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Lower Bounds on Multivariate Higher Order Derivatives of Differential Entropy †

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† This paper is an extended version of our paper published in 2021 IEEE International Symposium on Information Theory.

Abstract: This paper studies the properties of the derivatives of differential entropy $H(X_t)$ in Costa's entropy power inequality. For real-valued random variables, Cheng and Geng conjectured that for $m \geq 1$, $(-1)^{m+1}(\frac{d^m}{dt^m})H(X_t) \geq 0$, while McKean conjectured a stronger statement, whereby $(-1)^{m+1}(\frac{d^m}{dt^m})H(X_t) \geq (-1)^{m+1}(\frac{d^m}{dt^m})H(X_{Gt})$. Here, we study the higher dimensional analogues of these conjectures. In particular, we study the veracity of the following two statements: $C_1(m, n) : (-1)^{m+1}(\frac{d^m}{dt^m})H(X_t) \geq 0$, where n denotes that X_t is a random vector taking values in \mathbb{R}^n , and similarly, $C_2(m, n) : (-1)^{m+1}(\frac{d^m}{dt^m})H(X_t) \geq (-1)^{m+1}(\frac{d^m}{dt^m})H(X_{Gt}) \geq 0$. In this paper, we prove some new multivariate cases: $C_1(3, i), i = 2, 3, 4$. Motivated by our results, we further propose a weaker version of McKean's conjecture $C_3(m, n) : (-1)^{m+1}(\frac{d^m}{dt^m})H(X_t) \geq (-1)^{m+1}\frac{1}{n}(\frac{d^m}{dt^m})H(X_{Gt})$, which is implied by $C_2(m, n)$ and implies $C_1(m, n)$. We prove some multivariate cases of this conjecture under the log-concave condition: $C_3(3, i), i = 2, 3, 4$ and $C_3(4, 2)$. A systematic procedure to prove $C_i(m, n)$ is proposed based on symbolic computation and semidefinite programming, and all the new results mentioned above are explicitly and strictly proved using this procedure.



Citation: Guo, L.; Yuan, C.-M.; Gao, X.-S. Lower Bounds on Multivariate Higher Order Derivatives of Differential Entropy. *Entropy* **2022**, *24*, 1155. <https://doi.org/10.3390/e24081155>

Academic Editor: Philip Broadbridge

Received: 27 June 2022

Accepted: 17 August 2022

Published: 19 August 2022

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Keywords: differential entropy; completely monotone; McKean's conjecture; log-concavity; Gaussian optimality

1. Introduction

Shannon's entropy power inequality (EPI) is one of the most important information inequalities [1], which has many proofs, generalizations, and applications [2–11]. In particular, Costa presented a generalized version of the EPI in his seminal paper [12].

Let X be an n -dimensional random vector with finite variance and a probability density function $p(x)$. For $t > 0$, define $X_t \triangleq X + Z_t$, where $Z_t \sim N_n(0, tI)$ is an independent standard Gaussian random vector with the covariance matrix $t \times I$. The probability density of X_t is

$$p_t(x_t) = \frac{1}{(2\pi t)^{n/2}} \int_{\mathbb{R}^n} p(x) \exp\left(-\frac{\|x_t - x\|^2}{2t}\right) dx. \quad (1)$$

Thus, the heat equation holds for $p_t(x_t)$, i.e.,

$$\frac{dp_t}{dt} = \frac{1}{2} \nabla^2 p_t. \quad (2)$$

The differential entropy of X_t is defined as

$$H(X_t) = - \int_{\mathbb{R}^n} p_t(x_t) \log p_t(x_t) dx_t. \quad (3)$$

Costa [12] proved that the *entropy power* of X_t , given by $N(X_t) = \frac{1}{2\pi e} e^{(2/n)H(X_t)}$ is a concave function in t . More precisely, Costa proved $(d/dt)N(X_t) \geq 0$ and $(d^2/dt^2)N(X_t) \leq 0$.

Due to its importance, several new proofs and generalizations for Costa’s EPI have been given. Dembo [13] gave a simple proof for Costa’s EPI via the Fisher information inequality. Villani [14] proved Costa’s EPI with Cauchy–Schwarz inequality as well as the heat equation. Toscani [15] proved that $(d^3/dt^3)N(X_t) \geq 0$ if p_t is log-concave. Cheng and Geng proposed a conjecture [16]:

Conjecture 1. *The first derivative of $H(X_t)$ (i.e., the Fisher information) is completely monotone in t , that is,*

$$C_1(m, n) : (-1)^{m+1}(d^m/dt^m)H(X_t) \geq 0. \tag{4}$$

Costa’s EPI implies $C_1(1, n)$ and $C_1(2, n)$ [12], and Cheng–Geng proved $C_1(3, 1)$ and $C_1(4, 1)$ [16].

Let $X_G \sim N_n(\mu, \sigma^2 I)$ be an n -dimensional Gaussian random vector and $X_{Gt} \triangleq X_G + Z_t$ be the Gaussian X_t . McKean [17] proved that X_{Gt} achieves the minimum of $(d/dt)H(X_t)$ and $-(d^2/dt^2)H(X_t)$ is subject to $\text{Var}(X_t) = \sigma^2 + t$, and conjectured the general case:

Conjecture 2. *The following inequality holds subject to $\text{Var}(X_t) = \sigma^2 + t$,*

$$C_2(m, n) : (-1)^{m+1}(d^m/dt^m)H(X_t) \geq (-1)^{m+1}(d^m/dt^m)H(X_{Gt}) \geq 0. \tag{5}$$

McKean proved $C_2(1, 1)$ and $C_2(2, 1)$ [17]. Zhang–Anantharam–Geng [18] proved $C_2(3, 1)$, $C_2(4, 1)$ and $C_2(5, 1)$ if the probability density function of X_t is log-concave. Note that $C_2(1, n)$ and $C_2(2, n)$ are immediate consequences of Entropy Power Inequality and Costa’s concavity of entropy power result [12], respectively. In this paper, we notice that in the multivariate case, Conjecture 2 might not be true for $m > 2$ even under the log-concave condition, which motivates us to propose the following weaker conjecture:

Conjecture 3. *The following inequality holds subject to $\text{Var}(X_t) = \sigma^2 + t$,*

$$C_3(m, n) : (-1)^{m+1}(d^m/dt^m)H(X_t) \geq (-1)^{m+1}\frac{1}{n}(d^m/dt^m)H(X_{Gt}) \geq 0. \tag{6}$$

We see that Conjecture 3 coincides with Conjecture 2 for $n = 1$ (univariate case). Additionally, Conjecture 2 implies Conjecture 3 and Conjecture 3 implies Conjecture 1. The three conjectures give different lower bounds for the derivatives of $(-1)^{m+1}H(X_t)$.

Remark 1. *The authors in [14,16] proved some cases of Conjecture 1 by writing the left-hand formula in Conjecture 1 as sums of squares and, hence, concluded their sign. We provide a systematic way to explore this idea using symbolic computation and semidefinite programming and prove several new results in the multivariate cases.*

Our procedure for proving $C_s(m, n)$ consists of three main ingredients. First, a systematic method is proposed to compute the constraints $R_i, i = 1, \dots, N_1$ that are satisfied by $p_t(x_t)$ and its derivatives. The condition that p_t is log-concave can also be reduced to a set of constraints, i.e., $\mathcal{R}_j, j = 1, \dots, N_2$. Second, based on symbolic computation, proof for $C_s(m, n)$ is reduced to the following problem:

$$\exists p_i \in \mathbb{R} \text{ and } Q_j \text{ s.t. } (E - \sum_{i=1}^{N_1} p_i R_i - \sum_{j=1}^{N_2} Q_j \mathcal{R}_j = S) \tag{7}$$

where E, Q_j , and S are polynomials in p_t and its derivatives such that E represents the conjecture, $Q_j \geq 0$, and S is a sum of squares (SOS). Third, problem (7) can be solved with semidefinite programming (SDP) [19,20]. Note that from Equation (7), we can give an explicit and strict proof for $C_s(m, n)$.

Using the procedure proposed in this paper, we prove several new results about the three conjectures: $C_1(3,2)$, $C_1(3,3)$, $C_1(3,4)$, and $C_3(3,2)$, $C_3(3,3)$, $C_3(3,4)$, $C_3(4,2)$ under the log-concave condition.

In Table 1, we give the data for computing the SOS representation (7) using the Matlab software in Appendix A of [21], where Vars is the number of variables, and N_1 and N_2 are the numbers of constraints in (7).

Table 1. Data in computing the SOS with symbolic computation and SDP.

	$C_2(3,1)$	$C_1(3,2)$	$C_1(3,3)$	$C_1(3,4)$	$C_3(3,2)$	$C_3(3,3)$	$C_3(3,4)$	$C_3(4,2)$
Vars	3	14	38	80	14	38	38	33
N_1	6	63	512	1966	63	512	512	417
N_2	0	0	0	0	0	6	6	3

The procedure is inspired by the work of [12,14,16,18], and uses basic ideas introduced therein. The specific contributions in this paper are:

- (1) Based on symbolic computation and semidefinite programming, $C_s(m, n)$ can be automatically verified with the aid of the software systems Maple and Matlab, and analytical proofs for $C_s(m, n)$ can also be efficiently produced.
- (2) The new concept of differentially homogenous polynomials is introduced and used to reduce the computational complexity. Compared with the pure SDP-based approach (such as [18]), the computational efficiency of our procedure is, in general, much higher. See Procedure 2 for details.
- (3) The results in [16,18] are generalized from the univariate cases to the multivariate cases (new results). This is the first attempt for the multivariate high order cases of the conjectures.
- (4) In comparison to the literature (such as [12,15,16,18]), the constraints (integral or log-concave) considered in this paper are more general.

