Complementing Chentsov's characterization

Akio Fujiwara*
Department of Mathematics, Osaka University
Toyonaka, Osaka 560-0043, Japan

On the occasion of Professor Amari's 80th birthday.

Abstract

It is shown that Markov invariant tensor fields on the manifold of probability distributions are closed under the operations of raising and lowering indices with respect to the Fisher metric. As a result, every (r, s)-type Markov invariant tensor field can be obtained by raising indices of some $(0, r+s)$-type Markov invariant tensor field.

1 Introduction

In his seminal book [4], Chentsov characterized several covariant tensor fields on the manifold of probability distributions that fulfil certain invariance property, now referred to as the Markov invariance. Since Markov invariant $(0, 2)$- and $(0, 3)$-type tensor fields play essential roles in introducing a metric and affine connections on the manifold of probability distributions, Chentsov's theorem is regarded as one of the most fundamental achievements in information geometry [2].

Let, for each $n \in \mathbb{N}$,

$$\mathcal{S}_{n-1} := \left\{ p : \Omega_n \to \mathbb{R}_{++} \;\middle|\; \sum_{\omega \in \Omega_n} p(\omega) = 1 \right\}$$

be the manifold of probability distributions on a finite set $\Omega_n = \{1, 2, \ldots, n\}$, where $\mathbb{R}_{++}$ denotes the set of strictly positive real numbers. In what follows, each point $p \in \mathcal{S}_{n-1}$ is identified with the vector $(p(1), p(2), \ldots, p(n)) \in \mathbb{R}^n_{++}$.

Given natural numbers n and ℓ satisfying $2 \le n \le \ell$, let

$$\Omega_\ell = \bigsqcup_{i=1}^{n} C_{(i)} \tag{1}$$

be a direct sum decomposition of the index set $\Omega_\ell = \{1, \ldots, \ell\}$ into n mutually disjoint nonempty subsets $C_{(1)}, \ldots, C_{(n)}$. We put labels on elements of the ith subset $C_{(i)}$ as follows:

$$C_{(i)} = \{i_1, \ldots, i_{r_i}\},$$

*fujiwara@math.sci.osaka-u.ac.jp

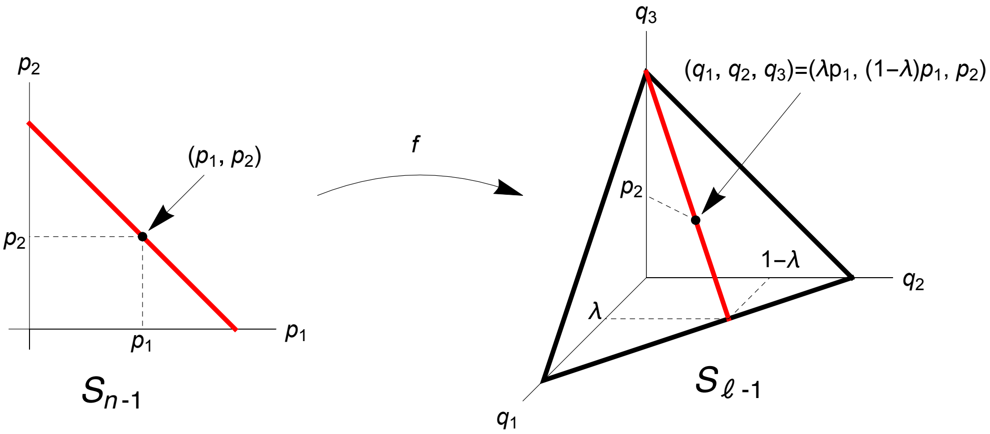

Figure 1: A Markov embedding $f : \mathcal{S}_{n-1} \to \mathcal{S}_{\ell-1}$ for $n = 2$ and $\ell = 3$ associated with the partition $\Omega_3 = C_{(1)} \sqcup C_{(2)}$, where $C_{(1)} = \{1, 2\}$ and $C_{(2)} = \{3\}$.

where r_i is the number of elements in $C_{(i)}$. A map

$$f : \mathcal{S}_{n-1} \longrightarrow \mathcal{S}_{\ell-1} : (p_1, \ldots, p_n) \longmapsto (q_1, \ldots, q_\ell)$$

is called a *Markov embedding* associated with the partition (1) if it takes the form

$$q_{i_s} := \lambda_{i_s} p_i \qquad \left(\lambda_{i_s} > 0, \ \sum_{s=1}^{r_i} \lambda_{i_s} = 1 \right) \tag{2}$$

for each $i = 1, \ldots, n$ and $s = 1, \ldots, r_i$. A simple example of a Markov embedding is illustrated in Figure 1, where $n = 2$ and $\ell = 3$.

