Who is today's speaker?

1. Name: Nobuki Takayama. Born: 1959
2. Lives in Kobe* and in Fukui† (after covid-19)

*https://en.wikipedia.org/wiki/Kobe
†https://en.wikipedia.org/wiki/Fukui_Prefecture

Who is today's speaker? 2.

1. 1984–Current: hypergeometric functions of several variables, A-hypergeometric system or GKZ HG. Special functions and computer algebra. "Askey-Bateman project, vol 2, Multivariable of special functions":
   https://www.cambridge.org/jp/academic/subjects/mathematics/abstract-analysis/encyclopedia-special-functions-askey-bateman-project-volume-2-1?format=HB&isbn=9781107003736
2. 1995–2005: D-modules algorithms and algebraic geometry.
3. 2010–Current: Statistics, computer algebra, numerical analysis. http://www.math.kobe-u.ac.jp/OpenXM/Math/hgm/ref-hgm.html
4. Software projects: Kan/sm1, Risa/Asir: http://www.openxm.org . HGM package on R: https://cran.r-project.org/package=hgm

Euler characteristic heuristic and computer algebra

Nobuki Takayama (Kobe Univ),
joint work with Lin Jiu, Satoshi Kuriki, Yi Zhang

Theorem

$$M_x = \{hg^T \mid g^T A h \geq x, h, g \in S^{m-1}\}$$

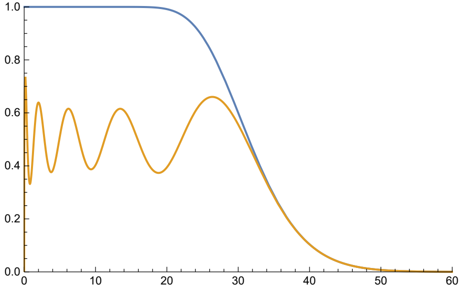
A is an $m \times m$ random matrix of the Gaussian distribution with the covariance E_m/s and the mean 0, i.e.,

$$p(A) \sim \exp\left(-\frac{1}{2}\mathrm{Tr}\,(sA^T A)\right).$$

Then, we have

$$E[\chi(M_x)] = \prod_{i=1}^{5} c_i \int_x^{+\infty} \exp\left(-\frac{s}{2}\sigma^2\right) {}_1F_1(-(m-1), 1; s\sigma^2) d\sigma$$

$E[\chi(M_x)]$ and the prob of the max eigenvalue of A is larger than x



$m = 10$, $s = 1$. The horizontal axis is x^2.
c_i are constants. Reference: "Computation of the expected Euler characteristic for the largest eigenvalue of a real non-central Wishart matrix",
`https://doi.org/10.1016/j.jmva.2020.104642`

Euler characteristic heuristic: Adler, Hosofer(1970's), Worsley(1994), Kuriki, Takemura(2000's)

Let $f(U)$ be a smooth random field on a manifold M.
$M_x = \{U \in M \mid f(U) \geq x\}$.

The expectation of the Euler characteristic $M_x \sim P\left(\max_{U \in M} f(U) \geq x\right)$

Notation: $P(\cdots) =$ (The probability of being $\cdots$).

If $M_x(f)$ is a simply connected domain or empty, then
$\chi(M_x(f)) = 1$ or $\chi(M_x(f)) = 0$ respectively.
On the other hand,

$$P(\max_{U \in M} f(U) \geq x) = \int h_{M_x(f)}(f)\mu(f) = E[h_{M_x(f)}]$$

where $\mu(f)$ is the probability measure on the f-space, $h_{M_x}(f)$ is the supporting function defined by

$$\begin{cases} h_{M_x}(f) & = 1, \qquad M_x \neq \emptyset \\ h_{M_x}(f) & = 0, \qquad M_x = \emptyset \end{cases}$$

Our problem

$A = (a_{ij})$: real $m \times n$ matrix valued random variable (random matrix), The probability density is

$$p(A)dA, \quad dA = \prod da_{ij}.$$

$$M = \{hg^T \mid g \in S^{m-1}, h \in S^{n-1}\} \simeq S^{m-1} \times S^{n-1}/\sim$$

h and g are column vectors. $(h, g) \sim (-h, -g)$. (hg^T is $n \times m$ matrix.) Put

$$f(U) = \mathrm{tr}(UA) = g^T A h, \quad U = hg^T \in M,$$

The random field f is determined by the random matrix A.

$$M_x = \{hg^T \in M \mid f(U) = g^T A h \geq x\}$$

We assume $p(A)$ is smooth and $n \geq m \geq 2$.

