Holonomic gradient descent for the Fisher–Bingham distribution on the $d$-dimensional sphere

Tamio Koyama · Hiromasa Nakayama · Kenta Nishiyama · Nobuki Takayama

Abstract We propose an accelerated version of the holonomic gradient descent and apply it to calculating the maximum likelihood estimate (MLE) of the Fisher–Bingham distribution on a $d$-dimensional sphere. We derive a Pfaffian system (an integrable connection) and a series expansion associated with the normalizing constant with an error estimation. These enable us to solve some MLE problems up to dimension $d = 7$ with a specified accuracy.

Keywords Fisher–Bingham distribution · Maximum likelihood estimate · Holonomic gradient descent · Integrable connection · Pfaffian system

1 Introduction

Let $x = (x_{ij})$ and $y = (y_i)$ be a symmetric matrix parameter of size $(d+1) \times (d+1)$ and a vector parameter of size $d+1$, respectively. We are interested in the Fisher–Bingham probability distribution

$$
\mu(t; x, y, r)|dt| := \frac{1}{Z(x, y, r)} \exp \left( \sum_{1 \leq i \leq j \leq d+1} x_{ij} t_i t_j + \sum_{i=1}^{d+1} y_i t_i \right) |dt|
$$

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on the $d$-dimensional sphere $S^d(r) = \{(t_1, \ldots, t_{d+1}) | \sum_{i=1}^{d+1} t_i^2 = r^2, r > 0\}$ and the maximum likelihood estimate of the parameters $x$ and $y$ of this probability distribution. Here, the function $Z$ is the normalizing constant defined as

$$Z(x, y, r) = \int_{S^d(r)} \exp\left( \sum_{1 \leq i \leq j \leq d+1} x_{ij} t_i t_j + \sum_{i=1}^{d+1} y_i t_i \right) |dt| \quad (1)$$

and $|dt|$ denotes the standard measure on the sphere with the radius $r$ such that

$$\int_{S^d(r)} |dt| = r^d \frac{2\pi^{(d+1)/2}}{\Gamma((d+1)/2)}.$$

Solving the MLE problem involves finding the maximum of the function in $x, y$

$$\prod_{k=1}^{N} \mu(T^{(k)}; x, y, 1)$$

for given data vectors $T^{(k)}, k = 1, \ldots, N$ in the $t$-space $S^d(1)$. In order to compute the MLE, we need approximate values for the normalizing constant $Z$ and its derivatives. In the case of $d = 2$, the normalizing constant is expressed in terms of the Bessel function and for $d = 2$ there are several approaches for computing MLEs in directional statistics (see, e.g., Kent 1982; Mardia and Jupp 2000; Wood 1988). However, there are few studies on approximating the normalizing constant for the case of $d > 2$ and applications to the MLE. Among these, Kume and Wood (2005) proposed a method to evaluate the normalizing constant by utilizing the Laplace approximation of the integral for $d > 2$ and Kume and Walker (2009) gave a series approximation of the normalizing constant.

In this paper, we propose a different method for evaluating it and present applications to the MLE. Our method is based on the holonomic gradient descent (HGD) proposed in Nakayama et al. (2011), which utilizes a holonomic system of linear differential equations satisfied by the normalizing constant and gives the MLE accurately. The HGD consists of four steps. The first step is to derive a holonomic system of linear partial differential equations for the normalizing constant. The second step is to translate the holonomic system into a Pfaffian system, which is roughly speaking a set of ordinary differential equations with respect to the parameters $x_{ij}$ and $y_i$ for the normalizing constant. These two steps can be performed by a symbolic computation (the Gröbner basis method) if the size of the problem is moderate. The remaining steps utilize numerical computation. The third step is to evaluate the normalizing constant and its derivatives at an initial point. To do this, we can use numerical integration for a rough evaluation or a series expansion for a more accurate evaluation. The last step is to extend the evaluated values to other points needed for the MLE by using the Pfaffian system and a numerical solver of ordinary differential equations.

It is shown in Koyama (2013) and Nakayama et al. (2011) that the normalizing constant of the Fisher–Bingham distribution is a holonomic function in $x, y, r$ and further more it is annihilated by a holonomic ideal for which an explicit expression is given. This is the first step when applying the HGD. For the second step, we need to translate the ideal into a Pfaffian system.
This is performed on a computer for $d \leq 2$ in Nakayama et al. (2011); however, this is not possible for $d > 2$ on current computers using Gröbner basis algorithms due to the high computational complexity.

In this paper, we overcome the difficulty of high complexity and complete the remaining steps for a general dimension: we give an accelerated version of the HGD as a general method, we derive the Pfaffian system of the Fisher–Bingham distribution for general $d$ by hand, and we derive a series expansion of the normalizing constant with an error estimation. We demonstrate that the accelerated version of HGD on our Pfaffian system works well up to $d = 7$ to a specified accuracy for a certain class of problems. We also propose a general method for evaluating the numerical errors and apply it to the Fisher–Bingham distribution.

2 Holonomic gradient descent with Pfaffian system of factored form

The HGD introduced in Nakayama et al. (2011) is a general algorithm for solving MLE problems for holonomic unnormalized distributions accurately. We herein propose an accelerated version of the HGD. The modification is small, but it allows a drastic performance improvement as we will see in the case of the Fisher–Bingham distribution.

In this section, we maintain a general setting to explain our accelerated method. A function $f(y_1, \ldots, y_n)$ is called a holonomic function when it satisfies an ordinary differential equation with polynomial coefficients for each variable $y_i$. In other words, the function $f$ is a holonomic function when the function is annihilated by an ordinary differential operator of the form

$$\sum_{j=0}^{r_i} a_{ij}(y) \left( \frac{\partial}{\partial y_i} \right)^j, \quad a_{ij}(y) \in \mathbb{C}[y_1, \ldots, y_n].$$

By virtue of this ordinary differential operators, the function $f$ can be regarded as a solution of a Pfaffian system discussed below. An important property of holonomic functions is that the integral $\int_R f(y_1, \ldots, y_n)dy_n$ is a holonomic function with respect to $y_1, \ldots, y_{n-1}$ under a suitable condition on the integration domain $R$. In the landmark paper by Zeilberger (1990), he introduced the notion of holonomic functions and applied it to mechanically prove special function identities with systems of linear partial differential equations and this important property. It has been proved that the normalizing constant $Z$ of the Fisher–Bingham distribution is a holonomic function in $x, y, r$ (Nakayama et al. 2011). Let $f(t; \theta)$ be a holonomic unnormalized probability distribution with respect to $t$ and $\theta$ where $\theta = (\theta_1, \ldots, \theta_m)$ is a parameter vector and let $Z(\theta) = \int_U f(t; \theta) dt$ be the normalizing constant. Let $I$ be a holonomic ideal in the ring of differential operators in $\theta$ that annihilates $Z$. The operator $\partial/\partial \theta_i$ is denoted by $\partial_{\theta_i}$. In order to apply the HGD to MLE problems, we need an explicit expression for the Pfaffian system associated with the holonomic ideal $I$ as an input to a numerical solver. The Pfaffian system is used to numerically evaluate the likelihood function and its gradient or its Hessian. Let us review the definition of the Pfaffian system (see, e.g., Nakayama et al. 2011 for details). Let rank $(I)$ be the holonomic rank of the ideal $I$ and
let $F$ be a vector of the standard monomials of a Gröbner basis of $I$. The length of this vector is rank($I$). We denote the elements of $F$ by $\partial^\alpha$ where $\alpha \in S$. We assume that the first element of $F$ is $\partial^0 = 1$. The Pfaffian system is a set of differential operators which annihilate the vector-valued function $F(Z) = (\partial^\alpha Z | \alpha \in S)^T$ that are of the form $\partial^\alpha - P_i$ where $P_i$ are rank($I$) $\times$ rank($I$) matrices with rational function entries which satisfy

$$\nabla \circ \nabla = 0, \quad \nabla = d - \sum P_i d\theta_i.$$

In this section, the symbol $d$ in the definition of $\nabla$ indicates the exterior derivative with respect to the variables $\theta$. In some of the literatures, the definition of the Pfaffian system does not include the integrability condition $\nabla \circ \nabla = 0$, but we will call the integrable Pfaffian system of equations simply the Pfaffian system for short. Our Pfaffian system can be regarded as the integrable connection $\nabla$.