The rest of this paper is organized as follows. In Section 2, we give the proof procedure. In Section 3, we prove $C_1(3,2)$, $C_1(3,3)$ and $C_1(3,4)$. In Section 4 we prove $C_3(3,2)$, $C_3(3,3)$, and $C_3(3,4)$ under the log-concave condition. In Section 5, we prove $C_3(4,2)$ under the log-concave condition. In Section 6, the conclusions are presented.

2. Proof Procedure

In this section, we provide a general procedure to prove $C_s(m, n)$ for specific values of s, m , and n .

2.1. Some Notations

Let $[n]_0 = \{0, 1, \dots, n\}$, $[n] = \{1, \dots, n\}$, and $x_t = [x_{1,t}, \dots, x_{n,t}]$. To simplify the notations, we use p_t to denote $p_t(x_t)$ in the rest of the paper. Denote

$$\mathcal{P}_n = \left\{ \frac{\partial^h p_t}{\partial^{h_1} x_{1,t} \cdots \partial^{h_n} x_{n,t}} : h = \sum_{i=1}^n h_i, h_i \in \mathbb{N} \right\}$$

to be the set of all derivatives of p_t with respect to the differential operators $\frac{\partial}{\partial x_{i,t}}, i = 1, \dots, n$ and $\mathbb{R}[\mathcal{P}_n]$ to be the set of polynomials in \mathcal{P}_n with coefficients in \mathbb{R} . For $v \in \mathcal{P}_n$, let $\text{ord}(v)$ be the order of v . For a monomial $\prod_{i=1}^r v_i^{d_i}$ with $v_i \in \mathcal{P}_n$, its *degree*, *order*, and *total order* are defined as $\sum_{i=1}^r d_i$, $\max_{i=1}^r \text{ord}(v_i)$, and $\sum_{i=1}^r d_i \cdot \text{ord}(v_i)$, respectively.

A polynomial in $\mathbb{R}[\mathcal{P}_n]$ is called a *k*th-order *differentially homogeneous polynomial* or simply a *k*th-order *differential form*, if all its monomials have a degree of k and a total order of k . Let $\mathcal{M}_{k,n}$ be the set of all monomials which have a degree of k and a total order of k . Then, the set of *k*th-order differential forms is an \mathbb{R} -linear vector space generated by $\mathcal{M}_{k,n}$, which is denoted as $\text{Span}_{\mathbb{R}}(\mathcal{M}_{k,n})$.

We will use Gaussian elimination in $\text{Span}_{\mathbb{R}}(\mathcal{M}_{k,n})$ by treating the monomials as variables. We always use the *lexicographic order for the monomials* to be defined below unless mentioned otherwise. Consider two distinct derivatives $v_1 = \frac{\partial^h p_t}{\partial^{h_1} x_{1,t} \cdots \partial^{h_n} x_{n,t}}$ and $v_2 = \frac{\partial^s p_t}{\partial^{s_1} x_{1,t} \cdots \partial^{s_n} x_{n,t}}$. We say $v_1 > v_2$ if $h > s$, or $h = s, h_l > s_l$ and $h_j = s_j$ for $j = l + 1, \dots, n$. Consider the two distinct monomials $m_1 = \prod_{i=1}^r v_i^{d_i}$ and $m_2 = \prod_{i=1}^r v_i^{e_i}$, where $v_i \in \mathcal{P}_n$ and $v_i < v_j$ for $i < j$. We define $m_1 > m_2$ if $d_l > e_l$, and $d_i = e_i$ for $i = l + 1, \dots, r$.

From (1), $p_t : \mathbb{R}^{n+1} \rightarrow \mathbb{R}$ is a function in x_t and t . Therefore, each polynomial $f \in \mathbb{R}[\mathcal{P}_n]$ is also a function in x_t and t , $\tilde{f}(t) = \int_{\mathbb{R}^n} f dx_t$ is a function in t , and the expectation of f with respect to $x_t \mathbb{E}[f] \triangleq \int_{\mathbb{R}^n} p_t f dx_t$ is also a function in t . By $f \geq 0$, $\tilde{f} \geq 0$, and $\mathbb{E}[f] \geq 0$, we mean $f(x_t, t) \geq 0$, $\tilde{f}(t) \geq 0$, and $\mathbb{E}[f](t) \geq 0$ for all $x_t \in \mathbb{R}^n$ and $t > 0$.

2.2. Three Parts of the Proof

In this section, we give the procedure to prove $C_s(m, n)$, which consists of three parts.

2.2.1. Part I

In **step 1**, we reduce the proof of $C_s(m, n)$ into the proof of an integral inequality, as shown by the following lemma, whose proof will be given in Section 2.3:

Lemma 1. Proof that $C_s(m, n), s = 1, 2, 3$ can be reduced to show

$$\int_{\mathbb{R}^n} \frac{E_{s,m,n}}{p_t^{2m-1}} dx_t \geq 0 \tag{8}$$

where

$$E_{s,m,n} = \sum_{a_1=1}^n \cdots \sum_{a_m=1}^n E_{s,m,n,\mathbf{a}_m},$$

$$\mathbf{a}_m = (a_1, \dots, a_m),$$

E_{s,m,n,\mathbf{a}_m} is a $2m$ th-order differential form in $\mathbb{R}[\mathcal{P}_{m,n}]$, and

$$\mathcal{P}_{m,n} = \left\{ \frac{\partial^h p_t}{\partial^{h_1} x_{a_1,t} \cdots \partial^{h_m} x_{a_m,t}} : h \in [2m - 1]_0; a_i \in [n], i \in [m] \right\}. \tag{9}$$

2.2.2. Part II

In **step 2**, we compute the constraints which are relations satisfied by the probability density p_t of X_t . In this paper, we consider two types of constraints: integral constraints and log-concave constraints, which will be given in Lemmas 2 and 3, respectively. Since $E_{s,m,n}$ in (8) is a $2m$ th-order differential form, we need only the constraints which are $2m$ th-order differential forms.

Definition 1. An m th-order integral constraint is the $2m$ th-order differential form R in $\mathbb{R}[\mathcal{P}_n]$ such that

$$\int_{\mathbb{R}^n} \frac{R}{p_t^{2m-1}} dx_t = 0.$$

Lemma 2 ([22]). There is a systematic method to compute the m th-order integral constraints $\mathcal{C}_{m,n} = \{R_i, i = 1, \dots, N_1\}$.

A function $f : \mathbb{R}^n \rightarrow \mathbb{R}$ is called *log-concave* if $\log f$ is a concave function. In this paper, by the *log-concave condition*, we mean that the density function p_t is log-concave.

Definition 2. An m th-order log-concave constraint is a $2m$ th-order differential form \mathcal{R} in $\mathbb{R}[\mathcal{P}_n]$ such that $\mathcal{R} \geq 0$ under the log-concave condition.

The following lemma computes the log-concave constraints:

Lemma 3 ([22]). Let $\mathbf{H}(p_t) \in \mathbb{R}[\mathcal{P}_n]^{n \times n}$ be the Hessian matrix of p_t , $\nabla p_t = (\frac{\partial p_t}{\partial x_{1,t}}, \dots, \frac{\partial p_t}{\partial x_{n,t}})$,

$$\mathbf{L}(p_t) \triangleq p_t \mathbf{H}(p_t) - \nabla^T p_t \nabla p_t, \tag{10}$$

and $\Delta_{k,l}, l = 1, \dots, L_k$ be the k th-order principle minors of $\mathbf{L}(p_t)$. Then, the m th-order log-concave constraints are

$$\mathbb{C}_{m,n} = \left\{ \prod_{i=1}^l (-1)^{k_i} \Delta_{k_i, l_i} T_{k_1, \dots, k_l} \mid \sum_{i=1}^l k_i \leq m \right\} \tag{11}$$

where $T_{k_1, \dots, k_l} \in \text{Span}_{\mathbb{R}}(\mathcal{M}_{2m-2\sum_{i=1}^l k_i, n})$ and $T_{k_1, \dots, k_l} \geq 0$.

Note that T_{k_1, \dots, k_l} in (11) are not known. For convenience, denote

$$\mathbb{C}_{m,n} = \{P_j, j = 1, \dots, N_2\}, \tag{12}$$

where P_j represents $\prod_{i=1}^l (-1)^{k_i} \Delta_{k_i, l_i}$ in (11). From Lemma 3, it is easy to see that $\prod_{i=1}^l (-1)^{k_i} \Delta_{k_i, l_i}$ is a $(2\sum_{i=1}^l k_i)$ th-order log-concave constraint.

2.2.3. Part III

In step 3, we give a procedure to write $E_{s,m,n}$ as an SOS under the constraints, the details of which will be given in Section 2.4.

Procedure 1. For $E_{s,m,n}$ in Lemma 1, $\mathbb{C}_{m,n} = \{R_i, i = 1, \dots, N_1\}$ in Lemma 2, and $\mathbb{C}_{m,n} = \{P_j, j = 1, \dots, N_2\}$ in Lemma 3, the procedure computes $e_i \in \mathbb{R}$ and $Q_j \in \text{Span}_{\mathbb{R}}(\mathcal{M}_{2m-\deg P_j, n})$ such that

$$E_{s,m,n} - \sum_{i=1}^{N_1} e_i R_i - \sum_{j=1}^{N_2} P_j Q_j = S, \tag{13}$$

$$\text{and } Q_j \geq 0, j = 1, \dots, N_2, \tag{14}$$

where S is an SOS. If the log-concave condition is not needed, we may set $Q_j = 0$ for all j .