Evaluation of E of the Euler characteristic

We apply the Morse theory. Where are critical points?
$\chi(M_x) = \sum_{\text{critical points } c} \text{sign}\,|\text{Hess}(f)(c)|$

Proposition (Well-known)

Fix an $m \times n$ matrix A. The following conditions are equivalent

1. *The function $f(U) = g^T Ah$ has a critical point at $U = hg^T$.*
2. *Vectors $g \in S^{m-1}, h \in S^{n-1}$ are a left and a right eigenvector of A respectively, i.e., there exists a real number c s.t. $g^T A = ch^T$, $Ah = cg$*

f takes the value c at the critical point (g, h).

Proof sketch: Parametirze $g \in S^{m-1}$ by the local coordinate u_i, $1 \leq i \leq m-1$. Differentiate $g^T g = 1$ by u_i and we obtain $(\partial_i g^T)g + g^T(\partial_i g) = 0$. Parametrize $h \in S^{n-1}$ by v_a, $1 \leq a \leq n-1$. Differentiation w.r.t. v_a is written as ∂_a (we use it later). Differentiate $f(U)$ by u_i.

A new coordinate for the matrix A

Let $(g, G(g))$ be a family of elements of $SO(m)$ parametrized by $g \in S^{m-1}$. (G is an $m \times (m-1)$ matrix). $(h, H(h)) \in SO(n)$, $h \in S^{n-1}$. Put

$$\sigma = g^T A h, \;\; B = G^T(g) A H(h) \in M(m-1, n-1) \tag{1}$$

Then the $m \times n$ A matrix can be written as

$$A = \sigma g h^T + G B H^T, \tag{2}$$

Idea: Use the change of coordinates

$$A \Leftrightarrow (\sigma, h, g, B)$$

The case $m = n = 2$

Fix two unit vectors

$$g = (\cos\theta, \sin\theta)^T, h = (\cos\phi, \sin\phi)^T \in S^1$$

$0 \le \theta, \phi < 2\pi$.

$$G = \left(\cos\left(\theta + \frac{\pi}{2}\right), \sin\left(\theta + \frac{\pi}{2}\right)\right)^T = (-\sin\theta, \cos\theta)^T,$$

which satisfies

$$(g, G) = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} \in SO(2).$$

Define H similarly.

$$A = \sigma g h^T + G B H^T,$$

where B is 1×1 matrix (b). Parameters: $\sigma \ge b$, θ, ϕ. It is a $1:2$ correspondance.

Evaluation of E of the Euler characteristic

Theorem

Assume $x > 0$ and $f(U)$ is a Morse function at a.e. A. The expectation of the Euler characteristic $E[\chi(M_x)]$ is

$$\frac{1}{2}\int_x^\infty d\sigma \int_{\mathrm{R}^{(m-1)(n-1)}} dB \int_{S^{m-1}} G^T dg \int_{S^{n-1}} H^T dh \, \det(\sigma^2 I_{m-1} - BB^T) p(A). \quad (3)$$

$G^T dg = \wedge_{i=1}^{m-1} G_i^T dg$, $H^T dh = \wedge_{i=1}^{n-1} H_i^T dh$ (G_i is the i-th column vector of G) $dg = (dg_1, \ldots, dg_m)^T$, $dh = (dh_1, \ldots, dh_n)^T$.

Proof sketch when $m = n = 2$

$$\begin{cases} Ah = \sigma g h^T h + bGH^T h & = \sigma g; \\ g^T A = \sigma g^T g h^T + b g^T G H^T & = \sigma h^T; \\ AH = \sigma g h^T H + bGH^T H & = bG; \\ G^T A = \sigma G^T g h^T + b G^T G H^T & = bH^T. \end{cases}$$

Namely, the function f has two critical points on M, which are at

- the point $P = hg^T \in M \Leftrightarrow (\alpha, \beta) = (\theta, \phi)$;
- and the point $Q = HG^T \in M \Leftrightarrow (\alpha, \beta) = (\theta + \pi/2, \phi + \pi/2)$.

