

Asymptotic Approximation of Marginal Likelihood Integrals

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Introduction

Discrete Model

State space $[k] = \{1, 2, \dots, k\}$

Compact parameter space $\Omega \subset \mathbb{R}^d$

Polynomial map $p = (p_i), p : \Omega \rightarrow \Delta_{k-1}$

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* $q \in \text{Im } p$.

Find asymptotics of $E[\log Z_n(U)]$ as $n \rightarrow \infty$.

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)

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

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

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 $x \in \text{fiber}(q)$, 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 $\Gamma_{+}(Q)$: $\text{conv}(\{\alpha + \alpha' : c_{\alpha} \neq 0, \alpha' \in \mathbb{R}_{\geq 0}^d\})$.

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

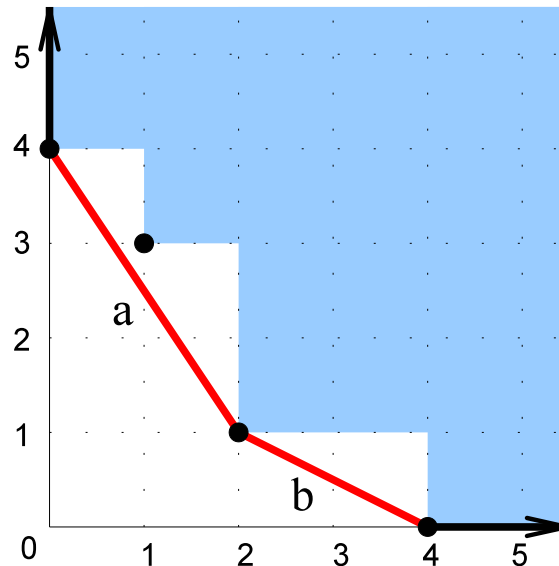
Example

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

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

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

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



Non-degeneracy

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

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

Example

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

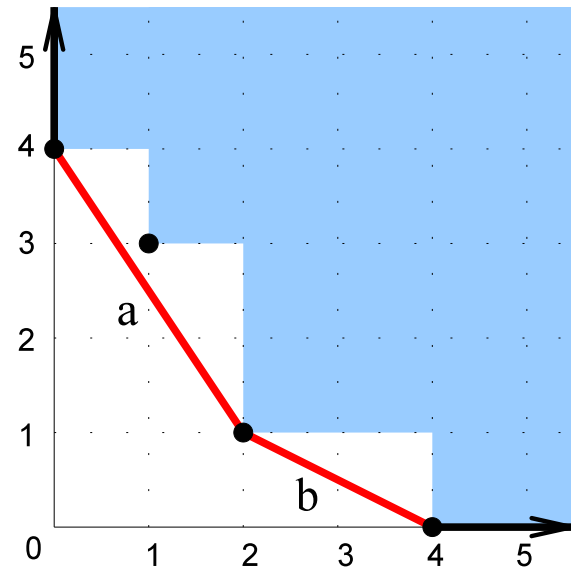
$Q(x, y) = (x + y)^2$ is degenerate.

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

Proposition 1

Suppose $Q(\omega)$ is non-degenerate.

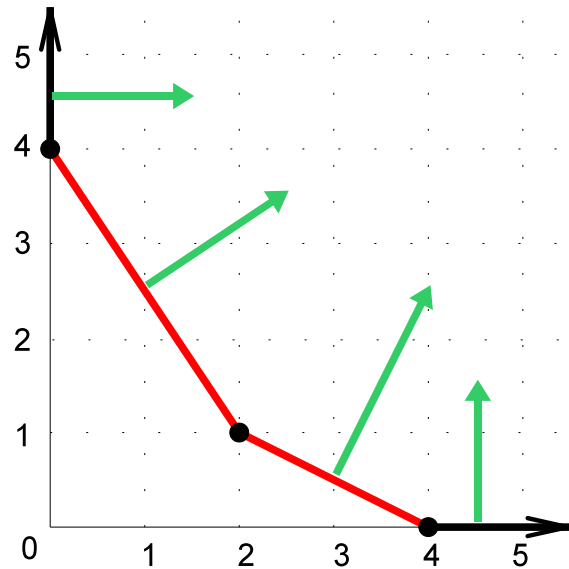
A regular subdivision of the normal fan of $\Gamma_+(Q)$ describes a local resolution of singularities at the origin via toric modifications.