A series $\{F^{[n]}\}_{n \in \mathbb{N}}$ of $(0, s)$-type tensor fields, each on $\mathcal{S}_{n-1}$, is said to be *Markov invariant* if

$$F_p^{[n]}(X_1, \ldots, X_s) = F_{f(p)}^{[\ell]}(f_* X_1, \ldots, f_* X_s)$$

holds for all Markov embeddings $f : \mathcal{S}_{n-1} \to \mathcal{S}_{\ell-1}$ with $2 \le n \le \ell$, points $p \in \mathcal{S}_{n-1}$, and tangent vectors $X_1, \ldots, X_s \in T_p \mathcal{S}_{n-1}$. When no confusion arises, we simply use an abridged notation F for $F^{[n]}$.

Now, the Chentsov theorem [4] (cf., [3, 5]) asserts that the only Markov invariant tensor fields of type $(0, s)$, with $s \in \{1, 2, 3\}$, on $\mathcal{S}_{n-1}$ are given, up to scaling, by

$$T_p(X) = E_p[(X \log p)] \ \ (= 0), \tag{3}$$

$$g_p(X, Y) = E_p[(X \log p)(Y \log p)], \tag{4}$$

$$S_p(X, Y, Z) = E_p[(X \log p)(Y \log p)(Z \log p)], \tag{5}$$

where $p \in \mathcal{S}_{n-1}$, and $E_p[\,\cdot\,]$ denotes the expectation with respect to p. In particular, the $(0, 2)$-type tensor field g is nothing but the Fisher metric, and the $(0, 3)$-type tensor field S yields the α-connection $\nabla^{(\alpha)}$ through the relation

$$g(\nabla_X^{(\alpha)} Y, Z) := g(\overline{\nabla}_X Y, Z) - \frac{\alpha}{2} S(X, Y, Z),$$

where $\overline{\nabla}$ is the Levi-Civita connection with respect to the Fisher metric g. Chentsov's theorem is thus a cornerstone of information geometry.

Despite this fact, it is curious that the above-mentioned formulation only concerns characterization of covariant tensor fields. Put differently, discussing the Markov invariance of contravariant and/or mixed-type tensor fields is beyond the scope. To the best of the author's knowledge, however, there have been no attempts toward such generalization. The objective of the present paper is to extend Chentsov's characterization to generic tensor fields.

2 Main results

Associated with each Markov embedding $f : \mathcal{S}_{n-1} \to \mathcal{S}_{\ell-1}$ is a unique affine map

$$\varphi_f : \mathcal{S}_{\ell-1} \longrightarrow \mathcal{S}_{n-1} : (q_1, \dots, q_\ell) \longmapsto (p_1, \dots, p_n)$$

that satisfies

$$\varphi_f \circ f = \mathrm{id}.$$

In fact, it is explicitly given by the following relations

$$p_i = \sum_{j \in C_{(i)}} q_j \qquad (i = 1, \dots, n)$$

that allocate each event $C_{(i)}\,(\subset \Omega_\ell)$ to the singleton $\{i\}\,(\subset \Omega_n)$, (cf., Appendix A). We shall call the map φ_f the *coarse-graining* associated with a Markov embedding f. Note that the coarse-graining φ_f is determined only by the partition (1), and is independent of the internal ratios $\{\lambda_{i_s}\}_{i,s}$ that specifies f as (2).

For example, let us consider a Markov embedding

$$f : \mathcal{S}_1 \longrightarrow \mathcal{S}_3 : (p_1, p_2) \longmapsto (\lambda p_1, (1-\lambda) p_1, \mu p_2, (1-\mu) p_2), \qquad (0 < \lambda, \mu < 1)$$

associated with the partition $\Omega_4 = C_{(1)} \sqcup C_{(2)}$, where

$$C_{(1)} = \{1, 2\}, \quad C_{(2)} = \{3, 4\}.$$

The coarse-graining $\varphi_f : \mathcal{S}_3 \to \mathcal{S}_1$ associated with f is given by

$$\varphi_f : (q_1, q_2, q_3, q_4) \longmapsto (q_1 + q_2, q_3 + q_4).$$

There are of course other affine maps $\overline{\varphi}_f : \mathcal{S}_3 \to \mathbb{R}^2_{++}$ that satisfy the relation $\overline{\varphi}_f \circ f = \mathrm{id}$ on $\mathcal{S}_1$: for example,

$$\overline{\varphi}_f : (q_1, q_2, q_3, q_4) \longmapsto \left(\frac{q_1}{\lambda}, \frac{q_3}{\mu} \right).$$

However, this is not a map of the form $\varphi_f : \mathcal{S}_3 \to \mathcal{S}_1$.

