Asymptotic Approximation of Marginal Likelihood Integrals

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17 Dec 2008, MSRI Algebraic Statistics Workshop

Introduction

Discrete Model
State space $[k] = \{1, 2, \ldots, k\}$
Compact parameter space $\Omega \subset \mathbb{R}^d$
Polynomial map $p = (p_i)$, $p : \Omega \to \Delta_{k-1}$

Example
Two-mixture of the independence model
with two ternary random variables

$$p_{ij}(a, b, c, d, e) = ab_i c_j + (1-a) d_i e_j, \quad i, j = 1, 2, 3$$

where $(a, 1-a) \in \Delta_1$, $(b_i), (c_j), (d_i), (e_j) \in \Delta_2$
and $\Omega = \Delta_1 \times \Delta_2 \times \Delta_2 \times \Delta_2 \times \Delta_2$.

Introduction

Let $u = (u_i)$ be a vector of counts for a sample of size n.

Marginal Likelihood Integral

$$Z_n(u) = \int_\Omega \prod_{i=1}^{k} p_i(\omega)^{u_i} d\omega$$

Plays important role in various practical applications, especially model selection.

Previous Work
Computed $Z_n(u)$ exactly for small samples.
(L.-Sturmfels-Xu 2008)

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Goal
Assume U drawn from *true distribution* $q \in \operatorname{Im} p$.
Find asymptotics of $\mathrm{E}[\log Z_n(U)]$ as $n \to \infty$.

Asymptotic Approximation

Notations

1. Define $Q(\omega) = \|p(\omega) - q\|^2 = \sum_{i=1}^{k} (p_i(\omega) - q_i)^2$.
2. Given $x \in \text{fiber}(q) = \{\omega : p(\omega) = q\}$,
   let $(-\lambda_x) \in \mathbb{Q}$ be the largest pole of the *zeta function*

   $$J_x(z) = \int_{\Omega_x} Q(\omega)^z d\omega$$

   for a sufficiently small neighborhood Ω_x of x.
   Let m_x be the multiplicity of this pole.
3. Define an ordering on $\mathbb{Q}_{>0} \times \mathbb{Z}_{>0}$:
   $(\lambda_2, m_2) > (\lambda_1, m_1) \;\Leftrightarrow\; \lambda_2 > \lambda_1$, or $\lambda_1 = \lambda_2$ and $m_2 < m_1$.

Asymptotic Approximation

Theorem (based on Watanabe 2001)

$$\mathrm{E}[\log Z_n] = n \sum_{i=1}^{k} q_i \log q_i - \lambda \log n + (m-1) \log\log n + O(1)$$

where (λ, m) is *smallest* among all (λ_x, m_x), $x \in \mathrm{fiber}(q)$.

Remarks

1. λ is the *real log canonical threshold* (RLCT) of the Q.
2. The (λ_x, m_x) can be found using *local* resolution of singularities, which exists by (Atiyah 1970).

Given $x \in \mathrm{fiber}(q)$, how do we compute (λ_x, m_x)?

Newton Diagrams

Let $Q(\omega) = \sum_\alpha c_\alpha \omega^\alpha$ be a polynomial in d variables.

Newton polyhedron $\Gamma_+(Q)$: $\mathrm{conv}(\{\alpha + \alpha' : c_\alpha \neq 0, \alpha' \in \mathbb{R}^d_{\geq 0}\})$.

Face polynomial $Q_\gamma(\omega)$: $\sum_{\alpha \in \gamma} c_\alpha \omega^\alpha$, γ compact face.

Newton diagram $\Gamma(Q)$: union of all compact faces.

Principal part $Q_\Gamma(\omega)$: $\sum_{\alpha \in \Gamma(Q)} c_\alpha \omega^\alpha$.