To summarize the proof procedure, we have the following:

Theorem 1. If Procedure 1 satisfies (13) and (14) for certain s, m , and n , then $C_s(m, n)$ is explicitly and strictly proved.

Proof. With Lemma 1, we have the following proof for $C_s(m, n)$:

$$\begin{aligned} \int_{\mathbb{R}} \frac{E_{t,m,n}}{p_t^{2m-1}} dx_t &\stackrel{(13)}{=} \int_{\mathbb{R}} \frac{\sum_{i=1}^{N_1} e_i R_i + \sum_{j=1}^{N_2} P_j Q_j + S}{p_t^{2m-1}} dx_t \\ &\stackrel{S1}{=} \int_{\mathbb{R}} \frac{\sum_{j=1}^{N_2} P_j Q_j + S}{p_t^{2m-1}} dx_t \\ &\stackrel{S2}{\geq} \int_{\mathbb{R}} \frac{S}{p_t^{2m-1}} dx_t \\ &\stackrel{S3}{\geq} 0. \end{aligned} \tag{15}$$

Equality S1 is true, because R_i is an integral constraint by Lemma 2. By Lemma 3 and (14), $P_j Q_j \geq 0$ is true under the log-concave condition, so inequality S2 is true under the log-concave condition. Finally, inequality S3 is true, because $S \geq 0$ is an SOS. \square

2.3. Proof of Lemma 1

Costa [12] proved the following basic properties for p_t and $H(X_t)$,

$$\begin{aligned} \frac{dH(X_t)}{dt} &= -\frac{1}{2}\mathbb{E}[\nabla^2 \log p_t] \\ &= \frac{1}{2} \int_{\mathbb{R}^n} \frac{\|\nabla p_t\|^2}{p_t} dx_t \\ &= \frac{1}{2}J(X_t), \end{aligned} \tag{16}$$

where

$$\nabla p_t = \left(\frac{\partial p_t}{\partial x_{1,t}}, \dots, \frac{\partial p_t}{\partial x_{n,t}} \right), \nabla^2 p_t = \sum_{i=1}^n \frac{\partial^2 p_t}{\partial^2 x_{i,t}}$$

and $J(X_t) \triangleq \mathbb{E}\left(\frac{\|\nabla p_t\|^2}{p_t^2}\right)$ is the Fisher information [6]. Equation (16) implies $C_1(1, n)$: $\frac{d}{dt}H(X_t) \geq 0$.

For $s = 1$, Lemma 1 was proved by

Lemma 4 ([22]). For $m \in \mathbb{N}_{m>1}$, we have

$$(-1)^{m+1}(d^m/dt^m)H(X_t) = \int_{\mathbb{R}^n} \frac{E_{1,m,n}}{p_t^{2m-1}(x_t)} dx_t, \tag{17}$$

where

$$\begin{aligned} E_{1,m,n} &= \frac{(-1)^{m+1}p_t^{2m-1}}{2} \frac{d^{m-1}}{dt^{m-1}} \left(\frac{\|\nabla p_t\|^2}{p_t} \right) \\ &= \sum_{a_1=1}^n \dots \sum_{a_m=1}^n E_{1,m,n,\mathbf{a}_m} \end{aligned}$$

is a 2mth-order differential form in $\mathbb{R}[\mathcal{P}_{m,n}]$.

To prove Lemma 1 for $s = 2, 3$, we need to compute $(d^m/dt^m)H(X_{Gt})$. Let $X_G \sim N_n(\mu, \sigma^2 I)$ be an n -dimensional Gaussian random vector and $X_{Gt} \triangleq X_G + Z_t$, where $Z_t \sim N_n(0, tI)$ is introduced in Section 1. Then, $X_{Gt} \sim N_n(\mu, (\sigma^2 + t)I)$ and the probability density of X_{Gt} is

$$\hat{p}_t = \frac{1}{(2\pi(\sigma^2 + t))^{n/2}} \exp\left(-\frac{1}{2(\sigma^2 + t)}\|x_t - \mu\|^2\right).$$

Lemma 5 ([22]). Let $T = \nabla^2 \log p_t$ and $T_G = \nabla^2 \log \hat{p}_t$. Then, under the log-concave condition, we have

$$\begin{aligned} \mathbb{E}[(-T)^m] &\stackrel{(a)}{\geq} [\mathbb{E}(-T)]^m \stackrel{(b)}{\geq} [\mathbb{E}(-T_G)]^m \\ &\stackrel{(c)}{=} (-1)^{m+1} \frac{2n^{m-1}}{(m-1)!} (d^m/dt^m)H(X_{Gt}). \end{aligned} \tag{18}$$

Lemma 6 ([22]). For $T = \nabla^2 \log p_t$ and $m \in \mathbb{N}_{m>1}$, we have

$$\mathbb{E}[(-T)^m] = \int_{\mathbb{R}} \frac{E_{0,m,n}}{p_t^{2m-1}} dx_t \tag{19}$$

where

$$\begin{aligned} E_{0,m,n} &= \sum_{a_1=1}^n \dots \sum_{a_m=1}^n E_{0,m,n,\mathbf{a}_m}, \\ \mathbf{a}_m &= (a_1, \dots, a_m), \end{aligned}$$

and E_{0,m,n,\mathbf{a}_m} is a 2mth-order differential form in $\mathbb{R}[\mathcal{P}_{m,n}]$.

We can now prove Lemma 1 for $s = 2, 3$. Let

$$\begin{aligned} E_{2,m,n} &= E_{1,m,n} - \frac{(m-1)!}{2n^{m-1}} E_{0,m,n}, \\ E_{3,m,n} &= E_{1,m,n} - \frac{(m-1)!}{2n^m} E_{0,m,n}, \end{aligned} \tag{20}$$

where $E_{1,m,n}$ and $E_{0,m,n}$ are from Lemmas 4 and 6, respectively. By Lemma 5, $C_s(m, n)$ is true if $\int_{\mathbb{R}^n} \frac{E_{s,m,n}}{p_t^{2m-1}} dx_t \geq 0$ for $l = 2, 3$. Together with Lemma 4, Lemma 1 is proved.

2.4. Main Result (Procedure 1)

In this section, we present the detailed Procedure 1, called Procedure 2, which is based on symbolic computation and the SOS theory.

Procedure 2. Input: $E_{s,m,n}$ and $R_i, i = 1, \dots, N_1$ are $2m$ th-order differential forms in $\mathbb{R}[\mathcal{P}_n]$; $P_j, j = 1, \dots, N_2$ are $2k_j$ th-order differential forms in $\mathbb{R}[\mathcal{P}_n]$.

Output: $e_i \in \mathbb{R}$ and $Q_j \in \text{Span}_{\mathbb{R}}(\mathcal{M}_{2(m-k_j),n})$ such that (13) and (14) are true, or fail meaning such that e_i and Q_j are not found.

S1. Treat the monomials in $\mathcal{M}_{m,n}$ as new variables $m_l, l = 1, \dots, N_{m,n}$, which are all the monomials in $\mathbb{R}[\mathcal{P}_n]$ with the degree m and the total order m . We call $m_l m_s$ a quadratic monomial.

S2. Write monomials in $\mathcal{C}_{m,n} = \{R_i, i = 1, \dots, N_1\}$ as quadratic monomials if possible. By performing Gaussian elimination on $\mathcal{C}_{m,n}$ by treating the monomials as variables and according to a monomial order such that a quadratic monomial is less than a non-quadratic monomial, we obtain

$$\tilde{\mathcal{C}}_{m,n} = \mathcal{C}_{m,n,1} \cup \mathcal{C}_{m,n,2},$$

where $\mathcal{C}_{m,n,1}$ is the set of quadratic forms in $m_i, \mathcal{C}_{m,n,2}$ is the set of non-quadratic forms, and $\text{Span}_{\mathbb{R}}(\mathcal{C}_{m,n}) = \text{Span}_{\mathbb{R}}(\tilde{\mathcal{C}}_{m,n})$.

S3. There may exist relationships among the variables m_i , which are called *intrinsic constraints*. For instance, for $m_1 = p_t^2 (\frac{\partial^2 p_t}{\partial^2 x_{1,t}})^2, m_2 = p_t (\frac{\partial p_t}{\partial x_{1,t}})^2 \frac{\partial^2 p_t}{\partial^2 x_{1,t}}$, and $m_3 = (\frac{\partial p_t}{\partial x_{1,t}})^4$ in $\mathcal{M}_{4,n}$, an intrinsic constraint is $m_1 m_3 - m_2^2 = 0$. By adding the intrinsic constraints which are quadratic forms in m_i to $\mathcal{C}_{m,n,1}$, we obtain

$$\hat{\mathcal{C}}_{m,n,1} = \{\hat{R}_i, i = 1, \dots, N_3\}.$$

S4. Let $\mathcal{M}_{2(m-k_j),n} = \{m_{j,k}, k = 1, \dots, V_j\}$ and $Q_j = \sum_{k=1}^{V_j} q_{j,k} m_{j,k}$, where $q_{j,k}$ are variables to be found later. Let $\bar{\mathcal{R}}_j$ be obtained from $P_j Q_j$ by writing monomials in $P_j Q_j$ as quadratic monomials in m_i , and eliminating the non-quadratic monomials with $\mathcal{C}_{m,n,2}$, such that $\bar{\mathcal{R}}_j - P_j Q_j \in \text{Span}_{\mathbb{R}}(\mathcal{C}_{m,n})$ and $\bar{\mathcal{R}}_j = \sum_{l=1}^{V_j} q_{j,l} h_{j,l}$, where $h_{j,l} \in \mathbb{R}[m_i, \mathcal{P}_n]$. If an $h_{j,l}$ is not a quadratic form in m_i , then delete $\bar{\mathcal{R}}_j$; hence, the $\bar{\mathcal{R}}_j$'s in quadratic form are selected. Then, denote these constraints as $\mathcal{R}_j, j = 1, \dots, N_2$, which form the reduced set $\hat{\mathcal{C}}_{m,n}$.

