

Data-Discriminants of Likelihood Equations

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Motivation

First Example



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Assume

- p_i is **probability** of observing side i ($i = 1, 2, 3, 4$)
- the die is **unfair** ($\Leftrightarrow \exists j$ such that p_j is not 25%)

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Given Constraints on p_1 , p_2 , p_3 and p_4

- $\{(p_1, p_2, p_3, p_4) \in \mathbb{R}_{>0}^4 \mid \sum_{i=1}^4 p_i = 1\}$
- We artificially assume $p_1 + 2p_2 + 3p_3 - 4p_4 = 0$

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Data Record

We toss the die 100 times and record the times of getting each side e.g. $[u_1 = 11, u_2 = 24, u_3 = 15, u_4 = 50]$

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Question

For given constraints and data, how to estimate p_1 , p_2 , p_3 and p_4 which BEST explains the data?

Answer

Maximize **likelihood function** $p_1^{11} p_2^{24} p_3^{15} p_4^{50}$ subjected to **given constraints**

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Answer.

It is equivalent to maximize $\log(p_1^{11} p_2^{24} p_3^{15} p_4^{50})$. By the [Lagrange Multiplier Method](#), we solve

$$p_1 \lambda_1 + p_1 \lambda_2 - 11 = 0$$

$$p_2 \lambda_1 + 2p_2 \lambda_2 - 24 = 0$$

$$p_3 \lambda_1 + 3p_3 \lambda_2 - 15 = 0$$

$$p_4 \lambda_1 - 4p_4 \lambda_2 - 50 = 0$$

$$p_1 + 2p_2 + 3p_3 - 4p_4 = 0$$

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$$p_1 + 2p_2 + 3p_3 - 4p_4 = 0$$

$$p_1 + p_2 + p_3 + p_4 - 1 = 0$$

and get 3 solutions

$$[p_1 = 1.2691, p_2 = -0.2903, p_3 = -0.0862, p_4 = 0.1075, \lambda_1 = 100, \lambda_2 = -91.3324],$$

$$[p_1 = 0.1857, p_2 = 1.2980, p_3 = -0.6737, p_4 = 0.1901, \lambda_1 = 100, \lambda_2 = -40.7547],$$

$$[p_1 = 0.1232, p_2 = 0.3057, p_3 = 0.2214, p_4 = 0.3497, \lambda_1 = 100, \lambda_2 = -10.7463].$$

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How to maximize likelihood function $p_1^{u_1} p_2^{u_2} p_3^{u_3} p_4^{u_4}$ subjected to given constraints?

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$$p_1 + 2p_2 + 3p_3 - 4p_4 = 0$$

$$p_1 + p_2 + p_3 + p_4 - 1 = 0$$

Remark

For general $[u_1, u_2, u_3, u_4]$, the system has 3 complex solutions.

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For which u_j , the system has 0, 1, 2 and 3 REAL/POSITIVE solutions?

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For which u_i , the system has 0, 1, 2 and 3 REAL/POSITIVE solutions?

Answer. Use real quantifier elimination/real root classification tools.

For example, by `RealRootClassification` in Maple2015 [C. Chen, J. H. Davenport, J. P. May, M. M. Maza, B. Xia and R. Xiao, 2010], for any $(u_1, u_2, u_3, u_4) \in \mathbb{R}_{>0}^4$,

- $D(u_1, u_2, u_3, u_4) > 0 \Rightarrow$ 3 distinct real solutions and 1 of them is positive;
- $D(u_1, u_2, u_3, u_4) < 0 \Rightarrow$ 1 real solution and it is positive.