The Pfaffian system can be obtained by an algorithmic method explained, e.g., in Nakayama et al. (2011). However, it requires heavy computation. For example, the computation for the Fisher–Bingham distribution could be performed within a reasonable time using current computer technology only up to the case of a 2-dimensional sphere. Moreover, the Pfaffian system obtained with this method requires heavy numerical computation in the HGD, because in general the entries of $P_i$ are huge rational functions. The latter drawback is removed by using our accelerated version of HGD introduced below.

**Algorithm 1**

1. Construct a Pfaffian system of the form

$$\partial^\theta_i - R_i^{-1}(\theta) Q_i(\theta)$$

(2)

where $Q_i$ and $R_i$ are rank($I$) $\times$ rank($I$) matrices with polynomial function entries.

2. Evaluate the normalizing constant $F(Z)$ at an initial parameter $\theta_0$.

3. $k = 0$

4. Evaluate the gradient of the likelihood function by $F(Z)$ at $\theta^k$ (see Nakayama et al. 2011). If the gradient is 0, then stop. Determine the value of the new parameter $\theta^{k+1}$ by standard procedures of gradient descent. $\theta^{k+1}$ must be sufficiently close to $\theta^k$.

5. Evaluate the approximate value of $F(Z)$ at $\theta^{k+1}$. It is, for instance, approximately equal to

$$F(Z)(\theta^k) + \sum_{i=1}^d R_i(\theta^k)^{-1} Q_i(\theta^k) F(Z)(\theta^k) \cdot (\theta_i^{k+1} - \theta_i^k).$$

(3)

6. $k \rightarrow k + 1$ and go to 4.

We call the Pfaffian system of the form (2) the Pfaffian system of *factored form*. The main difference between the HGD in Nakayama et al. (2011) and our proposed method is (3). In the original version, the factored matrix $R_i^{-1} Q_i$ is expressed as a single matrix with entries of (huge) rational functions, but in our proposed method, we express it
as the two matrices $Q_i$ and $R_i$ and the inverse of $R_i$ is calculated numerically in each iteration step. We note that the approximation in (3) should be replaced with a more accurate and efficient numerical scheme such as the Runge–Kutta method.

**Remark 1** When we have a Gröbner basis of $I$, the Pfaffian system of the form (2) can be obtained by the computation of normal forms by using the Gröbner basis and then solving linear equations in the ring of polynomials.

This procedure is general, but it can require a huge amount of computational resources. When we apply this method to problems, we need to find shortcuts based on individual problems in order to solve the problems efficiently. We will do this for the Fisher–Bingham distribution in the next section.

**Remark 2** The matrix $R_i^{-1} Q_i$ may have the form

$$\sum_j R_i^{-1} Q_{ij} T_i^{-1} S_{ij} \cdots$$

where $R_i, Q_{ij}, S_{ij}, T_{ij}, \ldots$ are rank$(I) \times$ rank$(I)$ matrices in polynomial function entries. This form is referred to as the multi-factored form or sometimes simply factored form.

In the following, we will sometimes call the accelerated version of HGD simply the HGD.

### 3 Pfaffian system for the normalizing constant

It is shown in Nakayama et al. (2011) and Koyama (2013) that the normalizing constant $Z$ in (1) of the Fisher–Bingham distribution is a holonomic function in $x, y, r$ and furthermore that it is annihilated by a holonomic ideal $I$.

The holonomic ideal $I$ is generated by the following operators in the ring of differential operators.

$$\partial_{ij} - \partial_i \partial_j \quad (1 \leq i \leq j \leq d + 1),$$

$$\sum_{i=1}^{d+1} \partial_i^2 - r^2,$$

$$x_{ij} \partial_{i}^2 + 2(x_{jj} - x_{ii}) \partial_i \partial_j - x_{ij} \partial_j^2 + \sum_{1 \leq k \leq d+1, k \neq i, j} (x_{kj} \partial_i \partial_k - x_{ik} \partial_j \partial_k)$$

$$+ y_j \partial_i - y_i \partial_j \quad (1 \leq i < j \leq d + 1),$$

$$r \partial_r - 2 \sum_{1 \leq i \leq j \leq d+1} x_{ij} \partial_i \partial_j - \sum_{i=1}^{d+1} y_i \partial_i - d$$

Here, $\partial_{ij}, \partial_i,$ and $\partial_r$ stand for $\frac{\partial}{\partial x_{ij}}, \frac{\partial}{\partial y_i},$ and $\frac{\partial}{\partial r}$ respectively. Note that we assume $x_{ij} = x_{ji}$. 

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We want to translate these into a Pfaffian system of the form (2) or (4) which is used in the accelerated HGD explained in the previous section.

Before proceeding to the discussion of the general \( d \)-dimensional case, we illustrate our method in the case of \( d = 1 \) and \( r = 1 \). Let \( I_1 \) be the left ideal generated by

\[
\partial_{11} - \partial_1^2, \quad \partial_{12} - \partial_1 \partial_2, \quad \partial_{22} - \partial_2^2, \quad \partial_1^2 + \partial_2^2 - 1, \quad x_{12} \partial_1^2 + 2(x_{22} - x_{11}) \partial_1 \partial_2 - x_{12} \partial_2^2 + y_2 \partial_1 - y_1 \partial_2
\]

in the ring of differential operators. The holonomic rank of \( I_1 \) is 4. Let \( F \) be a vector of operators \((1, \partial_1, \partial_2, \partial_1^2)^T\). We want to find a matrix \( P \) whose entries are rational functions such that \( \partial_1 F \equiv PF \) holds modulo the left ideal \( I_1 \). Here, \( s \equiv t \) means that each element of \( s - t \) belongs to \( I_1 \). Since \( \partial_1 F = (\partial_1, \partial_1^2, \partial_1 \partial_2, \partial_1^3)^T \), we need to express \( \partial_1 \partial_2 \) and \( \partial_1^2 \) in terms of \( F \) modulo \( I_1 \). Eliminating \( \partial_2^2 \) from (11) by (10), we obtain

\[
2(x_{22} - x_{11}) \partial_1 \partial_2 \equiv -x_{12} \partial_1^2 + x_{12} \partial_2^2 - y_2 \partial_1 + y_1 \partial_2
\]

\[
\equiv -x_{12} \partial_1^2 + x_{12}(1 - \partial_1^2) - y_2 \partial_1 + y_1 \partial_2
\]

\[
+ y_1 \partial_2 \text{ (the underlined term is reduced by (10))}
\]

\[
= (x_{12}, -y_2, y_1, -2x_{12}) F.
\]

Thus, we have expressed \( \partial_1 \partial_2 \) in terms of \( F \).