S5. Let $\hat{E}_{s,m,n}$ be obtained from $E_{s,m,n}$ by eliminating the non-quadratic monomials using $\mathcal{C}_{m,n,2}$ such that $E_{s,m,n} - \hat{E}_{s,m,n} \in \text{Span}_{\mathbb{R}}(\mathcal{C}_{m,n,2}) \subset \text{Span}_{\mathbb{R}}(\mathcal{C}_{m,n})$.

S6. Since $\hat{E}_{s,m,n}, \hat{R}_i, i = 1, \dots, N_3$ and $\mathcal{R}_j, j = 1, \dots, N_2$ are quadratic forms in m_i , we can use the Matlab codes given in Appendix A [21] to compute $p_i, q_{j,s} \in \mathbb{R}$ such that

$$\hat{E}_{s,m,n} - \sum_{i=1}^{N_3} p_i \hat{R}_i - \sum_{j=1}^{N_2} \mathcal{R}_j = S, \tag{21}$$

$$\mathcal{R}_j = \sum_{l=1}^{V_j} q_{j,l} h_{j,l}, j = 1, \dots, N_2$$

$$Q_j = \sum_{l=1}^{V_j} q_{j,l} m_{j,l} \geq 0, j = 1, \dots, N_2 \tag{22}$$

where

$$S = \sum_{i=1}^{N_{m,n}} c_i \left(\sum_{j=i}^{N_{m,n}} e_{ij} m_j \right)^2$$

is an SOS, $c_i, e_{ij} \in \mathbb{R}$ and $c_i \geq 0$. If (21) and (22) cannot be found, return FAIL.

S7. Since $\widehat{R}_i, E_{s,m,n} - \widehat{E}_{s,m,n}, \mathcal{R}_j - P_j Q_j$ are all in $\text{Span}_{\mathbb{R}}(\mathcal{C}_{m,n})$, Equations (13) and (14) can be obtained from (21) and (22), respectively.

Remark 2. Procedure 2 can be implemented automatically by Maple and Matlab on a computer. In Procedure 2, steps S2, S4 and S5 are based on the symbolic computation theory for reduction, which makes our method more efficient than the pure SDP-based method [18] or a direct theoretical proof [16]. The use of symbolic computation also ensures that our calculation is strict and free of numerical errors.

Remark 3. Let R be an intrinsic constraint. Then, R becomes zero when replacing m_i by its corresponding monomial in $\mathcal{M}_{m,n}$. Therefore, $\text{Span}_{\mathbb{R}}(\widehat{\mathcal{C}}_{m,n,1}) = \text{Span}_{\mathbb{R}}(\mathcal{C}_{m,n,1}) \subset \text{Span}_{\mathbb{R}}(\mathcal{C}_{m,n})$ in $\mathbb{R}[\mathcal{P}_n]$; that is, we do not need to include the intrinsic constraints in (21). However, these intrinsic constraints are needed when using the Matlab software in Appendix A of [21].

2.5. An Illustrative Example

As an illustrative example, we prove $C_2(3, 1)$ under the log-concave condition using the proof procedure given in Section 2.2. Since $n = 1$, denote

$$x_t = x_{1,t}, f := f_0 := p_t, f_n := \frac{\partial^n p_t}{\partial^n x_{1,t}}, n \in \mathbb{N}_{>0}.$$

In step 1, by Lemma 1 and (8), we have

$$\begin{aligned} & \frac{d^3 H(X_t)}{dt^3} - \frac{2!}{2} \mathbb{E} \left[\frac{(f_1^2 - f f_2)^3}{f^6} \right] \\ \stackrel{(16)}{=} & \int \left(\frac{1}{2} \frac{d^2}{dt^2} \left(\frac{f_1^2}{f} \right) - \frac{(f_1^2 - f f_2)^3}{f^5} \right) dx_t \\ \stackrel{(8)}{=} & \int \frac{E_{2,3,1}}{f^5} dx_t \end{aligned} \tag{23}$$

where

$$\begin{aligned} E_{2,3,1} = & \frac{1}{4} f^4 f_3^2 - \frac{1}{2} f^3 f_1 f_3 f_2 + \frac{1}{4} f^4 f_1 f_5 - \frac{11}{4} f^2 f_1^2 f_2^2 \\ & - \frac{1}{8} f^3 f_1^2 f_4 + f^3 f_2^3 + 3 f f_1^4 f_2 - f_1^6 \end{aligned}$$

is a sixth-order differential form.

In step 2, we compute the constraints with Lemmas 2 and 3. With Lemma 2, we find six third-order integral constraints: $\mathcal{C}_{3,1} = \{R_i, i = 1, \dots, 6\}$:

$$\begin{aligned} R_1 &= 5 f f_1^4 f_2 - 4 f_1^6, \\ R_2 &= 2 f^3 f_1 f_2 f_3 + f^3 f_2^3 - 2 f^2 f_1^2 f_2^2, \\ R_3 &= f^4 f_1 f_5 + f^4 f_2 f_4 - f^3 f_1^2 f_4, \\ R_4 &= f^3 f_1^2 f_4 + 2 f^3 f_1 f_2 f_3 - 2 f^2 f_1^3 f_3, \\ R_5 &= f^2 f_1^3 f_3 + 3 f^2 f_1^2 f_2^2 - 3 f f_1^4 f_2, \\ R_6 &= f^4 f_2 f_4 + f^4 f_3^2 - f^3 f_1 f_2 f_3. \end{aligned}$$

With Lemma 3, we obtain one third-order log-concave constraint: $\mathbf{C}_{3,1} = \{P_1 Q_1\}$, where

$$P_1 = f f_2 - f_1^2, Q_1 \in \text{Span}_{\mathbb{R}}(\mathcal{M}_{4,1}), \text{ and } Q_1 \geq 0.$$

In **step 3**, we use Procedure 2 to compute the SOS representation (13) and (14) with the input $E_{2,3,1}, C_{3,1} = \{R_i, i = 1, \dots, 6\}, P_1 = f_1^2 - ff_2$.

S1. The new variables are $\mathcal{M}_{3,1} = \{m_1 = f^2 f_3, m_2 = ff_1 f_2, m_3 = f_1^3\}$, which are listed from high to low in the lexicographical monomial order.

S2. By writing monomials in $C_{3,1}$ as quadratic monomials in m_i if possible and performing Gaussian elimination on $C_{3,1}$, we have

$$\begin{aligned} C_{3,1,1} &= \{\widehat{R}_1 = 5m_2 m_3 - 4m_3^2, \\ &\quad \widehat{R}_2 = m_1 m_3 + 3m_2^2 - \frac{12}{5}m_3^2\}, \\ C_{3,1,2} &= \{\widetilde{R}_1 = f^3 f_2^3 + 2m_1 m_2 - 2m_2^2, \\ &\quad \widetilde{R}_2 = f^4 f_1 f_5 - m_1^2 + 3m_1 m_2 + 6m_2^2 - \frac{24}{5}m_3^2, \\ &\quad \widetilde{R}_3 = f^4 f_2 f_4 + m_1^2 - m_1 m_2, \\ &\quad \widetilde{R}_4 = f^3 f_1^2 f_4 + 2m_1 m_2 + 6m_2^2 - \frac{24}{5}m_3^2\}. \end{aligned}$$

S3. There exist no intrinsic constraints and thus, $\widehat{C}_{3,1,1} = \{\widehat{R}_1, \widehat{R}_2\}$ and $N_3 = 2$.

S4. $\mathcal{M}_{4,1} = \{f^3 f_4, f^2 f_1 f_3, f^2 f_2^2, f f_1^2 f_2, f_1^4\}$. Then, $Q_1 = q_{1,1} f^2 f_2^2 + q_{1,2} f f_1^2 f_2 + q_{1,3} f_1^4$. Monomials $f^3 f_4, f^2 f_1 f_3$ do not appear in Q_1 due to $Q_1 \geq 0$. By writing monomials in $P_1 Q_1$ as quadratic monomials if possible and using $C_{3,1,2}$ to eliminate non-quadratic monomials, we obtain

$$\begin{aligned} \mathcal{R}_1 &= P_1 Q_1 - \left(\frac{1}{5}q_{1,2}\widehat{R}_1 - q_{1,1}\widetilde{R}_1 - \frac{1}{5}q_{1,3}\widehat{R}_1\right) \\ &= q_{1,1}(2m_1 m_2 - m_2^2) + q_{1,2}\left(\frac{4}{5}m_3^2 - m_2^2\right) + \frac{q_{1,3}}{5}m_3^2. \end{aligned}$$

S5. By writing $E_{2,3,1}$ as a quadratic form in m_i , we have

$$\begin{aligned} \widehat{E}_{2,3,1} &= E_{2,3,1} - \frac{3}{5}\widehat{R}_1 - \widetilde{R}_1 - \frac{1}{4}\widetilde{R}_2 + \frac{1}{8}\widetilde{R}_4 \\ &= \frac{1}{2}m_1^2 - 3m_1 m_2 - \frac{3}{2}m_2^2 + 2m_3^2. \end{aligned}$$