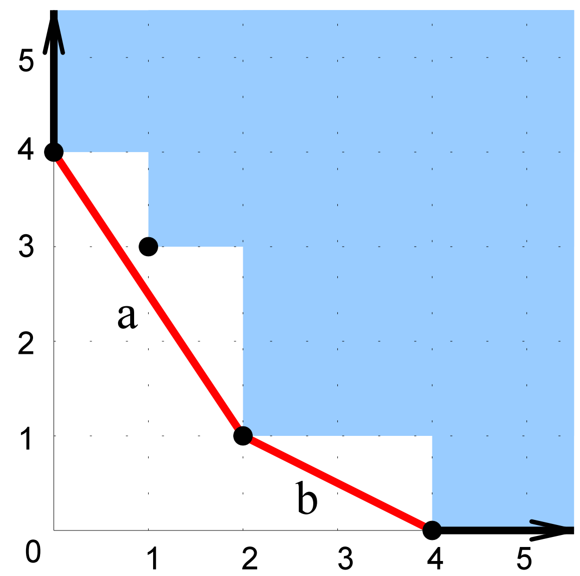
Example

$$Q(x, y) = x^4 + x^2 y + x y^3 + y^4$$

$$Q_a(x, y) = x^2 y + y^4$$

$$Q_b(x, y) = x^4 + x^2 y$$

$$Q_\Gamma(x, y) = x^4 + x^2 y + y^4$$



Non-degeneracy

$Q(\omega)$ is *non-degenerate* if for all compact faces γ,

$$\mathcal{V}\left(\frac{\partial Q_\gamma}{\partial \omega_1}, \frac{\partial Q_\gamma}{\partial \omega_2}, \ldots, \frac{\partial Q_\gamma}{\partial \omega_d}\right) \quad \subseteq \quad \mathcal{V}(\omega_1\omega_2\cdots\omega_d)$$

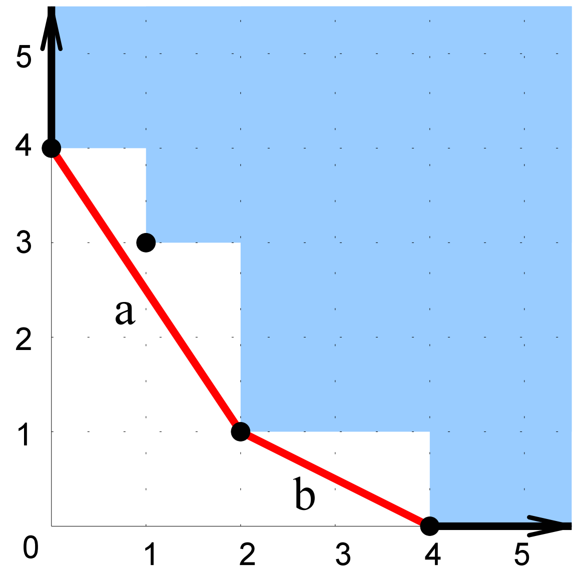
Example

$Q(x,y) = x^4 + x^2y + xy^3 + y^4$ is non-degenerate.
$Q(x,y) = (x+y)^2$ is degenerate.

We now present three tools which allow us to compute resolution of singularities using Newton diagrams.

Proposition 1

Suppose $Q(\omega)$ is non-degenerate.
A regular subdivision of the normal fan of $\Gamma_+(Q)$ describes a local resolution of singularities at the origin via toric modifications.



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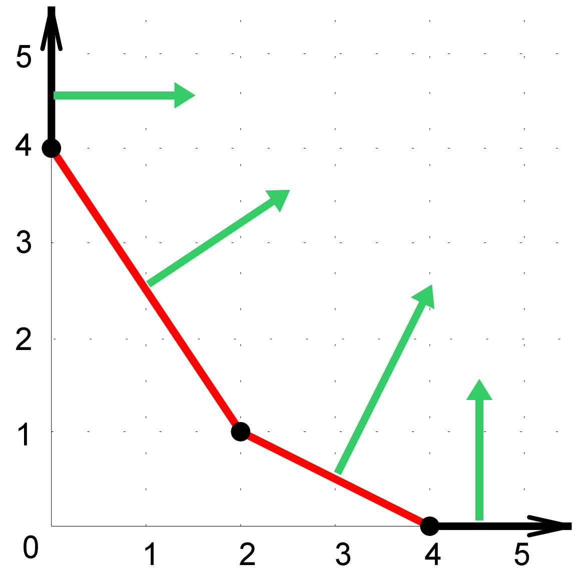