We now try to express \( \partial_1^3 \) in terms of \( F \). From \( \partial_1 \times (11) \), we obtain

\[
x_{12} \partial_1^3 + 2(x_{22} - x_{11}) \partial_1^2 \partial_2 \equiv x_{12} \partial_1 \partial_1^2 - y_2 \partial_1^2 + y_1 \partial_1 \partial_2 + \partial_2
\]

\[
\equiv x_{12} \partial_1 (1 - \partial_1^2) - y_2 \partial_1^2 + \frac{y_1}{2(x_{22} - x_{11})} (x_{12} - y_2 \partial_1 + y_1 \partial_2 - 2x_{12} \partial_1^2)
\]

\[
+ \partial_2 \text{ (the underlined terms are reduced by (10) and (12))},
\]

and consequently we have

\[
2x_{12} \partial_1^3 + 2(x_{22} - x_{11}) \partial_1^2 \partial_2 \equiv (a, b, c, d) F,
\]

where

\[
a = \frac{y_1 x_{12}}{2(x_{22} - x_{11})}, \quad b = x_{12} - \frac{y_1 y_2}{2(x_{22} - x_{11})},
\]

\[
c = 1 + \frac{y_1^2}{2(x_{22} - x_{11})}, \quad d = -y_2 - \frac{x_{12} y_1}{x_{22} - x_{11}}.
\]

By a similar computation for \( \partial_2 \times (11) \), we have

\[
2(x_{22} - x_{11}) \partial_1^3 - 2x_{12} \partial_1^2 \partial_2 \equiv (a', b', c', d') F,
\]

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where
\[
a' = -y_1 + \frac{x_{12}y_2}{2(x_{22} - x_{11})}, \quad b' = 1 + 2(x_{22} - x_{11}) - \frac{y_2^2}{2(x_{22} - x_{11})},
\]
\[
c' = -x_{12} + \frac{y_1y_2}{2(x_{22} - x_{11})}, \quad d' = y_1 - \frac{x_{12}y_2}{x_{22} - x_{11}}.
\]

Therefore, we have
\[
\begin{pmatrix}
2x_{12} & 2(x_{22} - x_{11}) \\
2(x_{22} - x_{11}) & -2x_{12}
\end{pmatrix}
\begin{pmatrix}
\partial_3^1 \\
\partial_2^1
\end{pmatrix}
= \begin{pmatrix} a & b & c & d \\
\alpha' & \beta' & \gamma' & \delta'
\end{pmatrix} F.
\]

Multiplying the both sides by the inverse matrix \( \begin{pmatrix} 2x_{12} & 2(x_{22} - x_{11}) \\
2(x_{22} - x_{11}) & -2x_{12}\end{pmatrix}^{-1} \), we can express \( \partial_1^3 \) in terms of \( F \). Thus we have obtained a factored form of \( P \) in \( \partial_1 F \equiv PF \). The identity \( \partial_1 F \equiv PF \) gives a Pfaffian equation for the direction \( y_1 \). In other words, the differential equation
\[
\frac{\partial F(Z)}{\partial y_1} = PF(Z), \quad F(Z) = \begin{pmatrix} Z, & \frac{\partial Z}{\partial y_1}, & \frac{\partial Z}{\partial y_2}, & \frac{\partial^2 Z}{\partial y_1^2} \end{pmatrix}^T
\]
holds. This is an ordinary differential equation for the vector-valued function \( F(Z) \) with respect to the variable \( y_1 \). It is easy to see that \( P \) is of the form (4). Ordinary differential equations for the other directions \( \partial_2, \partial_{11}, \partial_{12}, \partial_{22} \) can be obtained analogously.

For the general \( d \), let \( F \) be the vector of operators
\[
(1, \partial_1, \ldots, \partial_{d+1}, \partial_1^2, \ldots, \partial_d^2)^T.
\]

**Theorem 1** There exists a \((2d + 2) \times (2d + 2)\) matrix \( H_i \) which has a factored form (4) and satisfies the relation \( \partial_i F \equiv H_i F \mod I \).

An expression of \( H_i \) as a factored form and a proof of this theorem, which is technical, will be given in the “Appendix”.

The relation between \( \partial_{ij} F \) and \( F \) can be easily obtained by Theorem 1.

In fact, since \( \partial_{ij} F \equiv \partial_i \partial_j F \equiv \partial_j \partial_i F \) by (5), we have
\[
\partial_{ij} F \equiv \partial_j \partial_i F \equiv \partial_j (H_i F) \equiv \frac{\partial H_i}{\partial y_j} F + H_i (\partial_j F) \equiv \left( \frac{\partial H_i}{\partial y_j} + H_i H_j \right) F. \tag{14}
\]

We denote by \( H_{ij} \) the matrix \( \frac{\partial H_i}{\partial y_j} + H_i H_j \). The matrix such that \( \partial_r F \equiv H_r F \) can be obtained easily by utilizing (8). Thus, we have obtained the relations
\[
\partial_i F \equiv H_i F, \quad \partial_{ij} F \equiv H_{ij} F, \quad \partial_r F \equiv H_r F. \tag{15}
\]
In Koyama et al. (2012), we prove that the holonomic rank of $I$ is equal to $2d + 2$. Therefore, the Pfaffian equations are expressed in terms of $(2d+2) \times (2d+2)$ matrices. The matrices in (15) are exactly these matrices. The integrability conditions of Pfaffian equations imply $\frac{\partial H_i}{\partial y_j} + H_i H_j = \frac{\partial H_j}{\partial y_i} + H_j H_i$.

In Nakayama et al. (2011), the differential equations satisfied by the likelihood function for $d = 1$ and $d = 2$ are derived by a heavy Gröbner basis computation and we could not obtain them for $d \geq 3$. It is known that the Gröbner basis computation has the double-exponential complexity with respect to the number of variables (see, e.g., Bayer and Stillman 1988) and we usually have to avoid deriving Gröbner bases by a computer for large problems. Instead, we can sometimes derive Gröbner bases by hand and apply them to interesting applications. By virtue of Theorem 1 for the general dimension, we can describe the differential equation satisfied by the likelihood function with matrices in factored form of which factors are relatively small matrices with polynomial entries. If we calculate the inverse matrices in the factored forms by symbolic computation, we would obtain the same result with the Gröbner basis method. In order to apply for the HGD, we do not need to calculate these inverse matrices with polynomial entries symbolically, instead we need only calculate inverse matrices numerically when variables are restricted to real number values in each step of the Runge–Kutta method. This will become a key ingredient of our algorithm, which will be discussed in Sect. 6.

Remark 3 The matrices $H_i, H_{ij}, H_r$ have simple forms when $x$ is a diagonal matrix. In Sei et al. (2013), the MLE of the Fisher distribution on $SO(3)$ is obtained by the HGD with differential equations for the normalizing constant with diagonalized arguments. It is a natural question to ask whether a simplification analogous to the diagonal $x$ case is possible. Unfortunately, an analog of Lemma 2 of Sei et al. (2013) does not hold except for the case of $y = 0$. It is possible to evaluate the gradient of $Z$ from values of $Z$ for diagonal $x$ by Proposition 1 given later, however this requires computation of a transformation matrix to diagonalize the matrix $x$ at each step of the gradient descent. On the other hand, we do not need to do this computation for the diagonal form in the HGD by the Pfaffian system for the full parameters $x, y, r$.