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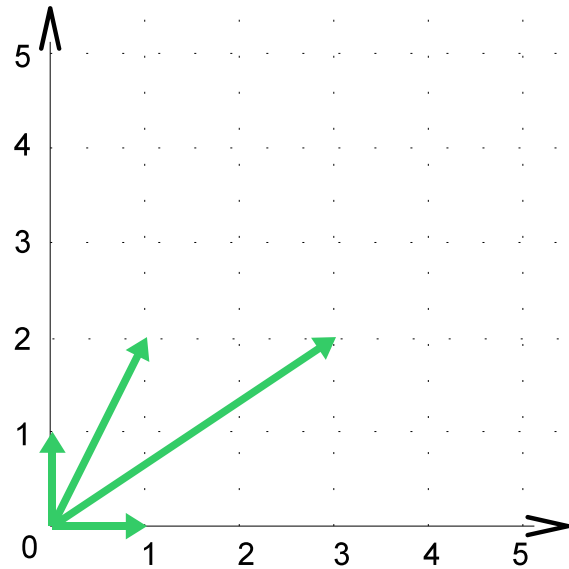
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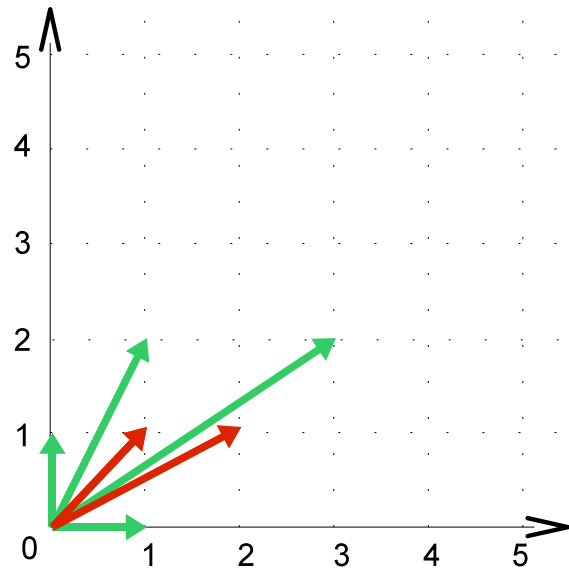
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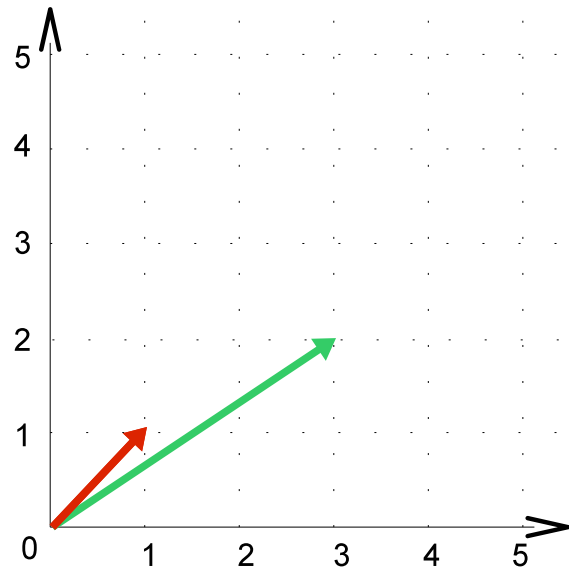
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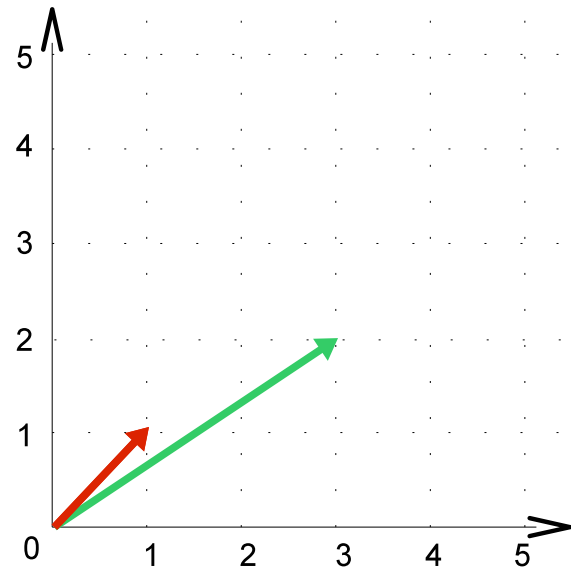
A regular subdivision of the normal fan of $\Gamma_+(Q)$ describes a local resolution of singularities at the origin via toric modifications.