where

$$D = u_1 u_2 u_3 u_4 (u_1 + u_2 + u_3 + u_4) (441 u_1^4 + 4998 u_1^3 u_2 + 20041 u_1^2 u_2^2 + 33320 u_1 u_2^3 + 19600 u_2^4 - 756 u_1^3 u_3 + 20034 u_1^2 u_2 u_3 + 83370 u_1 u_2^2 u_3 + 79800 u_2^3 u_3 - 5346 u_1^2 u_3^2 + 55890 u_1 u_2 u_3^2 + 119025 u_2^2 u_3^2 + 4860 u_1 u_3^3 + 76950 u_2 u_3^3 + 18225 u_3^4 - 1596 u_1^3 u_4 - 11116 u_1^2 u_2 u_4 - 17808 u_1 u_2^2 u_4 + 4480 u_2^3 u_4 + 7452 u_1^2 u_3 u_4 - 7752 u_1 u_2 u_3 u_4 + 49680 u_2^2 u_3 u_4 - 17172 u_1 u_3^2 u_4 + 71460 u_2 u_3^2 u_4 + 27540 u_3^3 u_4 + 2116 u_1^2 u_4^2 + 6624 u_1 u_2 u_4^2 - 4224 u_2^2 u_4^2 - 9528 u_1 u_3 u_4^2 + 15264 u_2 u_3 u_4^2 + 14724 u_3^2 u_4^2 - 1216 u_1 u_4^3 - 512 u_2 u_4^3 + 3264 u_3 u_4^3 + 256 u_4^4)$$

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For which u_i , the system has 0, 1, 2 and 3 REAL/POSITIVE solutions?

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Question

How to compute D EFFICIENTLY?

Maximum Likelihood Estimation Problem

Algebraic Statistical Model

$$X = \mathcal{V} \cap \Delta_n$$

where

\mathcal{V} : irreducible and generically reduced projective variety

$$\{(p_0, \dots, p_n) \in \mathbb{C}^{n+1} \mid g_1(p_0, \dots, p_n) = 0, \dots, g_s(p_0, \dots, p_n) = 0\}$$

Δ_n : probability simplex

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Data Vector

$$[u_0, u_1, \dots, u_n]$$

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Maximum Likelihood Estimation Problem

For given **model** and **data**, how to estimate p_0, \dots, p_n which BEST explains the data?

Method

Maximize **likelihood function** $\prod_{i=0}^n p_i^{u_i}$ subject to the **algebraic statistical model**.

Lagrange Likelihood Equations

Question

How to maximize likelihood function $\prod_{i=0}^n p_i^{u_i}$ subject to the algebraic statistical model $\mathcal{V}(g_1, \dots, g_s) \cap \Delta_n$?

Answer

For every critical point (p_0, \dots, p_n) of the likelihood function, there exists $(\lambda_1, \dots, \lambda_{s+1}) \in \mathbb{C}^{s+1}$ such that $(p_0, \dots, p_n, \lambda_1, \dots, \lambda_{s+1})$ is a solution to the Lagrange likelihood equations [S. Hosten, A. Khetan and B. Sturmfels, 2005; E. Gross and J. I. Rodriguez, 2014]:

$$\begin{aligned} F_0 &= p_0(\lambda_1 + \frac{\partial g_1}{\partial p_0} \lambda_2 + \dots + \frac{\partial g_s}{\partial p_0} \lambda_{s+1}) - u_0 = 0 \\ &\dots \\ F_n &= p_n(\lambda_1 + \frac{\partial g_1}{\partial p_n} \lambda_2 + \dots + \frac{\partial g_s}{\partial p_n} \lambda_{s+1}) - u_n = 0 \\ F_{n+1} &= g_1(p_0, \dots, p_n) = 0 \\ &\dots \\ F_{n+s} &= g_s(p_0, \dots, p_n) = 0 \\ F_{n+s+1} &= p_0 + \dots + p_n - 1 = 0 \end{aligned}$$

where

- $p_0, \dots, p_n, \lambda_1, \dots, \lambda_{s+1}$ are unknowns,
- u_0, \dots, u_n are parameters.

Real/Positive Root Classification Problem

Theorem 1 (System of Lagrange likelihood equations is generically zero-dimensional) [S. Hosten, A. Khetan and B. Sturmfels, 2009]

For a given algebraic statistical model, for general data (u_0, \dots, u_n) , the number of complex solutions of Lagrange likelihood equations is a non-negative constant (ML-Degree).