4 Series expansion for the normalizing constant

Let us define the function $\tilde{Z}$ by the integral

$$\tilde{Z}(\tilde{x}, \tilde{y}, \tilde{r}) = \int_{S^d(r)} \exp \left( \sum_{i=1}^{d+1} (\tilde{x}_i t_i^2 + \tilde{y}_i t_i) \right) |dt|.$$  \hfill (16)

The function satisfies the invariance relation

$$\tilde{Z}(\tilde{x}, \tilde{y}, 1) = \tilde{Z}(r^{-2} \tilde{x}, r^{-1} \tilde{y}, r).$$ \hfill (17)

This function is the restriction of the normalizing constant $Z$ to the diagonalized $\tilde{x}$. Since the normalizing constant is invariant under the action of the orthogonal group
Suppose that the real symmetric matrix $x$ is diagonalized by an orthogonal matrix $P = (p_{ij})$, and set $\tilde{x} = P^T x P$, $\tilde{y} = P^T y$, $\tilde{r} = r$. Then, we have

$$Z(x, y, r) = \tilde{Z} (\tilde{x}, \tilde{y}, \tilde{r})$$

$$\frac{\partial Z}{\partial y_i} (x, y, r) = \sum_{k=1}^{d+1} p_{ik} \frac{\partial \tilde{Z}}{\partial y_k} (\tilde{x}, \tilde{y}, \tilde{r})$$

$$\frac{\partial^2 Z}{\partial y_i^2} (x, y, r) = \sum_{k=1}^{d+1} p_{ik}^2 \frac{\partial^2 \tilde{Z}}{\partial y_k^2} (\tilde{x}, \tilde{y}, \tilde{r})$$

$$- \sum_{1 \leq k < \ell \leq d+1} p_{ik} p_{i\ell} \frac{\partial \tilde{Z}}{\partial y_k} \frac{\partial \tilde{Z}}{\partial y_\ell} (\tilde{x}, \tilde{y}, \tilde{r}) - \frac{\partial \tilde{Z}}{\partial y_k} (\tilde{x}, \tilde{y}, \tilde{r}) - \frac{\partial \tilde{Z}}{\partial y_\ell} (\tilde{x}, \tilde{y}, \tilde{r})$$

Kume and Walker (2009) give a series approximation of the Fisher–Bingham distribution and consequently that of the normalizing constant $\tilde{Z} (\tilde{x}, \tilde{y}, 1)$. Their expression is easily rescaled to the case including the parameter $r$. We will give an error estimate of this series approximation. We will omit the tilde symbol (‘~’) for $x$ and $y$ in the following where this should cause no confusion.

**Theorem 2** 1. (Kume and Walker 2009) The restricted normalizing constant has the following series expansion

$$\tilde{Z} (x, y, r) = S_d \cdot \sum_{\alpha, \beta \in \mathbb{N}_0^{d+1}} r^{d+2|\alpha+\beta|} \frac{(d-1)!! \prod_{i=1}^{d+1} (2\alpha_i + 2\beta_i - 1)!!}{(d-1 + 2|\alpha| + 2|\beta|)!! \alpha! \beta!} x^\alpha y^{2\beta}. \quad (18)$$

Here, $S_d = \int_{S^{d}(1)} |dt|$ denotes the surface area of the $d$-sphere of radius 1, and $\mathbb{N}_0 = \{0, 1, 2, \ldots\}$. For a multi-index $\alpha \in \mathbb{N}_0^{d+1}$, we put $\alpha! = \prod_{i=1}^{d+1} \alpha_i!$, $\alpha!! = \prod_{i=1}^{d+1} \alpha_i!!$, and $|\alpha| = \sum_{i=1}^{d+1} \alpha_i$.

2. The truncation error of the series is estimated as

$$\left| S_d \cdot \sum_{|\alpha+\beta| \geq N} r^{d+2|\alpha+\beta|} \frac{(d-1)!! \prod_{i=1}^{d+1} (2\alpha_i + 2\beta_i - 1)!!}{(d-1 + 2|\alpha| + 2|\beta|)!! \alpha! \beta!} x^\alpha y^{2\beta} \right|$$

$$\leq S_d \cdot \frac{r^d}{N!} \left( r^2 \sum_i (|x_i| + |y_i|^2) \right)^N \frac{N + 1}{N + 1 - r^2 \sum_i (|x_i| + |y_i|^2)} \quad (19)$$

when $N$ is sufficiently large.
We note that the series (18) converges slowly when \( r^2 \sum_i (|x_i| + |y_i|^2) > 1 \) and converges relatively rapidly when \( r^2 \sum_i (|x_i| + |y_i|^2) \leq 1 \). The derivatives of \( \tilde{Z} \) are expressed as derivatives of the right-hand side of (18).

**Proof of 2.**

We have the following estimates

\[
\left| \sum_{|\alpha+\beta| \geq N} r^{d+2|\alpha+\beta|} \frac{(d-1)! \prod_{i=1}^{d+1} (2\alpha_i + 2\beta_i - 1)! |x^\alpha y^{2\beta}|}{(d-1 + 2|\alpha| + 2|\beta|)!\alpha!(2\beta)!} \right|
\]

\[
\leq \sum_{|\alpha+\beta| \geq N} r^{d+2|\alpha+\beta|} \frac{(d-1)! \prod_{i=1}^{d+1} (2\alpha_i + 2\beta_i - 1)! |x^\alpha y^{2\beta}|}{(d-1 + 2|\alpha| + 2|\beta|)!\alpha!(2\beta)!}
\]

\[
\leq \sum_{|\alpha+\beta| \geq N} \left| \frac{r^{d+2|\alpha+\beta|}}{\alpha!(2\beta)!} \right| \frac{1}{\alpha! \beta!} \frac{1}{x^\alpha y^{2\beta}}
\]

\[
\leq \sum_{|\alpha+\beta| \geq N} r^{d+2|\alpha+\beta|} \frac{1}{\alpha! \beta!} \frac{1}{x^\alpha y^{2\beta}} \leq r^d \sum_{n \geq N} \frac{r^{2n}}{n!} \sum_{|\alpha+\beta|=n} \frac{n!}{\alpha! \beta!} |x^\alpha y^{2\beta}|
\]

\[
\leq r^d \sum_{n \geq N} \frac{r^{2n}}{n!} \left( \sum_{i=1}^{d+1} (|x_i| + |y_i|^2) \right)^n \leq r^d \sum_{n \geq N} \frac{1}{n!} \left( r^2 \sum_{i=1}^{d+1} (|x_i| + |y_i|^2) \right)^n.
\]

Set \( L(x, y, r) = r^2 \sum_{i=1}^{d+1} (|x_i| + |y_i|^2) \). Assume that \( N \) is sufficiently large so that \( L/(N+1) < 1 \). We have the estimate

\[
|L(x, y, r)| \leq \frac{r^d}{N!} |L(x, y, r)|^N \frac{N + 1}{N + 1 - L(x, y, r)}
\]

by the estimate

\[
\sum_{n \geq N} \frac{1}{n!} L^n = \frac{1}{N!} L^N \sum_{n \geq N} \frac{1}{(N+1)^{n-N}} L^{n-N}
\]

\[
= \frac{1}{N!} L^N \sum_{n=0}^{\infty} \frac{1}{(N+1)^n} L^n
\]

\[
\leq \frac{1}{N!} L^N \sum_{n=0}^{\infty} \frac{1}{(N+1)^n} L^n
\]

\[
= \frac{1}{N!} L^N \frac{N + 1}{N + 1 - L}.
\]

\( \Box \)
5 Numerical evaluation of the normalizing constant

In order to efficiently evaluate \( \tilde{Z} \) numerically, we use the holonomic gradient method (HGM) (see, e.g., Hashiguchi et al. 2013). The HGM is a method for evaluating the normalizing constant by utilizing a system of differential equations. In the case of the Fisher–Bingham distribution, we numerically evaluate the series (2) in the domain \( r^2 \sum_i (|x_i| + |y_i|^2) \leq 1 \) and extend the numerical evaluation outside this domain by using a differential equation with respect to \( r \). To use this method, we prepare the following theorem.