Now we introduce a generalized Markov invariance. A series $\{F^{[n]}\}_{n\in\mathbb{N}}$ of (r,s)-type tensor fields, each on $\mathcal{S}_{n-1}$, is said to be *Markov invariant* if

$$F_p^{[n]}(\omega^1,\dots,\omega^r,X_1,\dots,X_s)=F_{f(p)}^{[\ell]}(\varphi_f^*\omega^1,\dots,\varphi_f^*\omega^r,f_*X_1,\dots,f_*X_s)$$

holds for all Markov embeddings $f:\mathcal{S}_{n-1}\to\mathcal{S}_{\ell-1}$ with $2\le n\le\ell$, points $p\in\mathcal{S}_{n-1}$, cotangent vectors $\omega^1,\dots,\omega^r\in T_p^*\mathcal{S}_{n-1}$, and tangent vectors $X_1,\dots,X_s\in T_p\mathcal{S}_{n-1}$. When no confusion arises, we simply use an abridged notation F for $F^{[n]}$.

The main result of the present paper is the following.

Theorem 1. *Markov invariant tensor fields are closed under the operations of raising and lowering indices with respect to the Fisher metric g.*

Theorem 1 has a remarkable consequence: every (r,s)-type Markov invariant tensor field can be obtained by raising indices of some $(0,r+s)$-type Markov invariant tensor field. This fact could be paraphrased by saying that Chentsov's original approach was universal.

3 Proof of Theorem 1

We first prove that raising indices with respect to the Fisher metric preserves Markov invariance, and then prove that lowering indices also preserves Markov invariance.

3.1 Raising indices preserves Markov invariance

Suppose we want to know whether the $(1,2)$-type tensor field $F^i{}_{jk}:=g^{im}S_{mjk}$ is Markov invariant, where S is the Markov invariant $(0,3)$-type tensor field defined by (5). Put differently, we want to investigate if, for some (then any) local coordinate system (x^a) of $\mathcal{S}_{n-1}$, the $(1,2)$-type tensor field F defined by $F\left(dx^a,\dfrac{\partial}{\partial x^b},\dfrac{\partial}{\partial x^c}\right):=g^{ae}S_{ebc}$ exhibits

$$F_p\left(dx^a,\frac{\partial}{\partial x^b},\frac{\partial}{\partial x^c}\right)=F_{f(p)}\left(\varphi_f^*dx^a,f_*\frac{\partial}{\partial x^b},f_*\frac{\partial}{\partial x^c}\right). \tag{6}$$

In order to handle such a relation, it is useful to identify the Fisher metric g on the manifold $\mathcal{S}_{n-1}$ and its inverse g^{-1} with the following linear maps:

$$g\ :\ T\mathcal{S}_{n-1}\longrightarrow T^*\mathcal{S}_{n-1}:\ \frac{\partial}{\partial x^a}\longmapsto g_{ab}\,dx^b,$$
$$g^{-1}\ :\ T^*\mathcal{S}_{n-1}\longrightarrow T\mathcal{S}_{n-1}:\ dx^a\longmapsto g^{ab}\frac{\partial}{\partial x^b}.$$

Note that these maps do not depend on the choice of a local coordinate system (x^a) of $\mathcal{S}_{n-1}$.