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Standard Method for Real/Positive Root Classification [L. Yang, X. Hou and B. Xia, 2001; D. Lazard and F. Rouillier, 2005; C. Chen, J. H. Davenport, J. P. May, M. M. Maza, B. Xia and R. Xiao, 2010]

- **Step 1** Compute **discriminant variety** (REMARK: generally discriminant variety is not a hypersurface [D. Lazard and F. Rouillier, 2005])

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- **Step 1** Compute **discriminant variety** (REMARK: generally discriminant variety is not a hypersurface [D. Lazard and F. Rouillier, 2005])
- **Step 2** Compute **cells** determined by discriminant variety and number of real/positive solutions over each cell [Tarski, 1951; Collins, 1975; Arnon et al., 1988; McCallum, 1988, 1999, 2001; Grigoriev, 1988; Collins and Hong, 1991; Renegar, 1992; Basu et al., 1996, 1999, 2006; Dolzmann and Sturm 1997; Brown, 2001, 2012, 2013, 2015; McCallum and Brown 2005; Strzebonski, 2000, 2005, 2006, 2011; Hong and Safey El Din, 2012; Bradford et al., 2013; M. England et al. 2015; R. Fukasaku et al. 2015...]

Data-Discriminant and Problem Statement

Proposition (See propositions 1–2 in [J. I. Rodriguez and X. Tang, 2015].)

Discriminant varieties of Lagrange likelihood equations are projective varieties.

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Data-Discriminant (Remark that we do need some extra assumptions for this definition. See Definition 5 in [J. I. Rodriguez and X. Tang, 2015].)

For a given algebraic statistics model X , the homogeneous polynomial that generates the reduced codimension 1 component of discriminant variety of Lagrange likelihood equations is said to be **data-discriminant** of Lagrange likelihood equations of X .

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Problem Statement: Design Algorithm

- **Input:** Lagrange likelihood equations
- **Output:** Data-Discriminant

Algorithm 1 (Standard Algorithm)

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Input. $F = u_0p^2 + u_1p + u_2,$

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$$\{u_1^2 - 4u_0 u_2\}$$

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Step 2. Compute the codimension 1 component of the equidimensional radical decomposition of $\langle u_1^2 - 4u_0 u_2 \rangle$

$$u_1^2 - 4u_0 u_2$$

Output. $u_1^2 - 4u_0 u_2$

Algorithm 2 (Probabilistic Algorithm)

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Step 1 (Compute the degree and get the possible terms). We assume our output is $D(u_0, u_1, u_2)$. Substitute

$$u_0 = 1 \cdot t + 11,$$

$$u_1 = 3 \cdot t + 2,$$

$$u_2 = 5 \cdot t + 6$$

(the red coefficients are "randomly" chosen)

into F, J

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into F, J and compute the radical of the elimination ideal $\langle F(t, p), J(t, p) \rangle \cap \mathbb{Q}[t]$

$$\langle 11t^2 + 232t + 260 \rangle$$

(that means $D(t + 11, 3t + 2, 5t + 6) = 11t^2 + 232t + 260$)

So the **total degree** of D is **2**.

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So the **total degree** of D is **2**. Similarly, we compute

$$\text{degree}(D, u_0) = 1, \quad \text{degree}(D, u_1) = 2 \quad \text{degree}(D, u_2) = 1$$

(so all the possible monomials in D are $u_1^2, u_0 u_1, u_1 u_2, u_0 u_2$)

Algorithm 2 (Probabilistic Algorithm)

Step 2 (Evaluation/Interpolation). Assume

$$D(u_0, u_1, u_2) = u_1^2 + (C_1 u_0 + C_2 u_2) u_1 + C_3 u_0 u_2 \quad (1)$$

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Step 2.1. Substitute $u_0 = 13$, $u_2 = 4$ into F, J and compute the radical of the elimination ideal $\langle F(u_1, p), J(u_1, p) \rangle \cap \mathbb{Q}[u_1]$

$$\langle u_1^2 - 208 \rangle \quad (2)$$

(that means $D(13, u_1, 4) = u_1^2 - 208$)

Comparing (1) and (2), we see

$$13C_1 + 4C_2 = 0 \quad (3)$$

and $52C_3 = -208$. Therefore, $C_3 = -4$.