**Theorem 3**

1. The function \( \tilde{Z} \) is annihilated by the left ideal \( \tilde{I} \) generated by

\[
A_i = \partial^2_{y_i} - \partial_{x_i} \quad (1 \leq i \leq d + 1),
\]

\[
B = \partial^2_{y_1} + \cdots + \partial^2_{y_{d+1}} - r^2,
\]

\[
C_{ij} = 2(x_i - x_j)\partial_{y_i}\partial_{y_j} + y_i\partial_{y_j} - y_j\partial_{y_i} \quad (1 \leq i < j \leq d + 1),
\]

\[
E = r\partial_r - 2 \sum_{i=1}^{d+1} x_i \partial^2_{y_i} - \sum_{i=1}^{d+1} y_i \partial_{y_i} - d.
\]

2. Set \( \tilde{F} = (\partial_{y_1}, \ldots, \partial_{y_{d+1}}, \partial^2_{y_1}, \ldots, \partial^2_{y_{d+1}})^T \). Then, we have \( \partial_r \tilde{F} \equiv P^{(r)} \tilde{F} \mod \tilde{I} \).

Here, the matrix \( P^{(r)} = (p^{(r)}_{ij}) \) is defined by

\[
r p^{(r)}_{ij} = (2x_i r^2 + 1)\delta_{ij} + \sum_{k=1}^{d+1} y_i \delta_{j(k+d+1)} \quad (1 \leq i \leq d + 1),
\]

\[
r p^{(r)}_{(i+d+1)j} = y_j r^2 \delta_{ij} + (2x_i r^2 + 2)\delta_{(i+d+1)j} + \sum_{k \neq i} \delta_{j(k+d+1)} \quad (1 \leq i \leq d + 1)
\]

for \( 1 \leq j \leq 2d + 2 \).

The proof of this theorem is analogous to that for the non-diagonal \( x \) case.

**Example 1** In the case of \( d = 1 \), the matrix \( P^{(r)} \) is

\[
\frac{1}{r} \begin{pmatrix}
2r^2 x_1 + 1 & 0 & y_1 & y_1 \\
0 & 2r^2 x_2 + 1 & y_2 & y_2 \\
r^2 y_1 & 0 & 2r^2 x_1 + 2 & 1 \\
0 & r^2 y_2 & 1 & 2r^2 x_2 + 2
\end{pmatrix}.
\]
We note that the largest eigenvalue of $P(r)$ is $O(r)$. Our implementation of the HGM numerically solves the ordinary differential equation

$$\frac{\partial G}{\partial r} = (P(r) - r\lambda E)G$$

instead of solving $\partial_r \tilde{F}(\tilde{Z}) = P(r) \tilde{F}(\tilde{Z})$, where $\lambda$ is the largest eigenvalue of $\lim_{r \to +\infty} P(r)/r$ and the vector-valued function $G$ is defined by $F(\tilde{Z}) = \exp(\lambda r^2/2)G$. This scalar scaling is necessary, because the adaptive Runge–Kutta method requires an absolute error bound of the solution to automatically make meshes finer and when a solution grows exponentially, meshes become too small to maintain an absolute error bound.

Now let us discuss on the accuracy of the HGM. The truncation error of the series approximation is estimated in Theorem 2. We want to estimate the numerical error caused by applying the HGM. In other words, we want to estimate how much the truncation error is magnified by solving the ordinary differential equation numerically. We propose a practical method to do this. Note that this method can be applied to any HGM, but we will explain it in the case of the Fisher–Bingham distribution. In this method, we assume that initial values are governed by a probability measure. This assumption is natural in, e.g., molecular modeling and some classes of non-linear ordinary differential equations are studied under this assumption (see, e.g., Cano et al. 2001). In our case, the ordinary differential equation is linear and the problem is much easier. Since we have not found a reference relevant to our case, we include below a discussion on the behavior of solutions of a linear equation under random initial data.

For a given initial value vector $Z_0$ at $r = r_0$, we denote by $RZ_0$ the output obtained at $r = r_1$ by solving the ordinary differential equation where we may suppose that $R$ is a constant matrix, because the Runge–Kutta solver can be regarded as a linear map from the input to the output under the assumption that round-off errors and cancellation errors by floating point arithmetic are sufficiently small and that the automatic mesh refinement process is fixed. When $Z_0$ is regarded as a random vector distributed as a multivariate normal distribution, the output $RZ_0$ is also a random vector distributed as a multivariate normal distribution. In our implementation, we perturb $Z_0$ with random numbers of which the standard deviation is $\varepsilon/2$ where $\varepsilon$ is a truncation error and solve the ordinary differential equation for these perturbed initial values. We evaluate the mean and the standard deviation of the first component of $RZ_0$ and these give an evaluation of the normalizing constant and its statistical error bound. This bound is more practical than that by interval arithmetic.

For example, Fig. 1 shows a histogram of the normalizing constant which is generated by the above procedure with $\varepsilon/2 = 0.1$, $r_0 = 1$, $r_1 = \sum |x_i| + \sum y_i^2$, $d = 3$, $x = \text{diag}(1.2, 2.5, 3.2, 3.6)$, $y = (2.3, 5.3, 4.2, 0.1)$. The series is evaluated at $x/r_1^2$, $y/r_1$, $r = 1$ and extended to $r = r_1$. In this case, the standard derivation of the normalizing constant is evaluated as 156.6288 and the confidence interval with probability 0.95 is $[14065.6, 14679.6]$.

Kume and Wood (2005) gave a saddle point approximation of the normalizing constant for the Fisher–Bingham distribution. Our method evaluates the normalizing constant with an error bound. Table 1 shows values by the HGM.
and by the third order saddle point approximation by Kume and Wood. Here, \( d = 4 \) and \((x_{ij}) = \text{diag}(x_{11}, 2x_{11}, 3x_{11}, 4x_{11}, 5x_{11}), 0.5 \leq x_{11} \leq 10, (y_k) = (0.5y_0, 0.4y_0, 0.3y_0, 0.2y_0, 0.1y_0), y_0 = 3. The absolute error bound to solve (21)
by the adaptive Runge–Kutta method is set to $10^{-6} \sum_{i=1}^{2d+2} G_i/(2d+2)$ and $\varepsilon$ is $10^{-5}$. The values of the standard deviation imply that the values by the HGM have at least 6-digit accuracy with 95% confidence.

6 Algorithm and numerical results

In Nakayama et al. (2011 Algorithm 1 and Theorem 2), we give an algorithm to obtain the MLE for the Fisher–Bingham distribution. This algorithm is valid for general dimensions, but it cannot be used for more than two dimensions with the current level of computer technology because of the high computational complexity of the Gröbner basis computation. We replace the Gröbner basis computation part (steps 1, 2, 3 in Nakayama et al. (2011, Algorithm 1) with our derivation of the Pfaffian system of factored form given in Theorem 1 and replace the numerical integration part of (1) with the evaluation by the series (2) and extend values to slowly convergent domains of the series by the HGM. For efficiency, we calculate the inverse matrices in our expressions for $H_{ij}$ and $H_i$ numerically during the steps of the adaptive Runge–Kutta method as explained in Sect. 2 regarding the accelerated version of the HGD. This enables us to solve maximum likelihood estimation problems in more than two dimensions case with the HGD. More precisely, we have the following complexity result.