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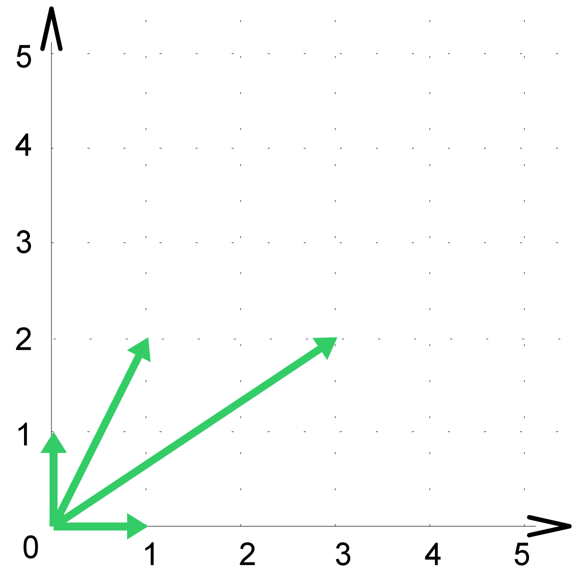

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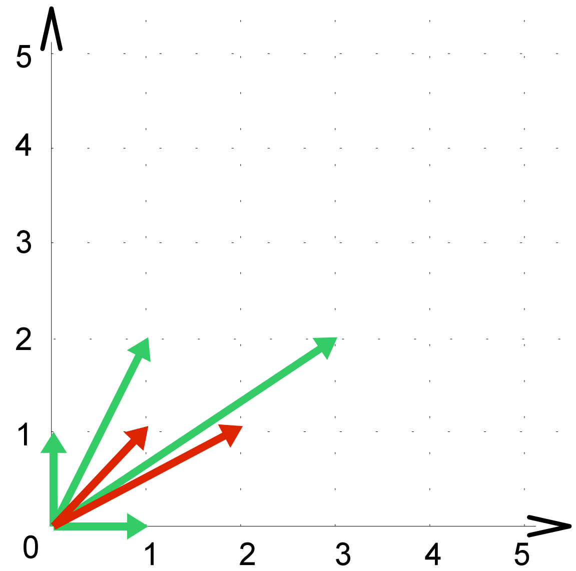

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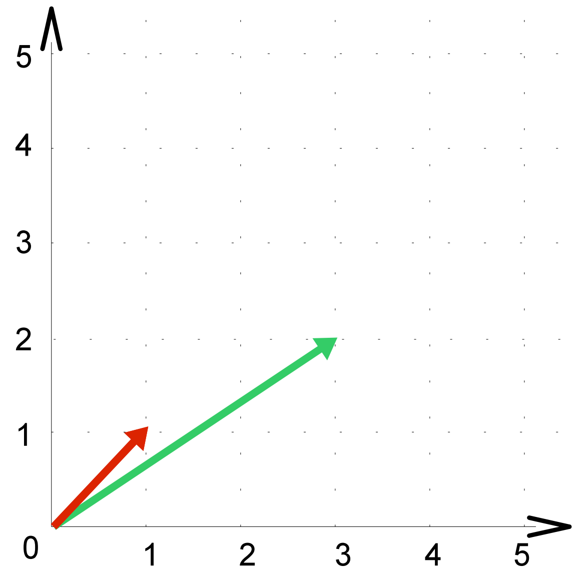

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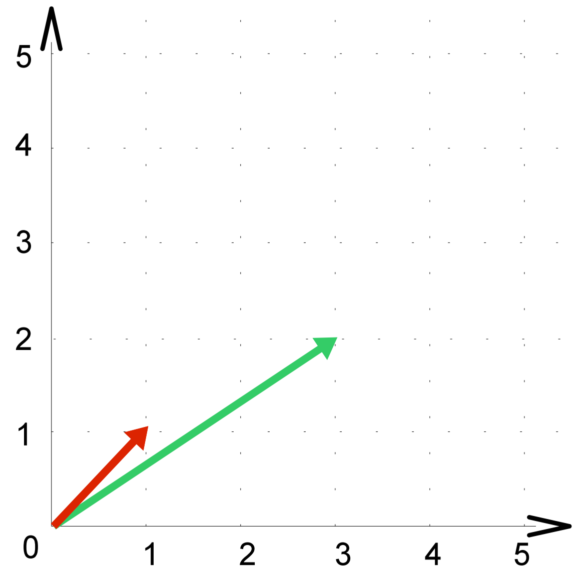
$$Q(x,y) \quad = \quad x^4 + x^2y + xy^3 + y^4$$

$$\begin{aligned} x &= u^3v^1 \\ y &= u^2v^1 \\ Q(u,v) &= u^8v^3(1+v+uv+u^4v) \end{aligned}$$