Proof sketch when $m = n = 2$ (continued)

$\det(\mathrm{Hess}_P f) = \sigma^2 - b^2$ and $\det(\mathrm{Hess}_Q f) = b^2 - \sigma^2$.
The only nontrivial case is $\sigma \geq x \geq b$, then

$$\chi(M_x) = 1(\sigma \geq x \geq b)\,\mathrm{sgn}\,\left(\sigma^2 - b^2\right).$$

$$\mathrm{d}A = \left(b^2 - \sigma^2\right)\mathrm{d}\sigma\mathrm{d}b\mathrm{d}\theta\mathrm{d}\phi.$$

Morse theory:

$$\chi(M_x) = \sum_{\text{critical points } c} \mathrm{sign}\,|\mathrm{Hess}(f)(c)|$$

Problem

Goal

For a given probability densitiy $p(A)$ of random matrices A, evaluate $E[\chi(M_x)]$ numerically. *It follows from the Euler characteristic heuristic that $E[\chi(M_x)]$ approximates*

$$P(\max_{g,h} g^T Ah \geq x) = P((\text{max singular value of } A) \geq x)$$

Interesting case (Gaussian distribution):

$$p(A) = \frac{1}{Z} \exp\left(-\frac{1}{2}\,\mathrm{Tr}(A-M)^T\Sigma^{-1}(A-M)\right) \qquad (4)$$

The $m \times n$ matrix M is the mean. The $n \times n$ positive definite matrix Σ is the covariance.

Result 1: When $M = 0$, Σ is a scalar matrix, the integral is studied by Aomoto and Kaneko.

The case of the Selberg type integral 1

Theorem

$$M_x = \{hg^T \mid g^T A h \geq x, h, g \in S^{m-1}\}$$

A is the $m \times m$ random matrix of the Gaussian distribution with the covariance E_m/s and the mean 0.

$$p(A) \sim \exp\left(-\frac{1}{2}\mathrm{Tr}\left(sA^T A\right)\right).$$

$$E[\chi(M_x)] = \prod_{i=1}^{5} c_i \int_x^{+\infty} \exp\left(-\frac{s}{2}\sigma^2\right) {}_1F_1(-(m-1), 1; s\sigma^2) d\sigma$$

Idea: Calculate the integral (3) by the SVD coordinate of B.

The case of the Selberg type integral 2

Proof sketch.

$$\tilde{G} = \left(\begin{array}{c|c} g & G \end{array} \right) \in O(m), \quad g \text{ is a column vector,}$$

Put $\tilde{H} = (h, H)$. Then the $m \times n$ matrix A is

$$A = \tilde{G} \left(\begin{array}{c|c} \sigma & 0 \\ \hline 0 & B \end{array} \right) \tilde{H}^T,$$

We denote the mid matrix above by $\tilde{B}$. $\mathrm{etr}(X)$ is $\exp(\mathrm{Tr}(X))$.
Note $\mathrm{tr}(PQ) = \mathrm{tr}(QP)$, $\tilde{H}^T\tilde{H} = E$.

$$\begin{aligned} \mathrm{etr}(-\frac{1}{2}sA^TA) &= \mathrm{etr}\left(-\frac{s}{2}\tilde{B}\tilde{B}^T\right) \\ &= \exp\left(-\frac{s}{2}\sigma^2\right)\exp\left(-\frac{s}{2}LL^T\right) \end{aligned}$$

The matrix B is expressed in the form of the singular value decomposition $B = PLQ^T$, $P, Q \in O(m-1)$,
$L = \mathrm{diag}(\ell_1, \ldots, \ell_{m-1})$.

The case of the Selberg type integral 3

$$c_1(S) = \frac{1}{2} \cdot \frac{1}{(2\pi)^{nm/2} \det(sE_m)^{n/2}}, \tag{5}$$

$$c_2(m) = \int_{S^{m-1}} G^T dg \int_{S^{m-1}} H^T dh \tag{6}$$

$$\tilde{c}_3(m; \sigma) = \frac{1}{(m-1)!} \exp\left(-\frac{s}{2}\sigma^2\right) \left(\int_{O(m-1)} \wedge_{i<j} P_j^T dP_i \right)^2 \tag{7}$$

$$\begin{aligned} q(s; \sigma) \quad = \quad & \tilde{c}_3(m, \sigma) \int_{L \in \mathrm{R}^{m-1}} \prod_{1 \le i < j \le m-1} |\ell_i^2 - \ell_j^2| \prod_{i=1}^{m-1} (\sigma^2 - \ell_i^2) \\ & \exp\left(-\frac{s}{2} \sum \ell_i^2\right) \prod_{i=1}^{m-1} d\ell_i \end{aligned} \tag{8}$$

Put $\ell_i^2 = \ell_i'$, then the integral is reduced to the Selberg type integral of Aomoto and Kaneko.