(We need one more evaluation to solve C_1 and C_2)

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Step 2.2. Substitute $u_0 = 7$ and $u_2 = 3$ into F and J . Similarly, we get

$$7C_1 + 3C_2 = 0 \quad (4)$$

By (3) and (4), $C_1 = C_2 = 0$.

Output. $u_1^2 - 4u_0 u_2$

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Remark: The EVALUATION/INTERPOLATION idea is NOT the first time investigated. See [M. Giusti, G. Lecerf and B. Salvy, 2001; E. Schost, 2003].

Experiment

Timings for Random Models (s: seconds; h: hours)

Random Degree 2-models			Random Degree 3-models		
Algorithm 1	Algorithm 2		Algorithm 1	Algorithm 2	
	Strategy 1	Strategy 2		Strategy 1	Strategy 2
4.9s	0.8s	0.6s	>2h	800.4s	901.2s
3.0s	0.7s	0.6s	>2h	777.3s	871.5s
5.0s	0.8s	0.6s	>2h	1428.9s	1499.5s
5.4s	0.8s	0.7s	>2h	1118.9s	1192.9s
6.3s	0.8s	0.7s	>2h	448.9s	489.8s
3.9s	0.7s	0.6s	>2h	1279.6s	1346.1s
2.0s	0.7s	0.5s	>2h	1286.5s	1409.0s
1.7s	0.7s	0.5s	>2h	1605.9s	1620.9s
3.8s	0.8s	0.6s	>2h	1099.4s	1242.6s
5.8s	0.8s	0.7s	>2h	1229.0s	1288.7s

Algebra System: Macaulay 2

Processor: 3.2 GHz Inter Core i5 (8GB total memory)

Computer System: Mac OS X 10.9.3

Experiment

Timings for Literature Models (s: seconds; h: hours; d: days)

Models	Algorithm 1	Algorithm 2	
		Strategy 1	Strategy 2
Example 3	11.1s	5.3s	6.4s
Example 4	36446.4s	360.2s	56.3s
Example 5	>16h	>16h	2768.2s
Example 6	>12d	>30d	30d

Example 3 (Random Censoring [M. Drton, B. Sturmfels and S. Sullivant, 2009]).

$$2p_0p_1p_2 + p_1^2p_2 + p_1p_2^2 - p_0^2p_{12} + p_1p_2p_{12}$$

Example 4 (3×3 Zero-Diagonal Matrix [E. Gross and J. I. Rodriguez, 2014]).

$$\det \begin{bmatrix} 0 & p_{12} & p_{13} \\ p_{21} & 0 & p_{23} \\ p_{31} & p_{32} & 0 \end{bmatrix}$$

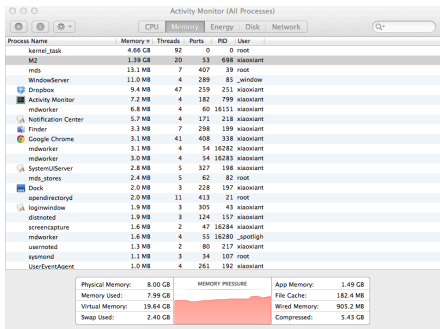
Example 5 (Grassmannian of 2-planes in \mathbb{C}^4 [S. Hosten, A. Khetan and B. Sturmfels, 2005]).

$$p_{12}p_{34} - p_{13}p_{24} + p_{14}p_{23}$$

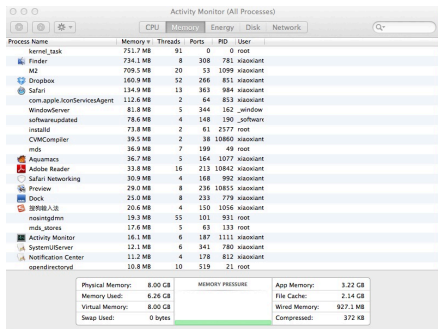
Example 6 (3×3 Symmetric Matrix Model [J. I. Rodriguez, 2014]).