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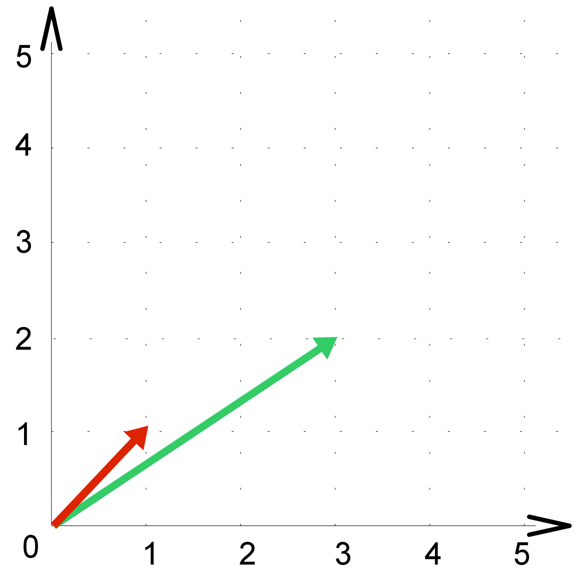
$$
\begin{aligned}
Q(x,y) &= x^4 + x^2y + xy^3 + y^4 \\
J_0(z) &= \int Q(x,y)^z \; dxdy \\
&= \int Q(u,v)^z \, u^4 v \; dudv \\
&= \int u^{8z+4} v^{3z+1} \\
&\quad\; (1+v+uv+u^4v)^z \; dudv \\
(\lambda, m) &= (\tfrac{5}{8},\; 1)
\end{aligned}
$$



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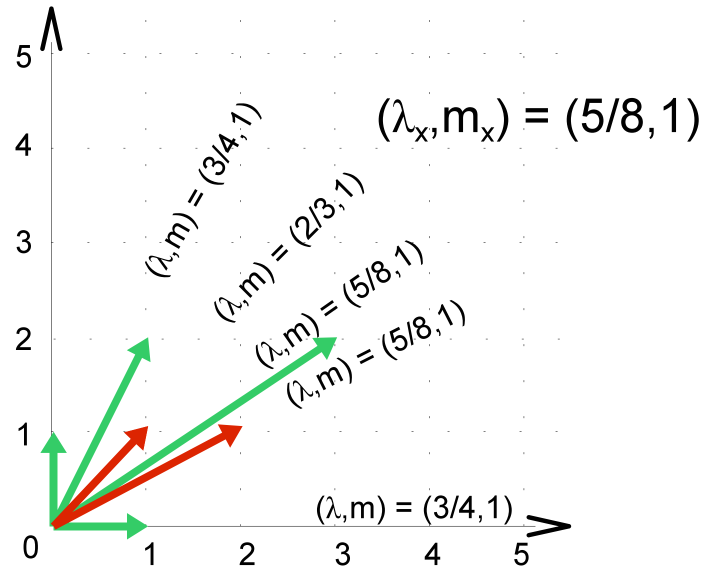