Now, observe that

$$\begin{aligned}\text{LHS of (6)}\quad &=\quad S_p\circ(g_p^{-1}\otimes I\otimes I)\left(dx^a,\frac{\partial}{\partial x^b},\frac{\partial}{\partial x^c}\right)\\ &=\quad S_p\left(g_p^{ae}\frac{\partial}{\partial x^e},\frac{\partial}{\partial x^b},\frac{\partial}{\partial x^c}\right)\end{aligned}$$

and

$$\begin{aligned}
\text{RHS of (6)} &= S_{f(p)} \circ (g^{-1}_{f(p)} \otimes I \otimes I) \left(\varphi_f^* dx^a, f_* \frac{\partial}{\partial x^b}, f_* \frac{\partial}{\partial x^c} \right) \\
&= S_{f(p)} \left(g^{-1}_{f(p)} (\varphi_f^* dx^a), f_* \frac{\partial}{\partial x^b}, f_* \frac{\partial}{\partial x^c} \right).
\end{aligned}$$

Since the $(0,3)$-type tensor field S is Markov invariant, the following Lemma establishes (6).

Lemma 2. *For any Markov embedding $f : \mathcal{S}_{n-1} \to \mathcal{S}_{\ell-1}$, it holds that*

$$f_* \left(g_p^{ae} \frac{\partial}{\partial x^e} \right) = g^{-1}_{f(p)} (\varphi_f^* dx^a). \tag{7}$$

In other words, the diagram

$$\begin{array}{ccc}
T_p^* \mathcal{S}_{n-1} & \xrightarrow{\varphi_f^*} & T^*_{f(p)} \mathcal{S}_{\ell-1} \\
{\scriptstyle g^{-1}} \downarrow & & {\scriptstyle g^{-1}} \downarrow \\
T_p \mathcal{S}_{n-1} & \xrightarrow{f_*} & T_{f(p)} \mathcal{S}_{\ell-1}
\end{array}$$

is commutative.

Proof. In view of a smooth link with the expression (2) of a Markov embedding, we make use of the $\nabla^{(m)}$-affine coordinate system

$$\hat{\eta}_i := p_i \qquad (i = 1, \dots, n-1)$$

as a coordinate system of $\mathcal{S}_{n-1}$, and the $\nabla^{(m)}$-affine coordinate system

$$\eta_{i_s} := q_{i_s} \qquad (i = 1, \dots, n-1;\ s = 1, \dots, r_i \ \text{ and } \ i = n;\ s = 1, \dots, r_n - 1)$$

as a coordinate system of $\mathcal{S}_{\ell-1}$, given a Markov embedding $f : \mathcal{S}_{n-1} \to \mathcal{S}_{\ell-1}$. Note that the component $q_{n_{r_n}}$ that corresponds to the last element n_{r_n} of $C_{(n)}$ is excluded in this coordinate system because of the normalisation.

We shall prove (7) by showing the identity

$$\hat{h}_{im} \, f_* \frac{\partial}{\partial \hat{\eta}_m} = g^{-1}_{f(p)} (\varphi_f^* d\hat{\eta}_i), \tag{8}$$

where $\hat{h}_{im} := h_p(d\hat{\eta}_i, d\hat{\eta}_m)$, with h being the $(2,0)$-type tensor field defined by

$$h(dx^a, dx^b) := g^{ab}.$$

Note that, due to the duality of the η- and θ-coordinate systems, $\hat{h}_{im}$ is identical to the component $\hat{g}_{im}$ of the Fisher metric g with respect to the θ-coordinate system $(\hat{\theta}^i)$ of $\mathcal{S}_{n-1}$, and is explicitly given by

$$\hat{g}_{im} = \hat{\eta}_i \delta_{im} - \hat{\eta}_i \hat{\eta}_m.$$

Similarly, the components of h with respect to the η-coordinate system (η_j) of $\mathcal{S}_{\ell-1}$ is simply denoted by $h_{ij} := h_{f(p)}(d\eta_i, d\eta_j)$, and is identical to $g_{ij} = \eta_i\delta_{ij} - \eta_i\eta_j$.

Due to the choice of the coordinate systems $(\hat{\eta}_i)_i$ and $(\eta_{i_s})_{i,s}$, we have

$$\hat{\eta}_i = \sum_{j\in C_{(i)}} \eta_j = \sum_{s=1}^{r_i} \eta_{i_s} \qquad (i = 1, \ldots, n-1),$$

so that

$$\varphi_f^* d\hat{\eta}_i = \sum_j \frac{\partial \hat{\eta}_i}{\partial \eta_j}\, d\eta_j = \sum_{s=1}^{r_i} d\eta_{i_s}.$$

Thus

$$\text{RHS of (8)} = g_{f(p)}^{-1}\left(\sum_{s=1}^{r_i} d\eta_{i_s}\right) = \sum_{s=1}^{r_i}\left(\sum_j h_{i_s,j}\frac{\partial}{\partial \eta_j}\right). \tag{9}$$