Aomoto(1987), Kaneko(1993), Selberg type integral

$$\int_{[0,1]^{m-1}} \prod_{1\le i\le m-1, 1\le k\le r} (\ell_i - \sigma_k)^{\mu} D(\ell_1, \ldots, \ell_{m-1}) d\ell_1 \cdots d\ell_{m-1},$$

$$D = \prod_{i=1}^{m-1} \ell_i^{\lambda_1} (1-\ell_i)^{\lambda_2} \prod_{1\le i<j\le m-1} |\ell_i - \ell_j|^{\lambda}, \tag{9}$$

The system of differential equations, special values, and the series expansion is derived when $\mu = 1$ or$\mu = -\lambda/2$ (J.Kaneko, Selberg Integrals and Hypergeometric Functions associated with Jack Polynomials, SIAM Journal on Mathematical Analysis 24 (1993), 1086–1110).

Confluence

Make the change of coordinates $\ell_i = y_i/N$, $\lambda_2 = N$, $\sigma_i = \tau_i/N$. Then, we have $d\ell_i = dy_i/N$, $(1-\ell_i)^\lambda = (1-y_i/N)^N$. Take the limit $(1-y_i/N)^N \to \exp(-y_i), \quad N \to \infty$ and the (9) converges to

$$\int_{\mathrm{R}_{\geq 0}^{m-1}} \prod_{1\leq i\leq m-1, 1\leq k\leq r} (y_i - \tau_k)^\mu D(y_1, \ldots, y_{m-1}) dy_1 \cdots dy_{m-1},$$

$$D = \prod_{i=1}^{m-1} y_i^{\lambda_1} \exp(-\sum_{i=1}^{m-1} y_i) \prod_{1\leq i<j\leq m-1} |y_i - y_j|^\lambda,$$

When $r = 1$, $\mu = 1$, the differential equation converges to

$$\theta_{\tau_1}(\theta_{\tau_1} + \frac{2}{\lambda}(\lambda_1 + 1) - 1) - \frac{2}{\lambda}\tau_1(\theta_{\tau_1} - (m-1))$$

When $\lambda = 1$, $\lambda_1 = -1/2$, the integral is equal to

$$c_5 \cdot {}_1F_1(-(m-1), 1; 2\tau_1)$$

Non-central, $m = n = 2$

$m = n = 2$. 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

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

Then

$$p(A) = \frac{s_1 s_2}{(2\pi)^2} e^{-\frac{R}{2}},$$

where

$$\begin{aligned} R =& s_1 (b \sin\theta \sin\phi + \sigma \cos\theta \cos\phi - m_{11})^2 + s_2 (\sigma \sin\theta \cos\phi - b \cos\theta \sin\phi - m_{21})^2 \\ &+ s_1 (\sigma \cos\theta \sin\phi - b \sin\theta \cos\phi)^2 + s_2 (b \cos\theta \cos\phi + \sigma \sin\theta \sin\phi - m_{22})^2 . \end{aligned}$$

$$\begin{aligned} \mathrm{E}[\chi(M_x)] =& F(s_1, s_2, m_{11}, m_{21}, m_{22}; x) \\ =& \frac{1}{2} \int_x^{\infty} d\sigma \int_{-\infty}^{\infty} db \int_0^{2\pi} d\theta \int_0^{2\pi} d\phi (\sigma^2 - b^2) \frac{s_1 s_2}{(2\pi)^2} \exp\left\{-\frac{1}{2} R\right\}, \end{aligned} \tag{10}$$

A linear ODE for $E[\chi(M_x)]$

It follows from the theory of holonomic D-modules, there exists a linear ODE of polynomial coefficients of x satisfied by $E[\chi(M_x)]$.