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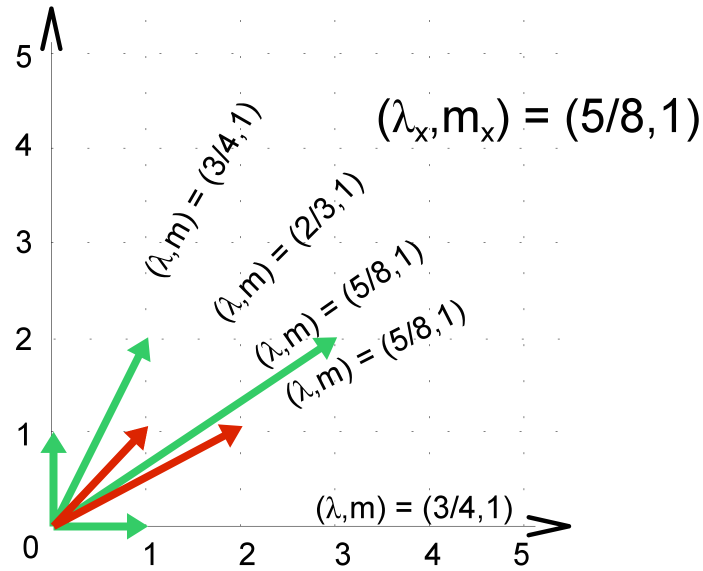
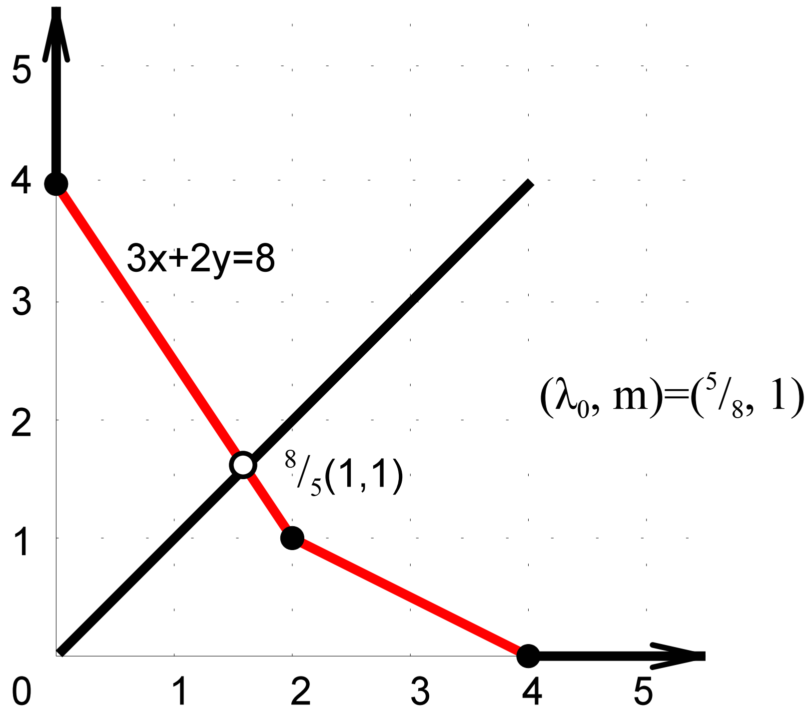
A regular subdivision of the normal fan of $\Gamma_+(Q)$ describes a local resolution of singularities at the origin via toric modifications.

The regular subdivision describes a resolution map $g : \mathcal{M} \to W$, where $\mathcal{M}$ is a manifold and W is an open nbhd of the origin.

In particular, each maximal cone gives a chart map $U \to W$ defined by monomials.



Proposition 2
Suppose $Q(\omega)$ is non-degenerate.
The RLCT λ_0 of $Q(\omega)$ comes from
the intersection $\frac{1}{\lambda_0}(1,1,\ldots,1) = \frac{1}{\lambda_0}\mathbf{1}$
of the diagonal $\{t\mathbf{1}\}$ with the boundary of $\Gamma_+(Q)$.



Proposition 3
Regardless of the degeneracy of $Q(\omega)$,
the RLCT and its multiplicity (λ_0, m_0) of $Q(\omega)$
is the same as that of the principal part $Q_\Gamma(\omega)$.

(Afternote: this proposition is false.
I will address this in a new paper.)

$$Q(\omega) = x^4 + x^2 y + x y^3 + y^4$$

$$Q_\Gamma(x, y) = x^4 + x^2 y + y^4$$

Example

Discrete model

$$p_{ij}(a,b,c,d,e) = ab_ic_j + (1-a)d_ie_j, \quad i,j = 1,2,3$$

True distribution

$$q_{11} = q_{12} = \ldots = q_{33} = \tfrac{1}{9}$$

$Q(a,b,c,d,e) = \sum_{i,j}(ab_ic_j + (1-a)d_ie_j - \frac{1}{9})^2$

Pick $x = (a^*, b^*, c^*, d^*, e^*) \in \mathrm{fiber}(q)$.

Shift the origin to x.

$$\begin{aligned} Q(a,b,c,d,e) = \textstyle\sum_{i,j}[&(a+a^*)(b_i+b_i^*)(c_j+c_j^*) \\ &+(1-a-a^*)(d_i+d_i^*)(e_j+e_j^*) - \tfrac{1}{9})]^2 \end{aligned}$$

Example

$Q = \sum_{i,j} [(a + a^*)(b_i + b_i^*)(c_j + c_j^*) + (1 - a - a^*)(d_i + d_i^*)(e_j + e_j^*) - \frac{1}{9}]^2$

Toric Modification

Suppose $a^* = 0$, $b^* = c^* = (0, 0, 1)$, $d^* = e^* = (\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$.