S6. Since $\widehat{E}_{3,1}, \widehat{R}_1, \widehat{R}_2, \mathcal{R}_1$ are quadratic forms in m_i , we can use the Matlab software in Appendix A of [21] to obtain the following SOS representation

$$\begin{aligned} \widehat{E}_{2,3,1} &= \sum_{i=1}^2 p_i \widehat{R}_i + \mathcal{R}_1 + \sum_{i=1}^3 c_i \left(\sum_{j=i}^3 e_{i,j} m_j\right)^2, \\ Q_1 &\geq 0, \end{aligned} \tag{24}$$

where

$$\begin{aligned} p_1 &= \frac{6}{5}, p_2 = -2, c_1 = \frac{1}{2}, e_{1,1} = 1, e_{1,2} = -3, e_{1,3} = 2, \\ q_{1,1} &= q_{1,2} = q_{1,3} = c_2 = c_3 = 0. \end{aligned}$$

S7. We obtain

$$\begin{aligned} E_{2,3,1} &= \frac{3}{4}R_1 + R_2 + \frac{1}{4}R_3 + \frac{1}{8}R_4 - \frac{7}{4}R_5 - \frac{1}{4}R_6 \\ &\quad + \sum_{i=1}^3 c_i \left(\sum_{j=i}^3 e_{i,j} m_j\right)^2. \end{aligned}$$

From Theorem 1 and (23), we have

$$\begin{aligned}
 & \frac{d^3 H(X_t)}{dt^3} - \frac{2!}{2} \mathbb{E} \left[\frac{(f_1^2 - f f_2)^3}{f^6} \right] \\
 &= \int_{\mathbb{R}} \frac{E_{2,3,1}}{p_t^5} dx_t \\
 &= \int_{\mathbb{R}} \frac{1}{p_t^5} \left(\frac{3}{4} R_1 + R_2 + \frac{1}{4} R_3 + \frac{1}{8} R_4 \right. \\
 & \quad \left. - \frac{7}{4} R_5 - \frac{1}{4} R_6 + \sum_{i=1}^3 c_i \left(\sum_{j=i}^3 e_{i,j} m_j \right)^2 \right) dx_t \\
 &= \int_{\mathbb{R}} \frac{(m_1 - 3m_2 + 2m_3)^2}{2p_t^5} dx_t \\
 &\geq 0.
 \end{aligned} \tag{25}$$

Thus, an explicit and strict proof is given for $C_2(3, 1)$. Note that this example is also considered in [18] by the pure SDP-based method, which is a semi-automatic algorithm. See Table 1 for the time used to provide analytical proof of this example by our automatic method on a computer.

3. Proof of $C_1(3, n)$ for $n = 2, 3, 4$

In this section, we use the procedure in Section 2.2 to prove $C_1(3, n)$ for $n = 2, 3, 4$.

3.1. Compute $E_{1,3,n}$

In step 1, we compute $E_{1,3,n}$ in (8) and (20):

$$\frac{1}{2} \frac{d^2}{dt^2} \left(\int_{\mathbb{R}^n} \frac{\|\nabla p_t\|^2}{p_t} dx_t \right) \stackrel{(2)}{=} \int_{\mathbb{R}^n} \frac{E_{1,3,n}}{p_t^5} dx_t, \tag{26}$$

where

$$E_{1,3,n} = \sum_{a=1}^n \sum_{b=1}^n \sum_{c=1}^n F_{3,a,b,c}$$

and

$$\begin{aligned}
 F_{3,a,b,c} &= \frac{p_t^4}{4} \frac{\partial^3 p_t}{\partial x_{a,t} \partial^2 x_{c,t}} \frac{\partial^3 p_t}{\partial x_{a,t} \partial^2 x_{b,t}} - \frac{p_t^3}{4} \frac{\partial p_t}{\partial x_{a,t}} \frac{\partial^3 p_t}{\partial x_{a,t} \partial^2 x_{b,t}} \frac{\partial^2 p_t}{\partial^2 x_{c,t}} \\
 &+ \frac{p_t^4}{4} \frac{\partial p_t}{\partial x_{a,t}} \frac{\partial^5 p_t}{\partial x_{a,t} \partial^2 x_{b,t} \partial^2 x_{c,t}} - \frac{p_t^3}{4} \frac{\partial p_t}{\partial x_{a,t}} \frac{\partial^3 p_t}{\partial x_{a,t} \partial^2 x_{c,t}} \frac{\partial^2 p_t}{\partial^2 x_{b,t}} \\
 &+ \frac{p_t^2}{4} \left(\frac{\partial p_t}{\partial x_{a,t}} \right)^2 \frac{\partial^2 p_t}{\partial^2 x_{b,t}} \frac{\partial^2 p_t}{\partial^2 x_{c,t}} - \frac{p_t^3}{8} \left(\frac{\partial p_t}{\partial x_{a,t}} \right)^2 \frac{\partial^4 p_t}{\partial^2 x_{b,t} \partial^2 x_{c,t}}.
 \end{aligned}$$

3.2. Compute the Third-Order Constraints

In step 2, we obtain the third-order constraints. We introduce the notation

$$\mathcal{V}_{a,b,c} = \left\{ \frac{\partial^h p_t}{\partial^{h_1} x_{a,t} \partial^{h_2} x_{b,t} \partial^{h_3} x_{c,t}} : h = h_1 + h_2 + h_3 \in [5]_0 \right\}, \tag{27}$$

where a, b, c are variables taking values in $[n]$. Then,

$$\mathcal{P}_{3,n} = \cup_{a=1}^n \cup_{b=1}^n \cup_{c=1}^n \mathcal{V}_{a,b,c}.$$

The third-order integral constraints are:

$$\mathcal{C}_{3,n} = \{ R_{i,a,b,c}^{(3)} : i = 1, \dots, 955; a, b, c \in [n] \}, \tag{28}$$

where $R_{i,a,b,c}^{(3)}$ in the form of lengthy formulas can be found in [23]. Note that we do not use all the third-order constraints in [23].

3.3. Proof of $C_1(3,2)$

The proof follows Procedure 2 with $E_{1,3,2}$ given in (26) as the input. To make the proof explicit, we will give the key expressions.

In Step S1, the new variables are $\mathcal{M}_{3,2}$ and are listed in the lexicographical monomial order:

$$\begin{aligned}
 m_1 &= p_t^2 \frac{\partial p_t^3}{\partial^3 x_{2,t}}, \quad m_2 = p_t^2 \frac{\partial^3 p_t}{\partial x_{1,t} \partial^2 x_{2,t}}, \\
 m_3 &= p_t^2 \frac{\partial^3 p_t}{\partial^2 x_{1,t} \partial x_{2,t}}, \quad m_4 = p_t^2 \frac{\partial p_t^3}{\partial^3 x_{1,t}}, \\
 m_5 &= p_t \frac{\partial^2 p_t}{\partial^2 x_{2,t}} \frac{\partial p_t}{\partial x_{2,t}}, \quad m_6 = p_t \frac{\partial^2 p_t}{\partial^2 x_{2,t}} \frac{\partial p_t}{\partial x_{1,t}}, \\
 m_7 &= p_t \frac{\partial^2 p_t}{\partial x_{1,t} \partial x_{2,t}} \frac{\partial p_t}{\partial x_{2,t}}, \quad m_8 = p_t \frac{\partial^2 p_t}{\partial x_{1,t} \partial x_{2,t}} \frac{\partial p_t}{\partial x_{1,t}}, \\
 m_9 &= p_t \frac{\partial^2 p_t}{\partial x_{1,t}^2} \frac{\partial p_t}{\partial x_{2,t}}, \quad m_{10} = p_t \frac{\partial^2 p_t}{\partial x_{1,t}^2} \frac{\partial p_t}{\partial x_{1,t}}, \\
 m_{11} &= \left(\frac{\partial p_t}{\partial x_{2,t}} \right)^3, \quad m_{12} = \left(\frac{\partial p_t}{\partial x_{2,t}} \right)^2 \frac{\partial p_t}{\partial x_{1,t}}, \\
 m_{13} &= \frac{\partial p_t}{\partial x_{2,t}} \left(\frac{\partial p_t}{\partial x_{1,t}} \right)^2, \quad m_{14} = \left(\frac{\partial p_t}{\partial x_{1,t}} \right)^3.
 \end{aligned}$$

In Step S2, the constraints are

$$\mathcal{C}_{3,2} = \{R_{j,a,b,c}^{(3)} : j = 1, \dots, 955; a, b, c \in [2]\}.$$

Removing the repeated ones, we have $N_1 = 135$. We obtain $\mathcal{C}_{3,2,1}$ and $\mathcal{C}_{3,2,2}$, which contain 48 and 52 constraints, respectively.

In Step S3, there exist 15 intrinsic constraints:

$$\begin{aligned}
 m_5 m_8 &= m_6 m_7, \quad m_5 m_{10} = m_6 m_9, \quad m_5 m_{12} = m_6 m_{11}, \\
 m_5 m_{13} &= m_6 m_{12}, \quad m_5 m_{14} = m_6 m_{13}, \quad m_7 m_{10} = m_8 m_9, \\
 m_7 m_{12} &= m_8 m_{11}, \quad m_7 m_{13} = m_8 m_{12}, \quad m_7 m_{14} = m_8 m_{13}, \\
 m_9 m_{12} &= m_{10} m_{11}, \quad m_9 m_{13} = m_{10} m_{12}, \quad m_9 m_{14} = m_{10} m_{13}, \\
 m_{11} m_{13} &= m_{12}^2, \quad m_{11} m_{14} = m_{12} m_{13}, \quad m_{12} m_{14} = m_{13}^2.
 \end{aligned}$$

Thus, $\widehat{\mathcal{C}}_{3,2,1}$ contains 63 constraints and $N_3 = 63$.

Step S4 is not needed in the proof of this case.