On the other hand, since

$$\begin{cases} \eta_{i_s} = \lambda_{i_s}\hat{\eta}_i & (i = 1, \ldots, n-1;\ s = 1, \ldots, r_i) \\ \eta_{n_s} = \lambda_{n_s}\left(1 - \displaystyle\sum_{i=1}^{n-1}\hat{\eta}_i\right) & (s = 1, \ldots, r_n - 1) \end{cases},$$

we see that, for each $m = 1, \ldots, n-1$,

$$\begin{aligned} f_*\frac{\partial}{\partial \hat{\eta}_m} &= \sum_{i=1}^{n-1}\sum_{s=1}^{r_i}\frac{\partial \eta_{i_s}}{\partial \hat{\eta}_m}\frac{\partial}{\partial \eta_{i_s}} + \sum_{s=1}^{r_n-1}\frac{\partial \eta_{n_s}}{\partial \hat{\eta}_m}\frac{\partial}{\partial \eta_{n_s}} \\ &= \sum_{s=1}^{r_m}\lambda_{m_s}\frac{\partial}{\partial \eta_{m_s}} - \sum_{s=1}^{r_n-1}\lambda_{n_s}\frac{\partial}{\partial \eta_{n_s}}. \end{aligned}$$

Consequently,

$$\text{LHS of (8)} = \sum_{m=1}^{n-1}\hat{h}_{im}\sum_{s=1}^{r_m}\lambda_{m_s}\frac{\partial}{\partial \eta_{m_s}} - \left(\sum_{m=1}^{n-1}\hat{h}_{im}\right)\left(\sum_{s=1}^{r_n-1}\lambda_{n_s}\frac{\partial}{\partial \eta_{n_s}}\right). \tag{10}$$

To prove (8), let us compare, for each j, the coefficients of $\dfrac{\partial}{\partial \eta_j}$ in (9) and (10). The index j runs through

$$\left(\bigsqcup_{k=1}^{n-1} C_{(k)}\right) \sqcup \{n_s\}_{s=1}^{r_n-1}.$$

So suppose that $j = k_u$, the uth element of $C_{(k)}$, where $1 \le k \le n$. Then

$$\text{coefficient of } \frac{\partial}{\partial \eta_{k_u}} \text{ in (9)} = \sum_{s=1}^{r_i} h_{i_s,k_u}. \tag{11}$$

On the other hand,

$$\text{coefficient of } \frac{\partial}{\partial \eta_{k_u}} \text{ in (10)} = \begin{cases} \hat{h}_{ik}\lambda_{k_u} & (1 \le k \le n-1) \\ -\left(\displaystyle\sum_{m=1}^{n-1}\hat{h}_{im}\right)\lambda_{n_u} & (k = n) \end{cases}. \tag{12}$$

We show that (11) equals (12) for all indices i, k, and u.

When $1 \le k \le n-1$,

$$\begin{aligned}(11) &= \sum_{s=1}^{r_i} (\eta_{i_s} \delta_{i_s,k_u} - \eta_{i_s} \eta_{k_u}) \\ &= \delta_{ik} \eta_{k_u} - \hat{\eta}_i \eta_{k_u} \\ &= \lambda_{k_u} (\delta_{ik} \hat{\eta}_k - \hat{\eta}_i \hat{\eta}_k) \\ &= (12).\end{aligned}$$

When $k = n$, on the other hand,

$$\begin{aligned}(11) &= \sum_{s=1}^{r_i} (-\eta_{i_s} \eta_{n_u}) \\ &= -\hat{\eta}_i \, \lambda_{n_u} \left(1 - \sum_{m=1}^{n-1} \hat{\eta}_m \right) \\ &= -\lambda_{n_u} \sum_{m=1}^{n-1} (\hat{\eta}_i \delta_{im} - \hat{\eta}_i \hat{\eta}_m) \\ &= (12).\end{aligned}$$

This proves the identity (8). □

Now that Lemma 2 is established, a repeated use of the line of argument that precedes Lemma 2 leads us to the following general assertion: raising indices with respect to the Fisher metric preserves Markov invariance.