Result 2. Use of the creative telescoping when $m = n = 2$

$g = (\cos\theta, \sin\theta)^T$, $h = (\cos\phi, \sin\phi)^T$. We set

$$\sin\theta = \frac{2s}{1+s^2}, \quad \cos\theta = \frac{1-s^2}{1+s^2}, \quad \sin\phi = \frac{2t}{1+t^2}, \quad \cos\phi = \frac{1-t^2}{1+t^2}.$$

$$\begin{aligned} \mathrm{E}[\chi(M_x)] &= F(s_1, s_2, m_{11}, m_{21}, m_{22}; x) \\ &= \frac{1}{2\pi^2} \int_x^\infty d\sigma \int_{-\infty}^\infty db \int_{-\infty}^\infty ds \int_{-\infty}^\infty dt \\ &\qquad \frac{s_1 s_2 (\sigma^2 - b^2)}{(1+s^2)(1+t^2)} \exp\Big\{-\frac{1}{2}\tilde{R}\Big\}, \end{aligned}$$

where $\tilde{R}$ is a rational function in σ, b, s, t.
$\Sigma^{-1} = \mathrm{diag}(s_1, s_2)$, $M = [[m_{11}, 0], [m_{21}, m_{22}]]$.

Result 2. Use of the creative telescoping when $m = n = 2$

$E[\chi(M_x)]$ satisfies an ODE of rank 11 (26MB).

HolonomicFunctions.m by C.Koutschan.

ODE data: `https://yzhang1616.github.io/ec1/ec1.html`

$f(t,x)$ is annihilated by the left ideal I in D.

$$(I + \partial_t \mathbb{Q}[t,x,\partial_t,\partial_x]) \cap \mathbb{Q}[x,\partial_x]$$

Let $\ell \in \mathbb{Q}[x,\partial_x]$ be an element of above. Since

$$\ell = L + \partial_t T, \quad L \in I, T \in \mathbb{Q}[t,x,\partial_t,\partial_x]$$

$$\ell \int_C f(t,x)dt = \int_C \ell f(t,x) = \int_C \partial_t(Tf(t,x))dt = [Tf]_{\partial C}$$

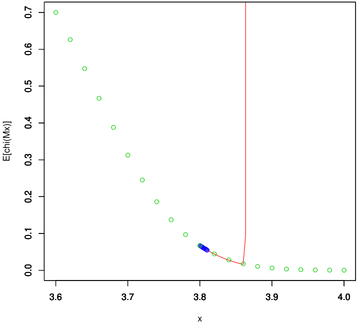
Computer algebra challenge: Derive an ODE when $m = 2, n = 3$.

Numerical Analysis of the huge ODE

We want to extrapolate simulation values by the ODE of rank 11. Standard numerical algorithms (implicit Runge-Kutta method, ...) does not work well, e.g., for
$m_{11} = 1, m_{21} = 2, m_{22} = 3, s_1 = 10^3, s_2 = 10^2$.

$$\Longrightarrow$$

Series solutions of 20,000 terms by rational arithmetics give



Problem

Computer algebra systems often output huge ODE's. Give algorithms and implementations to perform a numerical analysis of these equations.

Our rank 11 ODE:

$$hc_{11}(x)\partial_x^{11} + \cdots + c_1(x)\partial_x$$

where $c_{11}(x) = O(1)$, $c_1(x) = O(1)$, and $h \sim 10^{-33}$.

Sparse interpolation/extrapolation method

We solve an ODE $Lf = 0$ of rank r when (approximate) values of the solution $f(t)$ at $t = p_1, p_2, \ldots, p_r$ are known. We call the points $(p_i, q_i), q_i = f(p_i)$ *data points*.

We approximately expand the solution f by a given basis functions $\{e_k(t)\}$, $k = 0, 1, \ldots, M$ as

$$f(t) = \sum_{k=0}^{M} f_k e_k(t), \quad f_k \in \mathrm{R}. \tag{11}$$

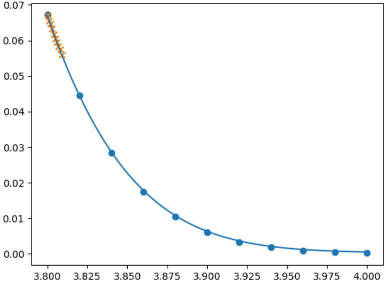
Put this expression into $Lf = 0$. We minimize the loss function $\int_{t_s}^{t_e} |Lf(t)|^2 dt$ with the constraints $f(p_i) = q_i$ w.r.t f_k's.

Or, minimize

$$\int_{t_s}^{t_e} |Lf(t)|^2 dt + \beta \sum_i |f(p_i) - q_i|$$

Sparse interpolation/extrapolation method

Solving the huge ODE of rank 11 by the sparse extrapolation method.



$$e_j(t) = (t - 3.8055)^j,\ j = 0, 1, \ldots, 29,\ t_s = 3.8,\ t_e = 4.0.$$