In Step S5, by eliminating the non-quadratic monomials in $E_{1,3,2}$ using $\mathcal{C}_{3,2,2}$ to obtain a quadratic form in m_i and then simplifying the quadratic form using $\mathcal{C}_{3,2,1}$, we have

$$\begin{aligned}
 \widehat{E}_{1,3,2} &= E_{1,3,2} - \left(\frac{3}{4}\widehat{R}_{17} - \frac{1}{6}\widehat{R}_{12} - \frac{1}{6}\widehat{R}_{13} + \frac{7}{6}\widehat{R}_{18} - \frac{1}{2}\widehat{R}_{32} \right. \\
 &\quad - \frac{1}{2}\widehat{R}_{34} - \frac{5}{8}\widehat{R}_{35} - \frac{1}{2}\widehat{R}_{40} - \frac{1}{12}\widehat{R}_2 - \frac{1}{8}\widehat{R}_5 - \frac{1}{4}\widehat{R}_6 \\
 &\quad + \frac{1}{2}\widetilde{R}_7 + \frac{1}{4}\widetilde{R}_8 + \frac{1}{2}\widetilde{R}_{18} + \frac{1}{4}\widetilde{R}_{19} - \frac{1}{8}\widetilde{R}_{39} - \frac{1}{4}\widetilde{R}_{46} \\
 &\quad \left. + \frac{1}{2}\widetilde{R}_{48} - \frac{1}{8}\widetilde{R}_{49} + \frac{1}{4}\widetilde{R}_{53} \right) \\
 &= \frac{1}{2}m_1^2 - m_1m_5 + \frac{3}{2}m_2^2 - 3m_2m_6 + \frac{3}{2}m_3^2 + \frac{1}{2}m_4^2 \\
 &\quad - 2m_4m_6 - m_4m_7 - m_4m_{10} - \frac{1}{2}m_5^2 + \frac{3}{2}m_6^2 - 3m_7^2 \\
 &\quad - 2m_7m_{10} + 3m_8^2 - \frac{5}{2}m_9^2 - \frac{3}{2}m_9m_{11} + 21m_9m_{13} \\
 &\quad - \frac{1}{2}m_{10}^2 + \frac{3}{5}m_{11}^2 + 3m_{12}^2 - 15m_{13}^2 + \frac{3}{5}m_{14}^2.
 \end{aligned}$$

In Step **S6**, using the Matlab program in [23] with $\widehat{E}_{1,3,2}$ and $\widehat{C}_{3,2,1}$ as the input, we find an SOS representation for $\widehat{E}_{1,3,2}$. Thus, by Theorem 1, $C_1(3,2)$ is strictly proved.

3.4. Proof of $C_1(3,3)$

The proof follows Procedure 2 with $E_{1,3,3}$ given in (29) as the input. The detailed lengthy formulas can be seen in [23].

In Step **S1**, the new variables are $\mathcal{M}_{3,3} = \{m_i, i = 1, \dots, 38\}$ which is the set of all monomials in $\mathbb{R}[\mathcal{P}_{3,3}]$ with a degree of 3 and a total order of 3, and which are listed in the lexicographical monomial order.

In Step **S2**, the constraints are: $\mathcal{C}_{3,n} = \{R_{i,a,b,c}^{(3)} : i = 1, \dots, 955\}$, $N_1 = 955$. We obtain $\mathcal{C}_{3,n,1}$ and $\mathcal{C}_{3,n,2}$, which contain 350 and 328 constraints, respectively.

In Step **S3**, there exist 189 intrinsic constraints. In total, $\widehat{\mathcal{C}}_{3,n,1}$ contains 539 constraints. Using \mathbb{R} -Gaussian elimination in $\text{Span}_{\mathbb{R}}(\widehat{\mathcal{C}}_{3,n,1})$ shows that 512 of these 539 constraints are linearly independent, so $N_3 = 512$.

Step **S4** is not needed in the proof of this case.

In Step **S5**, by eliminating the non-quadratic monomials in $E_{1,3,3}$ using $\mathcal{C}_{3,3,2}$ and then simplifying the expression using $\mathcal{C}_{3,3,1}$, we obtain $\widehat{E}_{1,3,3}$ written as a quadratic form in m_i .

In Step **S6**, using the Matlab program in [23] with $\widehat{E}_{1,3,3}$ and $\widehat{\mathcal{C}}_{3,3,1}$ as the input, we find an SOS representation for $\widehat{E}_{1,3,3}$. Thus, using Theorem 1, $C_1(3,3)$ is strictly proved.

3.5. Proof of $C_1(3,4)$

The proof follows Procedure 2 with $E_{1,3,4}$ given in (29) as the input. The detailed lengthy formulas can be seen in [23].

In Step **S1**, the new variables are $\mathcal{M}_{3,4} = \{m_i, i = 1, \dots, 80\}$ which is the set of all monomials in $\mathbb{R}[\mathcal{P}_{3,4}]$ with a degree of 3 and a total order of 3, and which are listed in the lexicographical monomial order.

In Step **S2**, we obtain $\mathcal{C}_{3,4} = \{R_{i,a,b,c}^{(3)}, R_j^{(0)}, R_{k,a,b'}^{(2)} : i = 1, \dots, 955, j = 1, \dots, 8, k = 1, \dots, 20, a, b, c \in [4]\}$. Removing the repeated ones, we have $N_1 = 3172$. We obtain $\mathcal{C}_{3,4,1}$ and $\mathcal{C}_{3,4,2}$ which contain 1120 and 975 constraints, respectively.

In Step **S3**, there exist 1080 intrinsic constraints. In total, $\widehat{\mathcal{C}}_{3,4,1}$ contains 2200 constraints. Only 1966 constraints in $\widehat{\mathcal{C}}_{3,4,1}$ are \mathbb{R} -linearly independent, so $N_2 = 1966$.

Step **S4** is not needed in the proof of this case.

In Step **S5**, by eliminating the non-quadratic monomials in $E_{1,3,4}$ using $\mathcal{C}_{3,4,2}$ to obtain a quadratic form in m_i and then simplifying the quadratic form with $\mathcal{C}_{3,4,1}$, we obtain $\widehat{E}_{1,3,4}$ which is written as a quadratic form in m_i .

In Step **S6**, using the Matlab program in [23] with $\widehat{E}_{1,3,4}$ and $\widehat{\mathcal{C}}_{3,4,1}$ as the input, we find an SOS representation for $\widehat{E}_{1,3,4}$. Thus, using Theorem 1, $C_1(3,4)$ is strictly proved.

4. Proof of $C_3(3, n)$ for $n = 2, 3, 4$ under the Log-Concave Condition

In this section, we use the procedure in Section 2.2 to prove $C_3(3, n)$ for $n = 2, 3, 4$ under the log-concave condition. The detailed lengthy formulas can be seen in [21].

4.1. Compute $E_{3,3,n}$

In step 1, we compute $E_{3,3,n}$ in (8) and (20):

$$\frac{1}{2} \frac{d^2}{dt^2} \left(\frac{\|\nabla p_t\|^2}{p_t} \right) - \frac{1}{n^3} \mathbb{E} \left(\frac{\|\nabla p_t\|^2 - p_t \nabla^2 p_t}{p_t^2} \right)^3 \tag{29}$$

$$\stackrel{(2)}{=} \int_{\mathbb{R}^n} \frac{E_{3,3,n}}{p_t^5} dx_t$$

where

$$E_{3,3,n} = \sum_{a=1}^n \sum_{b=1}^n \sum_{c=1}^n E_{3,a,b,c}$$

and

$$E_{3,a,b,c} = \frac{p_t^4}{4} \frac{\partial^3 p_t}{\partial x_{a,t} \partial^2 x_{c,t}} \frac{\partial^3 p_t}{\partial x_{a,t} \partial^2 x_{b,t}} - \frac{p_t^3}{4} \frac{\partial p_t}{\partial x_{a,t}} \frac{\partial^3 p_t}{\partial x_{a,t} \partial^2 x_{b,t}} \frac{\partial^2 p_t}{\partial^2 x_{c,t}}$$

$$+ \frac{p_t^4}{4} \frac{\partial p_t}{\partial x_{a,t}} \frac{\partial^5 p_t}{\partial x_{a,t} \partial^2 x_{b,t} \partial^2 x_{c,t}} - \frac{p_t^3}{4} \frac{\partial p_t}{\partial x_{a,t}} \frac{\partial^3 p_t}{\partial x_{a,t} \partial^2 x_{c,t}} \frac{\partial^2 p_t}{\partial^2 x_{b,t}}$$

$$+ \frac{p_t^2}{4} \left(\frac{\partial p_t}{\partial x_{a,t}} \right)^2 \frac{\partial^2 p_t}{\partial^2 x_{b,t}} \frac{\partial^2 p_t}{\partial^2 x_{c,t}} - \frac{p_t^3}{8} \left(\frac{\partial p_t}{\partial x_{a,t}} \right)^2 \frac{\partial^4 p_t}{\partial^2 x_{b,t} \partial^2 x_{c,t}}$$

$$- \frac{1}{n^3} \left[\left(\frac{\partial p_t}{\partial x_{a,t}} \right)^2 - p_t \left(\frac{\partial^2 p_t}{\partial^2 x_{a,t}} \right) \right] \left[\left(\frac{\partial p_t}{\partial x_{b,t}} \right)^2 - p_t \left(\frac{\partial^2 p_t}{\partial^2 x_{b,t}} \right) \right] \left[\left(\frac{\partial p_t}{\partial x_{c,t}} \right)^2 - p_t \left(\frac{\partial^2 p_t}{\partial^2 x_{c,t}} \right) \right].$$

4.2. Compute the Third-Order Log-Concave Constraints

In step 2, we obtain the third-order log-concave constraints.