Experiment

Comparing Memory Pressure for Computing Example 6



Left: running standard algorithm after 3 days



Right: running probabilistic algorithm after 3 days

3×3 Symmetric Matrix Model

A gambler has a coin and two pairs of three-sided dice. All the coin and dice are unfair. The two dice in the first pair have the same weights. The two dice in the second pair have the same weights.



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He plays the same game 1000 rounds

Toss the coin.

- If the coin lands on side 1, toss the first pair of dice.
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$[u_{11}, u_{12}, u_{13}, u_{22}, u_{23}, u_{33}]$

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Question

How to estimate the probability p_{ij} of getting the sides i and j with respect to the two dice?

3 × 3 Symmetric Matrix Model

Assume that the probabilities of observing the sides 1 and 2 of the coin are c_1 and c_2 , and the probabilities of observing the sides 1, 2 and 3 of one die in the first and second pair are $[b_1, b_2, b_3]$ and $[r_1, r_2, r_3]$, respectively. We know

$$\begin{bmatrix} p_{11} & \frac{p_{12}}{2} & \frac{p_{13}}{2} \\ \frac{p_{12}}{2} & p_{22} & \frac{p_{23}}{2} \\ \frac{p_{13}}{2} & \frac{p_{23}}{2} & p_{33} \end{bmatrix} = c_1 \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix} [b_1, b_2, b_3] + c_2 \begin{bmatrix} r_1 \\ r_2 \\ r_3 \end{bmatrix} [r_1, r_2, r_3]. \quad (5)$$

Therefore, the matrix on the left side has at most rank 2.

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Therefore, the matrix on the left side has at most rank 2. We have an algebraic statistical model below.

3 × 3 Symmetric Matrix Model

$$\mathcal{V}(g(p_{11}, p_{12}, p_{13}, p_{22}, p_{23}, p_{33})) \cap \Delta_5,$$

where

$$g = \det \begin{bmatrix} 2p_{11} & p_{12} & p_{13} \\ p_{12} & 2p_{22} & p_{23} \\ p_{13} & p_{23} & 2p_{33} \end{bmatrix},$$

$$\Delta_5 = \{(p_{11}, \dots, p_{33}) \in \mathbb{R}_{>0}^6 \mid p_{11} + p_{12} + p_{13} + p_{22} + p_{23} + p_{33} = 1\}$$

3 × 3 Symmetric Matrix Model

Question

How to maximize **likelihood function**

subject to the **algebraic statistical model** $\mathcal{V}(g) \cap \Delta_5$?

Answer.

Solve the **Lagrange likelihood equations**

$$F_0 = p_{11} \lambda_1 + p_{11} \lambda_2 (8p_{22}p_{33} - 2p_{23}^2) - u_{11} = 0$$

$$F_1 = p_{12} \lambda_1 + p_{12} \lambda_2 (2p_{13}p_{23} - 4p_{12}p_{33}) - u_{12} = 0$$

$$F_2 = p_{13} \lambda_1 + p_{13} \lambda_2 (2p_{12}p_{23} - 4p_{13}p_{22}) - u_{13} = 0$$

$$F_3 = p_{22} \lambda_1 + p_{22} \lambda_2 (8p_{11}p_{33} - 2p_{13}^2) - u_{22} = 0$$

$$F_4 = p_{23} \lambda_1 + p_{23} \lambda_2 (2p_{12}p_{13} - 4p_{11}p_{23}) - u_{23} = 0$$

$$F_5 = p_{33} \lambda_1 + p_{33} \lambda_2 (8p_{11}p_{22} - 2p_{12}^2) - u_{33} = 0$$

$$F_6 = g(p_{11}, p_{12}, p_{13}, p_{22}, p_{23}, p_{33}) = 0$$

$$F_7 = p_{11} + p_{12} + p_{13} + p_{22} + p_{23} + p_{33} - 1 = 0$$

where

- $p_{11}, p_{12}, p_{13}, p_{22}, p_{23}, p_{33}, \lambda_1$ and λ_2 are unknowns
- $u_{11}, u_{12}, u_{13}, u_{22}, u_{23}$ and u_{33} are parameters.