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

$$x = u^3v^1$$

$$y = u^2v^1$$

$$Q(u, v) = u^8v^3(1 + v + uv + u^4v)$$



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

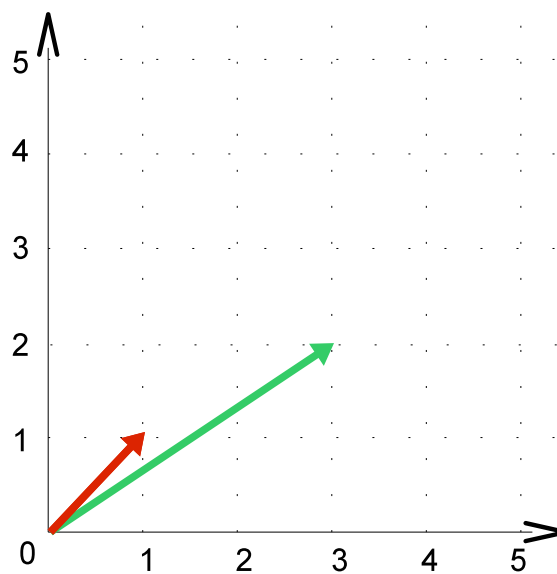
$$J_0(z) = \int Q(x, y)^z dx dy$$

$$= \int Q(u, v)^z u^4 v^3 du dv$$

$$= \int u^{8z+4} v^{3z+1}$$

$$(1 + v + uv + u^4v)^z du dv$$

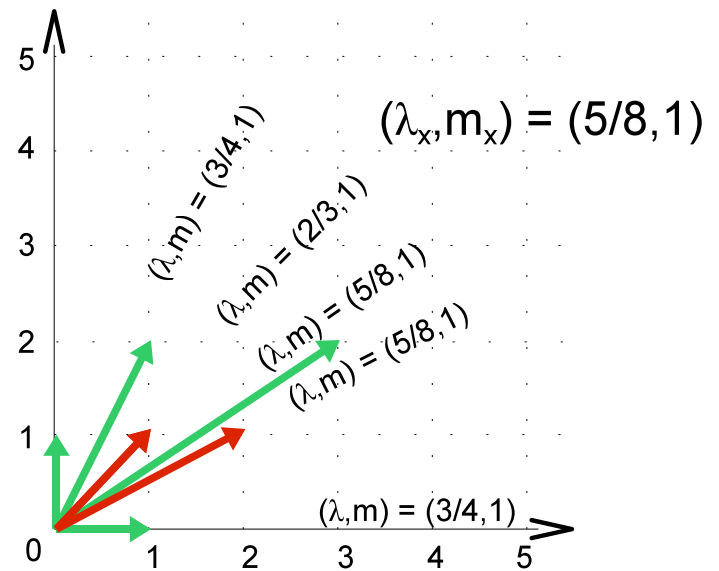
$$(\lambda, m) = \left(\frac{5}{8}, 1\right)$$



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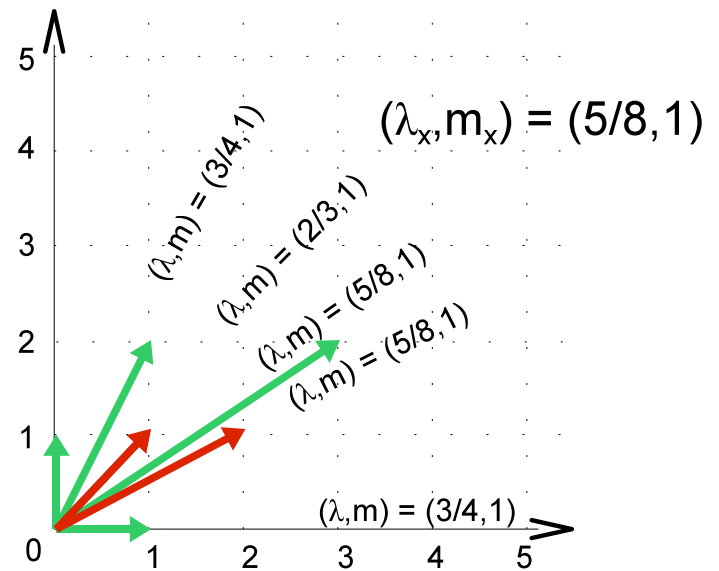
Proposition 1

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.