From Lemma 3, we can compute the third-order log-concave constraints:

$$\mathbb{C}_{3,2} = \{ \mathcal{R}_1 = -\Delta_{1,1} Q_1, \mathcal{R}_2 = -\Delta_{1,2} Q_2, \mathcal{R}_3 = \Delta_{2,1} Q_3 \}, \tag{30}$$

where $Q_1, Q_2 \in \text{Span}_{\mathbb{R}}(\mathcal{M}_{4,4})$ and $Q_3 \in \text{Span}_{\mathbb{R}}(\mathcal{M}_{2,2})$. Note that $\mathbb{C}_{3,2}$ does not contain all the log-concave constraints in Lemma 3. The constraints $\mathbb{C}_{3,2}$ are enough for our purpose in this paper.

For $n > 2$, we give certain log-concave constraints in a special form, which are needed in the proof procedure in Section 4.3. Let

$$\nabla_1 p_t = \left(\frac{\partial p_t}{\partial x_{a,t}}, \frac{\partial p_t}{\partial x_{b,t}}, \frac{\partial p_t}{\partial x_{c,t}} \right),$$

$$\mathbf{L}_1(p_t) \triangleq p_t \mathbf{H}_1(p_t) - \nabla_1^T p_t \nabla_1 p_t,$$

where

$$\mathbf{H}_1(p_t) = \begin{bmatrix} \frac{\partial^2 p_t}{\partial^2 x_{a,t}} & \frac{\partial^2 p_t}{\partial x_{a,t} \partial x_{b,t}} & \frac{\partial^2 p_t}{\partial x_{a,t} \partial x_{c,t}} \\ \frac{\partial^2 p_t}{\partial x_{a,t} \partial x_{b,t}} & \frac{\partial^2 p_t}{\partial^2 x_{b,t}} & \frac{\partial^2 p_t}{\partial x_{b,t} \partial x_{c,t}} \\ \frac{\partial^2 p_t}{\partial x_{a,t} \partial x_{c,t}} & \frac{\partial^2 p_t}{\partial x_{b,t} \partial x_{c,t}} & \frac{\partial^2 p_t}{\partial^2 x_{c,t}} \end{bmatrix},$$

and $\Delta'_{k,l}, l = 1, \dots, L_k$ the k th-order principle minors of $\mathbf{L}_1(p_t)$. Let \mathcal{M}'_k be the set of all monomials in $\mathcal{V}_{a,b,c}$ (defined in (27)) which have a degree of k and a total order of k . We have

$$\mathbb{C}_{3,n} = \{ -\Delta'_{1,1} Q_{1,1}, -\Delta'_{1,2} Q_{1,2}, -\Delta'_{1,3} Q_{1,3}, \Delta'_{2,1} Q_{2,1}, \Delta'_{2,2} Q_{2,2}, \Delta'_{2,3} Q_{2,3}, -\Delta'_{3,1} Q_{3,1} \} \tag{31}$$

where $Q_{1,i} \in \text{Span}_{\mathbb{R}}(\mathcal{M}'_4)$, $Q_{2,j} \in \text{Span}_{\mathbb{R}}(\mathcal{M}'_2)$, and $Q_{3,1} \in \mathbb{R}$.

4.3. Proof of $C_3(3,2)$

The proof follows Procedure 2 with $E_{3,3,2}$ given in (29) and the constraints in (28) and (30) as the input.

Steps S1–S3 are the same with the proof of the case $C_1(3,2)$.

In Step S4, we obtain $\widehat{C}(3,2)$ which contains three quadratic-form constraints.

In Step S5, by eliminating the non-quadratic monomials in $E_{3,3,2}$ using $C_{3,2,2}$ to obtain a quadratic form in m_i and then simplifying the quadratic form using $C_{3,2,1}$, we have

$$\begin{aligned} \widehat{E}_{3,3,2} = & \frac{31}{40}m_{14}^2 - \frac{147}{8}m_{13}^2 - \frac{5}{2}m_7m_{10} + \frac{15}{4}m_8^2 - \frac{25}{8}m_9^2 \\ & - \frac{31}{16}m_9m_{11} + \frac{207}{8}m_9m_{13} - \frac{5}{8}m_{10}^2 + \frac{1}{2}m_1^2 \\ & - \frac{5}{4}m_1m_5 + \frac{31}{40}m_{11}^2 + \frac{31}{8}m_{12}^2 + \frac{1}{2}m_4^2 - \frac{5}{2}m_4m_6 \\ & - \frac{5}{4}m_4m_7 + \frac{3}{2}m_3^2 - \frac{15}{4}m_7^2 - \frac{5}{4}m_4m_{10} \\ & - \frac{5}{8}m_5^2 + \frac{15}{8}m_6^2 + \frac{3}{2}m_2^2 - \frac{15}{4}m_2m_6. \end{aligned}$$

In Step S6, using the Matlab software in Appendix A [21] with $\widehat{E}_{3,3,2}$, $\widehat{C}_{3,2,1}$ and $\widehat{C}_{3,2}$ as the input, we find an SOS representation for $\widehat{E}_{3,3,2}$. Thus, $C_3(3,2)$ is proved under the log-concave condition. The Maple program for proving $C_3(3,2)$ can be found at <https://github.com/cmyuanmmrc/codeforepi/> (accessed on 15 July 2020).

Remark 4. We fail to prove $C_2(3,2)$ even under the log-concave condition using the above procedure. Specifically, we cannot find an SOS representation for $\widehat{E}_{2,3,2}$ in Step S6. Since the SDP algorithm is not complete for problem (21), we cannot say that an SOS representation does not exist for $\widehat{E}_{2,3,2}$. The Maple program for $C_2(3,2)$ can be found at <https://github.com/cmyuanmmrc/codeforepi/> (accessed on 15 July 2020).

4.4. Proof of $C_3(3,3)$ and $C_3(3,4)$

In this subsection, we prove $C_3(3,3)$, $C_3(3,4)$. Motivated by symmetric functions, for any function $f(a, b, c)$, we have

$$\begin{aligned} \sum_{a,b,c=1}^n f(a, b, c) = & \sum_{1 \leq a < b < c}^n \left\{ \frac{2}{(n-1)(n-2)} [f(a, a, a) \right. \\ & + f(b, b, b) + f(c, c, c)] + \frac{1}{n-2} [f(a, a, b) + f(a, b, a) \\ & + f(b, a, a) + f(a, a, c) + f(a, c, a) + f(c, a, a) \\ & + f(b, b, a) + f(b, a, b) + f(a, b, b) + f(b, b, c) \\ & + f(b, c, b) + f(c, b, b) + f(c, c, a) + f(c, a, c) \\ & + f(a, c, c) + f(c, c, b) + f(c, b, c) + f(b, c, c)] \\ & + [f(a, b, c) + f(a, c, b) + f(b, a, c) + f(b, c, a) \\ & \left. + f(c, a, b) + f(c, b, a)] \right\}. \end{aligned} \tag{32}$$

From (29) and (32), we obtain

$$E_{3,3,n} = \sum_{a=1}^n \sum_{b=1}^n \sum_{c=1}^n E_{3,a,b,c} = \sum_{1 \leq a < b < c \leq n} J_{3,3,n}$$

where

$$\begin{aligned}
 J_{3,3,n} = & \frac{2}{(n-1)(n-2)} [E_{3,a,a,a} + E_{3,b,b,b} + E_{3,c,c,c}] \\
 & + \frac{1}{n-2} [E_{3,a,a,b} + E_{3,a,b,a} + E_{3,b,a,a} + E_{3,a,a,c} \\
 & + E_{3,a,c,a} + E_{3,c,a,a} + E_{3,b,b,a} + E_{3,b,a,b} + E_{3,a,b,b} \\
 & + E_{3,b,b,c} + E_{3,b,c,b} + E_{3,c,b,b} + E_{3,c,c,a} + E_{3,c,a,c} \\
 & + E_{3,a,c,c} + E_{3,c,c,b} + E_{3,c,b,c} + E_{3,b,c,c}] \\
 & + [E_{3,a,b,c} + E_{3,a,c,b} + E_{3,b,a,c} + E_{3,b,c,a} \\
 & + E_{3,c,a,b} + E_{3,c,b,a}]
 \end{aligned} \tag{33}$$

From (33), if we prove $J_{3,3,n} \geq 0$, then $E_{3,3,n} \geq 0$. It is clear that $J_{3,3,n}$ has many fewer terms than $E_{3,3,n}$.

In $J_{3,3,n}$ given in (33) and the constraints in (28) and (31), we may consider $\frac{\partial}{\partial x_{a,t}}, \frac{\partial}{\partial x_{b,t}}$, and $\frac{\partial}{\partial x_{c,t}}$ as the differential operators without giving concrete values to a, b , and c .

First, we prove $C_3(3,3)$ using Procedure 2 with $J_{3,3,3}$ given in (33) and the constraints in (28) and (31) as the input.

In Step S1, the new variables are $\mathcal{M}'_3 = \{m_i, i = 1, \dots, 38\}$, which is the set of all the monomials in $\mathbb{R}[\mathcal{V}_{a,b,c}]$ with a degree of 3 and a total order of 3.

In Step S2, the constraints are: $\mathcal{C}_{3,n} = \{R_{i,a,b,c}^{(3)} : i = 1, \dots, 955\}$, $N_1 = 955$. We obtain $\mathcal{C}_{3,n,1}$ and $\mathcal{C}_{3,n,2}$, which contain 350 and 328 constraints, respectively.