3 × 3 Symmetric Matrix Model

Data-Discriminant (By Probabilistic Algorithm)

$$\begin{aligned} -\mathcal{D}_{X_p} &= u_{11} u_{12} u_{13} u_{22} u_{23} u_{33} \\ -\mathcal{D}_{X_\infty} &= (u_{11} + u_{22} + u_{33} + u_{12} + u_{13} + u_{23})(u_{11} + u_{22} + u_{12})(u_{11} + u_{33} + u_{13})(u_{22} + u_{33} + u_{23})(u_{12} + \\ & 2u_{22} + u_{23})(u_{13} + 2u_{33} + u_{23})(u_{13} + 2u_{11} + u_{12})(8u_{11}u_{22}u_{33} - 2u_{11}u_{23}^2 - 2u_{12}^2u_{33} + 2u_{12}u_{13}u_{23} - 2u_{13}^2u_{22}). \\ -\mathcal{D}_{X_J} &= \underbrace{-64u_{11}^5 u_{22}^3 u_{23}^4 + \dots + u_{13}^4 u_{22}^2 u_{23}^6}_{1307 \text{ terms}} \end{aligned}$$

3 × 3 Symmetric Matrix Model

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Real Root Classification

(Sample points of data-discriminant are computed by RAGlib

[M. Safey El Din and E. Schost, 2003; H. Hong and M. Safey El Din, 2012; A. Greuet and M. Safey El Din, 2014])

For $(u_{11}, \dots, u_{33}) \in \mathbb{R}_{>0}^6$, if $\mathcal{D}_{X_\infty}(u_{11}, \dots, u_{33}) \neq 0$, then

- $\mathcal{D}_{X_J}(u_{11}, \dots, u_{33}) > 0 \Rightarrow 6$ distinct real solutions
- $\mathcal{D}_{X_J}(u_{11}, \dots, u_{33}) < 0 \Rightarrow 2$ distinct real (positive) solutions.

3 × 3 Symmetric Matrix Model

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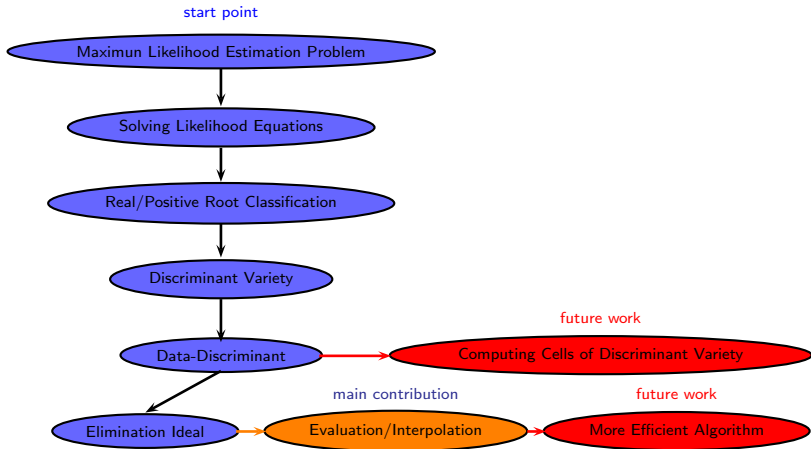
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- $\mathcal{D}_{X_J}(u_{11}, \dots, u_{33}) < 0 \Rightarrow 2$ distinct real (positive) solutions.

Remark. Sign of data-discriminant is NOT enough for classifying positive solutions.

- For data $(1, 1, \frac{280264116870825}{295147905179352825856}, 1, \frac{34089009205592922038535}{141080698675730650759168}, \frac{32898355113670387769001}{141080698675730650759168})$, the system has 6 distinct positive solutions.
- For data $(1, 1, 199008, 30, 2022, 1)$, the system has also 6 real solutions but only 2 positive solutions



Thank You for Your Attention!