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

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



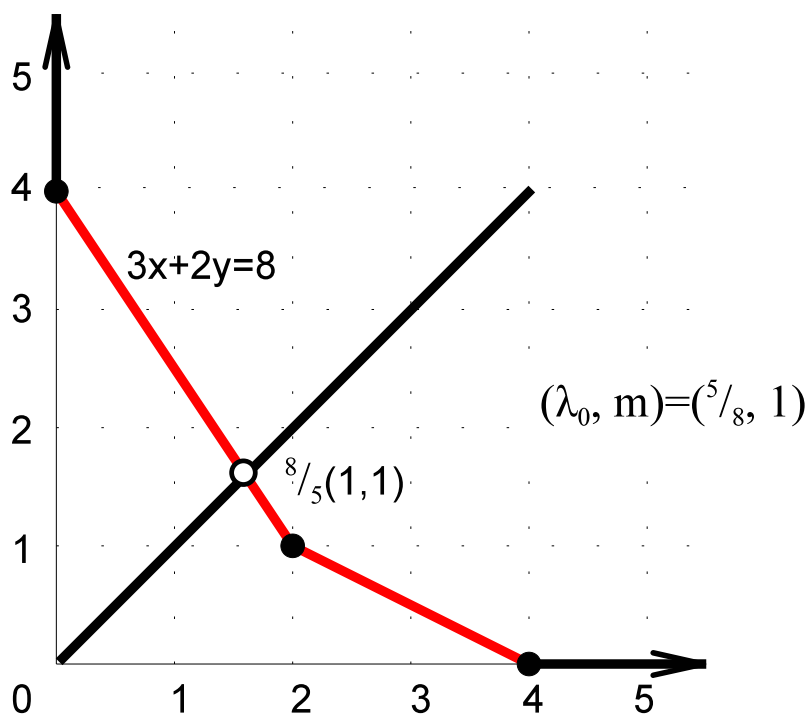
Proposition 2

Suppose $Q(\omega)$ is non-degenerate.

The RLCT λ_0 of $Q(\omega)$ comes from

the intersection $\frac{1}{\lambda_0}(1, 1, \dots, 1) = \frac{1}{\lambda_0}\mathbf{1}$

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.)

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

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

Example

Discrete model

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

True distribution

$$q_{11} = q_{12} = \dots = q_{33} = \frac{1}{9}$$

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

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

Shift the origin to x .

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

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

$$\begin{aligned} \text{Principal part } Q_\Gamma &= \frac{2}{3}(d_1 d_2 + e_1 e_2 + d_1^2 + d_2^2 + e_1^2 + e_2^2) \\ &\quad - \frac{2}{3}a(d_1 + d_2 + e_1 + e_2) + \frac{8}{9}a^2 \end{aligned}$$

From this, one can check that Q is non-degenerate.

Using the method of Newton diagrams, we derive

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

Example

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

Non-toric Modification

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

$$\begin{aligned} \text{Principal part } Q_\Gamma &= \frac{1}{6}(b_1^2 + b_2^2 + c_1^2 + c_2^2 + d_1^2 + d_2^2 + e_1^2 + e_2^2 \\ &\quad + b_1b_2 + c_1c_2 + d_1d_2 + e_1e_2 + c_1e_2 + c_2e_1 + b_1d_2 + b_2d_1) \\ &\quad + \frac{1}{3}(b_1d_1 + b_2d_2 + c_1e_1 + c_2e_2) \end{aligned}$$

From this, one can check that Q is degenerate.

We do a linear change of variable.

Example

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

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

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

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

Comparison with Exact Evaluation

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

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

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

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

References

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3. S. Watanabe: Algebraic Analysis for Nonidentifiable Learning Machines, *Neural Computation* **13** (2001) 899–933.
4. K. Yamazaki and S. Watanabe: Newton Diagram and Stochastic Complexity in Mixture of Binomial Distributions, *Algorithmic Learning Theory* (2004) 350–364.