3.2 Lowering indices preserves Markov invariance

Suppose that, given a Markov invariant $(3,0)$-type tensor field T, we want to know whether the $(2,1)$-type tensor field F defined by

$$F\left(\frac{\partial}{\partial x^a}, dx^b, dx^c \right) := g_{ae} T^{ebc}$$

satisfies Markov invariance:

$$F_p \left(\frac{\partial}{\partial x^a}, dx^b, dx^c \right) = F_{f(p)} \left(f_* \frac{\partial}{\partial x^a}, \varphi_f^* dx^b, \varphi_f^* dx^c \right)$$

or equivalently

$$T_p \left(g_{ae} dx^e, dx^b, dx^c \right) = T_{f(p)} \left(g_{f(p)} \left(f_* \frac{\partial}{\partial x^a} \right), \varphi_f^* dx^b, \varphi_f^* dx^c \right).$$

This question is resolved affirmatively by the following

Lemma 3. *For any Markov embedding $f : \mathcal{S}_{n-1} \to \mathcal{S}_{\ell-1}$, it holds that*

$$\varphi_f^* \left((g_p)_{ae} \, dx^e \right) = g_{f(p)} \left(f_* \frac{\partial}{\partial x^a} \right).$$

In other words, the diagram

$$\begin{array}{ccc} T_p^*\mathcal{S}_{n-1} & \xrightarrow{\varphi_f^*} & T_{f(p)}^*\mathcal{S}_{\ell-1} \\ g\big\uparrow & & g\big\uparrow \\ T_p\mathcal{S}_{n-1} & \xrightarrow{f_*} & T_{f(p)}\mathcal{S}_{\ell-1} \end{array}$$

is commutative.

Proof. Since g is an isomorphism, this is a straightforward consequence of Lemma 2. □

Lemma 3 has the following implication: lowering indices with respect to the Fisher metric preserves Markov invariance.

Theorem 1 is now an immediate consequence of Lemmas 2 and 3.

4 Concluding remarks

We have proved that raising and lowering indices with respect to the Fisher metric preserve Markov invariance of tensor fields on the manifold of probability distributions. For example, g^{ij} is, up to scaling, the only $(2,0)$-type Markov invariant tensor field. It may be worthwhile to mention that not every operation in tensor calculus preserves Markov invariance. The following example is due to Amari [1].

With the $\nabla^{(e)}$-affine coordinate system $\theta = (\theta^1, \dots, \theta^{n-1})$ of $\mathcal{S}_{n-1}$ defined by

$$\log p(\omega) = \sum_{i=1}^{n-1} \theta^i \delta_i(\omega) - \log\left(1 + \sum_{k=1}^{n-1} \exp\theta^k\right),$$

the $(0,3)$-type tensor field (5) has the following components:

$$S_{ijk} = \begin{cases} \eta_i(1-\eta_i)(1-2\eta_i), & (i=j=k) \\ -\eta_i(1-2\eta_i)\eta_k, & (i=j\neq k) \\ -\eta_j(1-2\eta_j)\eta_i, & (j=k\neq i) \\ -\eta_k(1-2\eta_k)\eta_j, & (k=i\neq j) \\ 2\eta_i\eta_j\eta_k, & (i\neq j\neq k\neq i) \end{cases}.$$

Here, $\eta = (\eta_1, \dots, \eta_{n-1})$ is the $\nabla^{(m)}$-affine coordinate system of $\mathcal{S}_{n-1}$ that is dual to θ. By using the formula

$$g^{ij} = \frac{1}{\eta_0} + \frac{\delta^{ij}}{\eta_i}, \qquad \left(\eta_0 := 1 - \sum_{i=1}^{n-1}\eta_i\right),$$

the $(1,2)$-type tensor field $F^i{}_{jk} := g^{im}S_{mjk}$ is readily calculated as

$$F^i{}_{jk} = \begin{cases} 1-2\eta_i, & (i=j=k) \\ -\eta_k, & (i=j\neq k) \\ -\eta_j, & (i=k\neq j) \\ 0, & (i\neq j,\ i\neq k) \end{cases}.$$

We know from Theorem 1 that F is Markov invariant. However, the following contracted $(0,1)$-type tensor field

$$\tilde{T}_k := F^i{}_{ik} = 1 - n\eta_k$$

is non-zero, and hence is not Markov invariant; see (3). This demonstrates that the contraction, which is a standard operation in tensor calculus, does not always preserve Markov invariance.