Principal part $Q_\Gamma = \frac{2}{3}(d_1 d_2 + e_1 e_2 + d_1^2 + d_2^2 + e_1^2 + e_2^2)$
$\qquad - \frac{2}{3} a(d_1 + d_2 + e_1 + e_2) + \frac{8}{9} a^2$

From this, one can check that Q is non-degenerate.
Using the method of Newton diagrams, we derive

$$(\lambda_x, m_x) = (\frac{5}{2}, 1)$$

Example

$$Q = \sum_{i,j} [(a + a^*)(b_i + b_i^*)(c_j + c_j^*) + (1 - a - a^*)(d_i + d_i^*)(e_j + e_j^*) - \tfrac{1}{9}]^2$$

Non-toric Modification

Suppose $a^* = \frac{1}{2}$, $b^* = c^* = (\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$, $d^* = e^* = (\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$.

Principal part $Q_\Gamma = \frac{1}{6}(b_1^2 + b_2^2 + c_1^2 + c_2^2 + d_1^2 + d_2^2 + e_1^2 + e_2^2$

$$+ b_1 b_2 + c_1 c_2 + d_1 d_2 + e_1 e_2 + c_1 e_2 + c_2 e_1 + b_1 d_2 + b_2 d_1)$$

$$+ \tfrac{1}{3}(b_1 d_1 + b_2 d_2 + c_1 e_1 + c_2 e_2)$$

From this, one can check that Q is degenerate.

We do a linear change of variable.

Example

$$Q = \sum_{i,j}[(a+a^*)(b_i+b_i^*)(c_j+c_j^*) + (1-a-a^*)(d_i+d_i^*)(e_j+e_j^*) - \tfrac{1}{9}]^2$$

Non-toric Modification

Suppose $a^* = \frac{1}{2}$, $b^* = c^* = (\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$, $d^* = e^* = (\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$.

Let $d_1 = d_1' - b_1'$, $d_2 = d_2' - b_2'$, $e_1 = e_1' - c_1'$, $e_2 = e_2' - c_2'$.

Then, $Q_\Gamma = d_1'^2 + d_1'd_2' + d_2'^2 + e_1'^2 + e_1'e_2' + e_2'^2$.

In the new variables, Q_Γ is non-degenerate.

Using the method of Newton diagrams, we derive

$$(\lambda_x, m_x) = (2, 1)$$

Example

$$Q = \sum_{i,j}[(a+a^*)(b_i+b_i^*)(c_j+c_j^*)+(1-a-a^*)(d_i+d_i^*)(e_j+e_j^*)-\tfrac{1}{9}]^2$$

Conjecture

The RLCT and its multiplicity of the model is $(2,1)$.

Moral of the story (Watanabe-Yamazaki 2004)

1. Take principal part.
2. If non-degenerate, apply Newton diagram method.
3. If degenerate, apply change of variable and go to Step 1.

Critical Question

For which singularities $x \in \mathrm{fiber}(q)$ do we compute (λ_x, m_x)?

Comparison with Exact Evaluation

Model $\quad p_i(\sigma,\theta,\rho) = \binom{4}{i}(\sigma_0\theta_0^i\theta_1^{4-i} + \sigma_1\rho_0^i\rho_1^{4-i})$, $\quad 0 \le i \le 4$

True Distribution $\quad q_i = \frac{1}{16}\binom{4}{i}$

Asymptotics $\quad \log Z_n = n\sum_i q_i \log q_i - \frac{3}{4}\log n + O(1)$

We compute $G(n) = 16\sum_i q_i \log q_i + \log Z_n - \log Z_{16+n}$.

We expect it to be close to $g(n) = \frac{3}{4}(\log(16+n) - \log n)$.

n	$G(n)$	$g(n)$
16	0.21027043	0.225772497
32	0.12553837	0.132068444
48	0.08977938	0.093704053
64	0.06993586	0.072682510
80	0.05729553	0.059385934
96	0.04853292	0.050210092
112	0.04209916	0.043493960

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