**Theorem 4** The complexity of the series expansion method, the HGM and the HGD for the Fisher–Bingham distribution on the $d$-dimensional sphere is

$$O((2d + 2)^{N+1}/N!) + \text{(complexity of solving the ODE with respect to $r$)}$$

$$+ O((2d + 2)^3) \times \text{(steps of the convergence of gradient descent)}.$$

The first and the second terms are the complexity to evaluate the initial values $F(Z)$ up to degree $N$ and the third term is the complexity of the HGD.

**Proof** The number of terms of the truncated series of (18) is $inom{2d + 2 + N}{2d + 2} = (2d + 2 + N)^N/(2d + 2)!$. The coefficients of the series can be evaluated by a recursive relation. We need $2d + 1$ derivatives of $\tilde{Z}$. Thus, we obtain the first term.

Our HGD requires the computation of the inverses of $(2d + 2) \times (2d + 2)$ matrices in each step of the HGD by Theorem 1. This corresponds to the third term. □

Our computational experiments give an observation that giving a practical bound for the complexity of numerically solving the ordinary differential equation with respect to $r$ with a prescribed accuracy does not seem to be easy.

We implemented our algorithm firstly in Maple and next in the C language using the GNU scientific library (GSL 2012). The prototype written in Maple is useful for debugging our C codes. Our C code is automatically generated by our code generation program pfngenc2.rr, which can be obtained from the URL in the Example 3, on Risa/Asir (2012).
In order to apply the HGD, we need to find a good starting point $\theta^0 = (x^0, y^0)$. We use the following method.

**Algorithm 2**

1. Take a random point $\tilde{\theta}^0 = (x, y)$ satisfying $0 < x_{ij} < 1$ and $0 < y_k < 1$.
2. Apply the Nelder–Mead algorithm, which does not require the gradient and may also be replaced with other methods, to find an approximate optimal point $\theta^0$ of the likelihood function from the starting point $\tilde{\theta}^0$ (see, e.g., Nocedal and Wright 2007). Normalizing constants are evaluated by the HGM, which may be replaced by other methods.
3. Apply the HGD with the starting point $\theta^0$. If the HGD stops normally, we are done. If the HGD stops at $\theta^1$ because of a numerical instability, go to the step 2 with $\tilde{\theta}^0 = a$ point in a neighborhood of $\theta^1$.

An alternative and heuristic way to avoid the retry in the last step is to abort the computation when a numerical instability occurs and then restart the algorithm with a new randomly chosen starting point. This procedure can be implemented in parallel.

We present some examples to illustrate the performance of our new algorithm and its implementation.

**Example 2** The problem “Astronomical data” given in Nakayama et al. (2011) is solved in 2.58 s on a 32-bit virtual machine, the host machine of which is an Intel Xeon E5410 (2.33GHz) processor based computer.

In contrast, our implementation in Nakayama et al. (2011) spends 17.3 s for the HGD and more than an hour for computing a Gröbner basis and deriving a Pfaffian system.

**Example 3** Problem names beginning with sk_’s in Table 2 are problems on the $k$-dimensional sphere. These problems are generated by a random number generator according to the Fisher–Bingham distribution. We chose 8 random points in the parameter space as starting points for Algorithm 2. The HGD aborts 2 times in the 8 tries in the worse case on $S^3$. This rate increases to 7 aborts of 8 tries in the worse case on $S^7$. The timing data shown are those for the first successful HGD among the 8 starting points. The first step time in the table is that of the step of applying the Nelder–Mead algorithm with the HGM.

These sample data and programs are obtainable from our web page.¹

### 7 Conclusion and open problems

We show that the HGD can solve some MLE problems up to dimension $d = 7$ by utilizing an explicit expression of the the Pfaffian system of factored form and the series expansion of the normalizing constant. However, there are two problems in applying our method efficiently to arbitrary data.

¹ [http://www.math.kobe-u.ac.jp/OpenXM/Math/Fisher--Bingham-2](http://www.math.kobe-u.ac.jp/OpenXM/Math/Fisher--Bingham-2).
Table 2 Performance of the accelerated HGD

| Problem | Time (1st step) | Time of the HGD and steps | Total |
|---------|-----------------|----------------------------|-------|
| s3_e1   | 9.8             | 3.2(73)                    | 13    |
| s3_e3   | 10              | 3.1(66)                    | 13    |
| s4_e1   | 50              | 14(93)                     | 64    |
| s4_e2   | 50              | 28(183)                    | 78    |
| s4_e3   | 50              | 11(75)                     | 61    |
| s5_e1   | 220             | 80(142)                    | 300   |
| s5_e2   | 221             | 140(121)                   | 361   |
| s5_e3   | 222             | 66(117)                    | 288   |
| s6_e1   | 828             | 247(172)                   | 1075  |
| s7_e1   | 2679            | 571(183)                   | 3250  |

1. In examples, we find a starting point for applying the HGD by the Nelder–Mead algorithm with the HGM for evaluating the normalizing constant. This method seems to work well for our examples, but it is not very efficient. Finding a good starting point efficiently for arbitrary data is an open question.

2. There are domains in \((x, y)\)-space where the normalizing constant cannot be evaluated to a given accuracy within a reasonable time by the HGM, because the normalizing constant is huge in these domains, which includes domains where \(|y|\) is large.

Although, there still remain important open problems, our proposed method evaluates the normalizing constant and its derivatives to a specified accuracy for a sufficiently broad set of parameters and solves MLE problems. We can easily control the accuracy of evaluations of the normalizing constant and so it is possible to apply our method for evaluations to other approximation methods.

8 Appendix: Proof of Theorem 1

We define two auxiliary vectors of operators to present the expression. We sort the set of the square free second order operators

\[
\{\partial_i \partial_j | 1 \leq i < j \leq d + 1\}
\]

by the lexicographic order. This gives a vector of operators of the length \(d(d + 1)/2\):

\[
F^{(2)} = (\partial_1 \partial_2, \partial_1 \partial_3, \ldots, \partial_d \partial_{d+1})^T.
\]  \(22\)

We sort the set of the third order operators

\[
\{\partial_i \partial_j \partial_k | 1 \leq i \leq j \leq k \leq d + 1, \ j \leq d\}
\]

by the lexicographic order.
We denote by $F^{(3)}$ the sorted vector

$$F^{(3)} = (\partial_1 \partial_1 \partial_1, \partial_1 \partial_1 \partial_2, \ldots, \partial_1 \partial_1 \partial_{d+1}, \partial_2 \partial_2 \partial_2, \ldots, \partial_d \partial_d \partial_{d+1})^T.$$  \hfill (23)

The length of this vector $d(d + 1)(d + 5)/6$ is denoted by $m$.

When two operators $\ell_1$ and $\ell_2$ are the same modulo the ideal $I$, we denote it by $\ell_1 \equiv \ell_2$. By examining the proof of Lemmas 2 and 3 of Nakayama et al. (2011), we obtain the following two lemmas which give an expression of the second and the third order operators $F^{(2)}$ and $F^{(3)}$ in terms of $F$.