In Step S3, there exist 189 intrinsic constraints. In total, $\widehat{\mathcal{C}}_{3,n,1}$ contains 539 constraints. Using \mathbb{R} -Gaussian elimination in $\text{Span}_{\mathbb{R}}(\widehat{\mathcal{C}}_{3,n,1})$ shows that 512 of these 539 constraints are linearly independent, thus $N_3 = 512$.

In Step S4, we obtain $\widehat{\mathcal{C}}_{3,n}$ from $\mathcal{C}_{3,n}$ which contains six constraints.

In Step S5, eliminating the non-quadratic monomials in $J_{3,3,3}$ using $\mathcal{C}_{3,n,2}$ and then simplifying the expression using $\mathcal{C}_{3,n,1}$, we obtain $\widehat{J}_{3,3,3}$, which is written as a quadratic form in m_i .

In Step S6, using the Matlab software in Appendix A [21] with $\widehat{J}_{3,3,3}$, $\widehat{\mathcal{C}}_{3,n,1}$ and $\widehat{\mathcal{C}}_{3,n}$ as the input, we find an SOS representation for $\widehat{J}_{3,3,3}$. Thus, using Theorem 1, $C_3(3,3)$ is strictly proved. The Maple program used to prove $C_3(3,3)$ can be found at <https://github.com/cmuyanmmrc/codeforepi/> (accessed on 15 July 2020).

To prove $C_3(3,4)$, we just need to replace the input from $J_{3,3,3}$ with $J_{3,3,4}$ in Step S5 in the above procedure. In the same way, $C_3(3,4)$ can be strictly proved. The Maple program used to prove $C_3(3,4)$ can be found at <https://github.com/cmuyanmmrc/codeforepi/> (accessed on 15 July 2020).

5. Proof of $C_3(4,2)$

In this section, we use the procedure in Section 2.2 to prove $C_3(4,2)$ under the log-concave condition.

In step 1, we compute $E_{3,4,n}$ in (8) and (20):

$$\begin{aligned}
 & \frac{1}{2} \frac{d^3}{dt^3} \left(\frac{\|\nabla p_t\|^2}{p_t} \right) - \frac{3}{n^4} \mathbb{E} \left(\frac{\|\nabla p_t\|^2 - p_t \nabla^2 p_t}{p_t^2} \right)^4 \\
 & \stackrel{(2)}{=} \int_{\mathbb{R}^n} \frac{E_{3,4,n}}{p_t^7} dx_t,
 \end{aligned} \tag{34}$$

where $E_{3,4,n} = \sum_{a=1}^n \sum_{b=1}^n \sum_{c=1}^n \sum_{d=1}^n E_{4,a,b,c,d}$. For brevity, we omit the concrete expression of $E_{4,a,b,c,d}$.

In step 2, based on Lemma 2, we obtain 589 fourth-order constraints:

$$\mathcal{C}_{4,2} = \{R_i^{(2)} : i = 1, \dots, 589\} \subset \mathbb{R}[\mathcal{P}_{4,2}] \text{ and } N_1 = 589. \tag{35}$$

Using Lemma 3, we obtain three fourth-order log-concave constraints:

$$\mathbb{C}_{4,2} = \{-\Delta_{1,1}Q_{1,1}, -\Delta_{1,2}Q_{1,2}, \Delta_{2,1}Q_{2,1}\}$$

where $Q_{1,1}, Q_{1,2} \in \text{Span}_{\mathbb{R}}(\mathcal{M}_{6,2})$ and $Q_{2,1} \in \text{Span}_{\mathbb{R}}(\mathcal{M}_{4,2})$.

In step 3, we use Procedure 2 to compute the SOS representations (13) and (14) with $E_{3,4,n}, \mathcal{C}_{4,2}$, and $\mathbb{C}_{4,2}$ as the input.

In Step S1, the new variables are $\mathcal{M}_{4,2} = \{m_i, i = 1, \dots, 33\}$, which is the set of all monomials in $\mathbb{R}[\mathcal{P}_{4,2}]$ with a degree of 4 and a total order of 4, and which is listed in the lexicographical monomial order.

In Step S2, using Gaussian elimination for $\mathcal{C}_{4,2} = \{R_i^{(2)} : i = 1, \dots, 589\}$, we obtain $\mathcal{C}_{4,2,1}$ and $\mathcal{C}_{4,2,2}$, which contain 266 and 182 constraints, respectively.

In Step S3, there exist 182 intrinsic constraints. Thus, $\hat{\mathcal{C}}_{4,2,1}$ contains 448 constraints. Using \mathbb{R} -Gaussian elimination in $\text{Span}_{\mathbb{R}}(\hat{\mathcal{C}}_{4,2,1})$ shows that 417 of these 448 constraints are linearly independent, so $N_3 = 417$.

In Step S4, we obtain $\hat{\mathbb{C}}(4,2)$, which contain three log-concave constraints, so $N_2 = 3$.

In Step S5, by eliminating the non-quadratic monomials in $E_{3,4,2}$ using $\mathcal{C}_{4,2,2}$ to obtain a quadratic form in m_i and then simplifying the quadratic form using $\mathcal{C}_{4,2,1}$, we obtain $\hat{E}_{3,4,2}$ which is written as a quadratic form in m_i .

In Step S6, using the Matlab software in Appendix A of [21] with $\hat{E}_{3,4,2}, \hat{\mathcal{C}}_{4,2,1}$ and $\hat{\mathbb{C}}(4,2)$ as the input, we find an SOS representation for $\hat{E}_{3,4,2}$. Thus, using Theorem 1, $C_3(4,2)$ is strictly proved under the log-concave condition. The Maple program used to prove $C_3(4,2)$ can be found at <https://github.com/cm yuanmmrc/codeforepi/> (accessed on 15 July 2020).

6. Conclusions

In this paper, three conjectures $C_l(m, n)$ for $l = 1, 2, 3$ concerning the lower bound for the derivatives of $H(X_t)$ are considered. We propose a general procedure to prove inequities similar to $C_l(m, n)$. We first consider one of the conjectures of McKean $C_1(m, n) : (-1)^{m+1}(d^m/dt^m)H(X_t) \geq 0$ in the multivariate case, and prove $C_1(3,2)$, $C_1(3,3)$ and $C_1(3,4)$. This conjecture is also mentioned in Villani's paper [14], and is named the super-H theorem. Motivated by $C_2(m, n)$, we further propose the following weaker conjecture $C_3(m, n) : (-1)^{m+1}(d^m/dt^m)H(X_t) \geq (-1)^{m+1}\frac{1}{n}(d^m/dt^m)H(X_{Gt})$. Using our procedure, we prove $C_3(3,2)$, $C_3(3,3)$, $C_3(3,4)$ and $C_3(4,2)$ under the log-concave condition.

In the univariate case ($n = 1$), $C_1(3,1)$ and $C_1(4,1)$ were proved [16] and $C_1(5,1)$ cannot be proved with the SDP approach (In this paper, when we say $C_s(m, n)$ cannot be proved with the SDP approach, we mean that the software in Appendix A of [21] terminates and gives a negative answer for problem (21)) [18,22]. $C_2(3,1)$, $C_2(4,1)$, and $C_2(5,1)$ were proved under the log-concave condition [18]. We try to prove $C_2(6,1)$ under the log-concave condition. However, due to the accuracy of the SDP software, we cannot find an explicit SOS representation. In the multivariate case, $C_1(3,2)$, $C_1(3,3)$, and $C_1(3,4)$ were proved and $C_1(4,2)$ cannot be proved with the SDP approach [22]. For $C_1(3, n), n > 4$, the corresponding SDP problem is too large for the Matlab software in Appendix A [23]. In this paper, $C_3(3,2)$, $C_3(3,3)$, $C_3(3,4)$, and $C_3(4,2)$ were proved under the log-concave condition, and $C_2(3,2)$, $C_2(3,3)$, $C_2(3,4)$, and $C_2(4,2)$ cannot be proved with the SDP approach under the log-concave condition. For $C_3(3, n), n > 4$ and $C_3(4, n), n > 2$, the corresponding SDP problems are too large for the Matlab software in Appendix A [21].

In order to use the SDP approach to prove more difficult problems, two kinds of improvements are needed. First, it is easy to see that the size of $E_s(m, n)$ and the numbers of the constraints increase exponentially as m and n become larger. Thus, we need to find certain rules which could be used to simplify the computation to solve problems such as $C_1(3, n)(n > 4)$ and $C_3(3, n)(n > 4)$ under the log-concave condition. Second, in many cases, such as $C_1(5,1)$ and $C_2(3,2)$ under the log-concave constraint, the SDP software terminates and gives a negative answer. Since the SDP method is not complete for our

problem, we do not know whether an SOS representation exists. We thus need a complete method to solve problem (13). Another problem is to find more constraints besides those used in this paper in order to increase the power of the approach.

Author Contributions: Conceptualization, L.G.; formal analysis, L.G., C.-M.Y. and X.-S.G.; funding acquisition, L.G., C.-M.Y. and X.-S.G.; investigation, L.G. and X.-S.G.; methodology, L.G.; project administration, X.-S.G.; resources, L.G.; software, L.G.; supervision, X.-S.G. All authors have read and agreed to the published version of the manuscript.

Funding: This work is supported by NSFC 11688101 and NKRDP 2018YFA0704705, Beijing Natural Science Foundation (No. Z190004), and the Fundamental Research Funds for the Central Universities 2021NTST32.

Institutional Review Board Statement: Not applicable.

Informed Consent Statement: Not applicable.

Data Availability Statement: Not applicable.

Acknowledgments: The authors would like to thank the reviewers for their invaluable comments.

Conflicts of Interest: The authors declare no conflict of interest.

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