Chentsov's idea of imposing the invariance of geometrical structures under Markov embeddings $f : \mathcal{S}_{n-1} \to \mathcal{S}_{\ell-1}$ is based on the fact that $\mathcal{S}_{n-1}$ is statistically isomorphic to $f(\mathcal{S}_{n-1})$. Put differently, the invariance only involves direct comparison between $\mathcal{S}_{n-1}$ and its image $f(\mathcal{S}_{n-1})$, and is nothing to do with the complement of $f(\mathcal{S}_{n-1})$ in the ambient space $\mathcal{S}_{\ell-1}$. On the other hand, the partial trace operation $F^i{}_{jk} \mapsto F^i{}_{ik}$ on $\mathcal{S}_{\ell-1}$ (more precisely, on $T_{f(p)}\mathcal{S}_{\ell-1} \otimes T^*_{f(p)}\mathcal{S}_{\ell-1}$) makes the output $F^i{}_{ik}$ "contaminated" with information from outside the submanifold $f(\mathcal{S}_{n-1})$. It is thus no wonder such an influx of extra information manifests itself as the non-preservation of Markov invariance. In this respect, a distinctive characteristic of Lemmas 2 and 3 lies in the fact that raising and lowering indices preserve Markov invariance although they are represented in the forms of contraction such as $g^{i\ell}S_{mjk} \mapsto g^{im}S_{mjk}$ or $g_{i\ell}T^{mjk} \mapsto g_{im}T^{mjk}$.

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Appendix

A Uniqueness of φ_f

A Markov embedding $f : \mathcal{S}_{n-1} \to \mathcal{S}_{\ell-1}$ defined by (1) and (2) uniquely extends to a linear map $\tilde{f} : \mathbb{R}^n \to \mathbb{R}^\ell : (x_1, \dots, x_n) \mapsto (y_1, \dots, y_\ell)$ as

$$y_{i_s} := \lambda_{i_s} x_i \qquad \left(\lambda_{i_s} > 0,\ \sum_{s=1}^{r_i} \lambda_{i_s} = 1 \right).$$

Similarly, let $\tilde{\varphi}_f : \mathbb{R}^\ell \to \mathbb{R}^n$ be the unique linear extension of $\varphi_f : \mathcal{S}_{\ell-1} \to \mathcal{S}_{n-1}$.

Since

$$\left(\sum_{k=1}^{\ell} (\tilde{\varphi}_f)_{ik}\, q_k \right)_{i=1,\dots,n} \in \mathcal{S}_{n-1} \tag{13}$$

for all $q = (q_1, \ldots, q_\ell) \in \mathcal{S}_{\ell-1}$, we see that the matrix elements of $\tilde{\varphi}_f$ are nonnegative:

$$(\tilde{\varphi}_f)_{ik} \geq 0 \qquad (\forall i = 1, \ldots, n;\ \forall k = 1, \ldots, \ell). \tag{14}$$

The relation (13) also entails that, for all $q \in \mathcal{S}_{\ell-1}$,

$$\sum_{k=1}^{\ell} q_k = 1 = \sum_{i=1}^{n} \left(\sum_{k=1}^{\ell} (\tilde{\varphi}_f)_{ik}\, q_k \right),$$

so that

$$\sum_{k=1}^{\ell} \left(\sum_{i=1}^{n} (\tilde{\varphi}_f)_{ik} - 1 \right) q_k = 0.$$

Consequently,

$$\sum_{i=1}^{n} (\tilde{\varphi}_f)_{ik} = 1 \qquad (\forall k = 1, \ldots, \ell). \tag{15}$$

It then follows from (14) and (15) that

$$0 \leq (\tilde{\varphi}_f)_{ik} \leq 1 \qquad (\forall i = 1, \ldots, n;\ \forall k = 1, \ldots, \ell). \tag{16}$$

Now, since $\tilde{\varphi}_f$ is a left inverse of $\tilde{f}$,

$$\delta_{ij} = \sum_{k=1}^{\ell} (\tilde{\varphi}_f)_{ik} \left(\tilde{f}\right)_{kj} = \sum_{k \in C_{(j)}} (\tilde{\varphi}_f)_{ik}\, \lambda_k = \sum_{s=1}^{r_j} (\tilde{\varphi}_f)_{i,j_s}\, \lambda_{j_s}.$$

Because of (16), we have

$$(\tilde{\varphi}_f)_{i,j_s} = \delta_{ij} \qquad (\forall s = 1, \ldots, r_j).$$

This proves that φ_f is unique and is given by the coarse-graining associated with f.

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