**Lemma 1** We have

$$P^{(2)} F^{(2)} + Q^{(2)} F \equiv 0.$$  \hfill (24)

Here, $P^{(2)}$ is an invertible $d(d + 1)/2 \times d(d + 1)/2$ matrix and $Q^{(2)}$ is a $d(d + 1)/2 \times (2d + 2)$ matrix of which entries are as follows.

$$P^{(2)}_{i,j,k,l} = \begin{cases} 2(x_{jj} - x_{ii}) & (i = k, j = l) \\ x_{jl} & (i = k, j \neq l) \\ x_{jk} & (i = l, j \neq k) \\ -x_{ik} & (i \neq k, j = l) \\ -x_{il} & (i \neq l, j = k) \end{cases}$$

$$Q^{(2)}_{i,j,k} = \begin{cases} y_j \delta_{k,i+1} - y_i \delta_{k,j+1} + x_{ij} \delta_{k,i+d+2} - x_{ij} \delta_{k,j+d+2} & (j \leq d) \\ y_j \delta_{k,i+1} - y_i \delta_{k,j+1} + x_{ij} \delta_{k,i+d+2} \\ -r^2 x_{i,d+1} \delta_{k,1} + \sum_{\ell=1}^{d} x_{i,d+1} \delta_{k,\ell+d+2} & (j = d + 1) \end{cases}$$

Here, $\delta$ is Kronecker’s $\delta$ and $P^{(2)}_{i,j,k,l}$ is the matrix element of $P^{(2)}$ standing for $\partial_i \partial_j$ and $\partial_k \partial_l$ in $F^{(2)}$. We use this notation of the index of the matrix element in the sequel.

**Lemma 2** We have

$$P^{(3)} F^{(3)} + Q^{(3)} F^{(2)} + R^{(3)} F \equiv 0.$$  \hfill (25)

Here, $P^{(3)}$, $Q^{(3)}$, and $R^{(3)}$ are an invertible $m \times m$ matrix, an $m \times d(d + 1)/2$ matrix and an $m \times (2d + 2)$ matrix of polynomial entries respectively. Entries are defined as follows.
Define a differential operator $G_{ijk}$ in $I$; we put

$$
C_{ij} = x_{ij} \partial_i^2 + 2(x_{jj} - x_{ii}) \partial_i \partial_j - x_{ij} \partial_j^2 + \sum_{k \neq i, j} (x_{kj} \partial_k \partial_j - x_{ik} \partial_j \partial_k) + y_j \partial_i - y_i \partial_j.
$$

Define a differential operator $G_{ijk}$ $(i \leq j \leq k \leq d + 1, j \leq d)$ by

$$
G_{ijk} = \begin{cases} 
\partial_i C_{jk} & (i \leq j < k \leq d + 1), \\
\partial_j C_{ij} & (i < j = k \leq d), \\
\partial_{d+1} C_{i,d+1} & (i = j = k \leq d).
\end{cases}
$$
We expand $G_{ijk}$ in the ring of differential operators and express it in terms of the elements of $F$, $F^{(2)}$, and $F^{(3)}$. For example, when $i < j < k < d + 1$, we have

$$G_{ijk} = \partial_i C_{jk} = \partial_i (x_{jk} \partial_j^2 + 2(x_{kk} - x_{jj}) \partial_j \partial_k - x_{jk} \partial_k^2)$$

$$+ \sum_{l \neq j, k} (x_{lk} \partial_j \partial_l - x_{lj} \partial_k \partial_l) + y_k \partial_j - y_j \partial_k$$

$$= x_{jk} \partial_i \partial_j^2 + 2(x_{kk} - x_{jj}) \partial_i \partial_j \partial_k - x_{jk} \partial_i \partial_k^2$$

$$+ \sum_{l \neq j, k} (x_{kl} \partial_i \partial_j \partial_l - x_{jl} \partial_i \partial_k \partial_l) + y_k \partial_i \partial_j - y_j \partial_i \partial_k$$

which yields $P_{ijk, ijj}^{(3)}, P_{ijk, ijk}^{(3)}, \ldots, Q_{ijk, ijj}^{(3)}, Q_{ijk, ijk}^{(3)}$. Analogous expansions and rewritings for the other cases give the conclusion. \qed

We denote by $\text{Mat}(k, l, S)$ the space of the $k \times l$ matrices with entries in the set $S$. Let $\mathbb{Q}[x, y, r]$ denote the ring of polynomials with coefficients in $\mathbb{Q}$.

**Lemma 3** The vector $F$ satisfies the identity

$$A \partial_i F = BF + CF^{(2)} + EF^{(3)}.$$  \hspace{1cm} (26)

Here, $A = (a_{pj}) \in \text{Mat}(2d + 2, 2d + 2, \mathbb{Q}[x, y, r])$, $B = (b_{pj}) \in \text{Mat}(2d + 2, 2d + 2, \mathbb{Q}[x, y, r])$, $C = (c_{p, jk}) \in \text{Mat}(2d + 2, d(d + 1)/2, \mathbb{Q}[x, y, r])$, $E = (e_{p, jk}) \in \text{Mat}(2d + 2, m, \mathbb{Q}[x, y, r])$ and $A$ is invertible in the space of the matrices with entries in the field of rational functions $\mathbb{Q}(x, y, r)$. Explicit expressions of these matrices are given in (27), (28), (29), (30), (31), (32), (33), (34). Note that $A$, $B$, $C$, $E$ depend on the index $i$.

Notation: $c_{p, jk}$ means the element at the $p$-th row of $C$ and the column of $C$ standing for $\partial_j \partial_k = \partial_k \partial_j$. $e_{p, jk}$ is defined analogously.

**Proof** The both sides of (26) is a column vector of the length $2d + 2$. We will determine the rows of $A$, $B$, $C$, $E$ from generators of $I$. Note that the index $i$ is fixed over the proof.

**The first rows.** The first element of the vector $\partial_i F$ is $\partial_i$, then we have

$$a_{11} = 1, \quad b_{1,i+1} = 1$$ \hspace{1cm} (27)

and the other elements of the first rows of $A$, $B$, $C$, $E$ are 0.

**The $(j + 1)$-th rows** $(1 \leq j \leq d, i \neq j)$. Using the differential operator (7) in $I$, we have

$$x_{ij} \partial_i^2 + 2(x_{jj} - x_{ii}) \partial_i \partial_j + \sum_{k \neq i, j} x_{kj} \partial_i \partial_k \equiv x_{ij} \partial_j^2 + \sum_{k \neq i, j} x_{ik} \partial_j \partial_k + y_i \partial_j - y_j \partial_i.$$ 

Therefore, we may put as
\[ a_{j+1,i+1} = x_{ij}, \quad a_{j+1,j+1} = 2(x_{jj} - x_{ii}), \]
\[ a_{j+1,k+1} = x_{kj} \quad (1 \leq k \leq d+1, k \neq i, k \neq j), \]
\[ b_{j+1,j+1} = y_{i}, \quad b_{j+1,i+1} = -y_{j}, \quad b_{j+1,j+d+2} = x_{ij}, \]
\[ c_{j+1,jk} = x_{ik} \quad (1 \leq k \leq d+1, k \neq i, k \neq j). \]

(28)

Notation: when an index is out of bound, ignore the setting. For example, we set \( b_{j+1,j+d+2} = x_{ij} \) when \( j + d + 2 \leq 2d + 2 \). The other elements of the \((j+1)\)-th rows of \( A, B, C, E \) are 0.

The \((i+1)\)-th rows. The \((i+1)\)-th element of the vector \( \partial_i F \) is \( \partial_i^2 \). When \( i \leq d \), we put
\[ a_{i+1,i+1} = 1, \quad b_{i+1,i+d+2} = 1 \]
and the other elements of the \((i+1)\)-th rows are 0. When \( i = d+1 \), we consider the operator (6) in the ideal \( I \). Then, we have
\[ \partial_{d+1}^2 = r^2 - \sum_{k=1}^{d} \partial_k^2 \]
and hence we put
\[ a_{d+2,d+2} = 1, \quad b_{d+2,1} = r^2, \quad b_{d+2,k+d+2} = -1 \quad (1 \leq k \leq d). \]

(30)

The other elements of the \((i+1)\)-th rows of \( A, B, C, E \) are 0.

