1} = \begin{pmatrix} 2 & 0 \\ 0 & 1 \end{pmatrix} \quad M = \begin{pmatrix} 1 & 0 \\ -1 & 1 \end{pmatrix}.$$

Using Heuristic, find an 11-th order ODE $P(F) = 0$ of $F(M,\Sigma;x)$. By numerical solving of $P(F) = 0$, get

x	1	2	3	4	5
HGM	0.745835	0.567729	0.144879	0.0146728	0.000582526
mc	0.745802	0.567623	0.144986	0.0146901	0.0005933

where mc is the result for a Monte Carlo study of $E[\chi(M_x)]$ with $10,000,000$ iterations.

Evaluation of the Expected Euler Characteristic

Example 2: Set

$$\Sigma^{-1} = \begin{pmatrix} 10^3 & 0 \\ 0 & 10^2 \end{pmatrix} \quad M = \begin{pmatrix} 1 & 0 \\ 2 & 3 \end{pmatrix}.$$

Using Heuristic, find an 11-th order ODE $P(F) = 0$ of $F(M, \Sigma; x)$.

Difficulty:

- Initial value: numerical integration is time-consuming and not reliable.
- Numerical solving of ODEs: the Runge-Kutta method only works locally since $F(M, \Sigma; x)$ is not dominant among solutions of $P(F) = 0$.

Recall: Let $f_1, \ldots, f_n$ be a basis of solutions of a linear ODE $L(y) = 0$. A solution f of $L(y) = 0$ is dominant if

$$\lim_{x \to \infty} \frac{|f_i(x)|}{|f(x)|} < \infty, \quad i = 1, \ldots, n.$$

Evaluation of the Expected Euler Characteristic

Let $P(y) = 0$ be the r-th order linear ODE of $F(M, \Sigma; x)$.

Idea: Compute approximation series solutions of the linear ODE $P(y) = 0$ and use them to extrapolate results by simulations.

1. Construct approximation series solutions $f_1, \ldots, f_r$ of $P(y) = 0$ up to $20,000$ terms.

2. Make an ansatz $f(x) = \sum_{i=0}^{r-1} t_i f_i(x)$, where t_i's are unknown. Chose $x = p_j$ for $j = 0, \ldots, r-1$. Then

$$f(p_j) = \sum_{i=0}^{r-1} t_i f_i(p_j), \quad j = 0, 1, \ldots, r-1.$$

Evaluation of the Expected Euler Characteristic

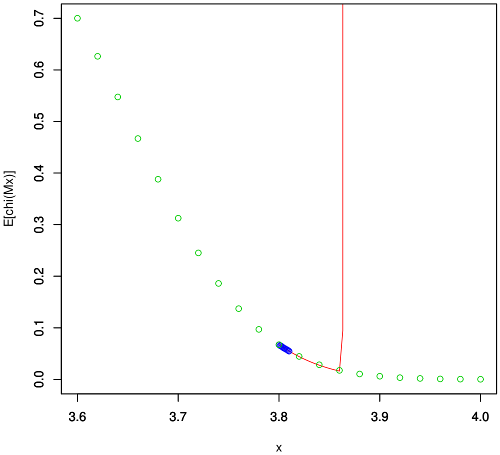
$$f(p_j) = \sum_{i=0}^{r-1} t_i f_i(p_j), \quad j = 0, 1, \ldots, r-1.$$

3. Compute $f(p_j)$ by Monte-Carlo simulation and then determine t_i's by solving linear equations.

4. Use $f(x) = \sum_{i=0}^{r-1} t_i f_i(x)$ to extrapolate $F(M, \Sigma; x)$ at target points.

x	$f(x)$	simulation
3.8133	0.051146	0.051176
3.8166	0.047517	0.047695
3.82	0.044120	0.044515

Evaluation of the Expected Euler Characteristic



The extrapolation function $f(x)$ with 20,000 terms. Solid line is $f(x)$, which diverges when $x > 3.8633$. Dots are values by simulations.

Conclusion

Let $W_m(n, \Sigma; \Omega)$ be non-central and W be a real matrix.

- Approximate formula of $\Pr(\lambda_1(W) \geq x)$ by Euler characteristic method
- Numerical evaluation for the integral formula by holonomic gradient method

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Thanks!