The \((d+2)\)-th rows. When \( i = d+1 \), it is reduced to the case of the \((i+1)\)-th rows. We assume that \( i \leq d \). Using the operators (7) and (6) in \( I \), we have
\[ x_{i,d+1} \partial_i^2 + 2(x_{d+1,d+1} - x_{ii}) \partial_i \partial_{d+1} + \sum_{k \neq i,d+1} x_{k,d+1} \partial_i \partial_k \equiv x_{i,d+1} \partial_{d+1}^2 + \sum_{k \neq i,d+1} x_{ik} \partial_{d+1} \partial_k + y_i \partial_{d+1} - y_{d+1} \partial_i \]
\[ \equiv x_{i,d+1} r^2 - \sum_{k=1}^{d} x_{i,d+1} \partial_k^2 + \sum_{k \neq i,d+1} x_{ik} \partial_{d+1} \partial_k + y_i \partial_{d+1} - y_{d+1} \partial_i. \]

Hence, we put
\[ a_{d+2,i+1} = x_{i,d+1}, \quad a_{d+2,d+2} = 2(x_{d+1,d+1} - x_{ii}), \]
\[ a_{d+2,k+1} = x_{k,d+1} \quad (1 \leq k \leq d, k \neq i), \]
\[ b_{d+2,1} = x_{i,d+1} r^2, \quad b_{d+2,d+2} = y_i, \quad b_{d+2,i+1} = -y_{d+1}, \]
\[ b_{d+2,l+d+2} = -x_{i,d+1}, \quad (1 \leq l \leq d), \]
\[ c_{d+2,k(d+1)} = x_{ik} \quad (1 \leq k \leq d, k \neq i). \]

(31)

The other elements of the \((d+2)\)-th rows of \( A, B, C, E \) are 0.
The \((j + d + 2)-th\) rows \((1 \leq j \leq d, i \neq j)\). Using the operator \((7)\) multiplied by \(\partial_j\) from the left hand side, we have

\[
-2(x_{jj} - x_{ii})\partial_i \partial_j^2 \equiv x_{ij} \partial_i^2 \partial_j - x_{ij} \partial_j^3 + \sum_{k \neq i,j} \left( x_{kj} \partial_i \partial_j \partial_k - x_{ik} \partial_j^2 \partial_k \right)
+ y_j \partial_i \partial_j - y_i \partial_j^2 + \partial_i.
\]

When \(i \leq d\), we put

\[
\begin{align*}
a_{j+d+2, j+d+2} &= -2(x_{jj} - x_{ii}), \\
b_{j+d+2, i+1} &= 1, \quad b_{j+d+2, j+d+2} = -y_i, \\
c_{j+d+2, ij} &= y_j, \\
e_{j+d+2, ijj} &= x_{ij}, \quad e_{j+d+2, jij} = -x_{ij}, \\
e_{j+d+2, ijk} &= x_{kj}, \quad e_{j+d+2, jkk} = -x_{ik} \quad (1 \leq k \leq d + 1, k \neq i, k \neq j).
\end{align*}
\]

The other elements in the \((j + d + 2)-th\) rows of \(A, B, C, E\) are 0.

When \(i = d + 1\), We use the operator \((6)\) and obtain

\[
-2(x_{jj} - x_{d+1,d+1})\partial_{d+1} \partial_j^2
\equiv x_{d+1, j} r^2 \partial_j - 2x_{d+1, j} \partial_j^3 + y_j \partial_{d+1} \partial_j - y_{d+1} \partial_j^2 + \partial_{d+1}
+ \sum_{k \neq d+1, j} \left( x_{kj} \partial_{d+1} \partial_j \partial_k - x_{d+1, k} \partial_j^2 \partial_k - x_{d+1, j} \partial_j \partial_k^2 \right).
\]

Therefore, we may put as

\[
\begin{align*}
a_{j+d+2, j+d+2} &= -2(x_{jj} - x_{d+1,d+1}), \\
b_{j+d+2, j+1} &= x_{d+1, j} r^2, \quad b_{j+d+2, j+d+2} = -y_{d+1}, \\
c_{j+d+2, j(d+1)} &= y_j, \\
e_{j+d+2, jjj} &= -2x_{ij}, \\
e_{j+d+2, ijk} &= x_{kj}, \quad e_{j+d+2, jkk} = -x_{ik}, \quad e_{j+d+2, jk} = -x_{ij} \quad (1 \leq k \leq d, k \neq j).
\end{align*}
\]

The other elements of the \((j + d + 2)-th\) rows of \(A, B, C, E\) are 0.

The \((i + d + 2)-th\) rows. We may assume that \(i \leq d\). Since the \((i + d + 2)-th\) element of the vector \(\partial_i F\) is \(\partial_i^3\), we put

\[
\begin{align*}
a_{i+d+2, i+d+2} &= 1, \quad e_{i+d+2, iii} = 1.
\end{align*}
\]

The other elements of the \((i + d + 2)-th\) rows of \(A, B, C, E\) are 0.

From Lemmas 1, 2, and 3, we have Theorem 1, which gives a differential equation satisfied by the normalizing constant with respect to the variable \(y_i\). As we remarked in Lemma 3, we note that \(A, B, C, E\) depend on the index \(i\) and we omit to denote the dependency.

\[\square\]
Proof of Theorem 1

\[ \partial_i F \equiv A^{-1}(BF + CF^{(2)} + EF^{(3)}) \] by Lemma 3

\[ \equiv A^{-1}\left(BF + CF^{(2)} - E(P^{(3)})^{-1}\left(Q^{(3)}F^{(2)} + R^{(3)}F\right)\right) \] by Lemma 2

\[ \equiv A^{-1}\left(BF - C(P^{(2)})^{-1}Q^{(2)}F - E(P^{(3)})^{-1}\left(-Q^{(3)}(P^{(2)})^{-1}Q^{(2)}F + R^{(3)}F\right)\right) \] by Lemma 1

\[ \equiv A^{-1}\left(B - C(P^{(2)})^{-1}Q^{(2)} + E(P^{(3)})^{-1}\left(Q^{(3)}(P^{(2)})^{-1}Q^{(2)} - R^{(3)}\right)\right)F. \]

\[ \Box \]

Example 4  In the case of \( d = 1 \) and for the \( y_1 \) direction, these matrices are as follows.

\[ F = (1 \partial_1 \partial_2 \partial_1^2)^T, \]

\[ F^{(2)} = (\partial_1 \partial_2), \]

\[ F^{(3)} = (\partial_1^3 \partial_1^2 \partial_1^2)^T, \]

\[ A = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & x_{12} & -2x_{11} + 2x_{22} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \]

\[ B = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ r^2x_{12} & -y_2 & y_1 & -x_{12} \end{pmatrix}, \]

\[ C = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}, \]

\[ E = \begin{pmatrix} 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 1 & 0 \end{pmatrix}, \]

\[ P^{(2)} = (-2x_{11} + 2x_{22}), \quad Q^{(2)} = (-r^2x_{12} y_2 - y_1 2x_{12}), \]

\[ P^{(3)} = \begin{pmatrix} 2x_{11} - 2x_{22} \\ 2x_{12} \\ -2x_{11} + 2x_{22} \end{pmatrix}, \quad Q^{(3)} = \begin{pmatrix} y_2 \\ -y_1 \end{pmatrix}, \]

\[ R^{(3)} = \begin{pmatrix} -r^2y_1 - 2r^2x_{11} + 2x_{22}r^2 + 1 -r^2x_{12} y_1 \\ 0 \end{pmatrix}. \]

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