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# A mathematical modeling of *n*-state systems

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ABSTRACT

In this paper, we assign a Riemannian manifold to *n*-state systems by using a canonical ensemble in equilibrium statistical mechanics. We consider discrete states with equal intervals, i.e., we assume equal energy intervals between the states of non-interacting particles. Since there are many important quantities on a Riemannian manifold, we may define them for *n*-state systems. We define a distance between different equilibrium statistical states of an *n*-state system. We also give a lower bound for the mean square error of an unbiased estimator for the temperature of an *n*-state system.

## 1. Introduction

Equilibrium statistical mechanics aims to elucidate the physical macroscopic properties (such as number of particles $N$, volume $V$ or energy $E$) of a system from the microscopic properties of matter by employing physics theories at classical mechanics, electromagnetism, quantum mechanics, or relativity in a probabilistic framework [1].

A particular microscopic configuration specifies a microstate with a certain probability, and a macroscopic state is associated with a large number of microstates. The possible microstates of a system are known as the ensemble of states. Depending on the system's thermodynamic condition, there are different ensembles to obtain equilibrium properties of the system. The microcanonical ensemble has an equal probability for each microstate which clarifies a set of microstates with the same macrostate energy. The canonical ensemble is specified by a set of microstates with the same number of particles and volume. In this condition, the system is in contact with a heat bath and can exchange its energy. The grand canonical ensemble is related to an open system that can exchange energy and particles with its environment. It is in fact a canonical subensemble with different particle numbers [2]. One may also see [3,4] to study the quantum mechanical canonical ensemble.

To study chemo-physical phenomena with mathematical models, one can employ some tools of different branches of mathematics [5–7]. Theory of dynamical systems [8], catastrophe theory [9], Shannon information theory [10,11], Fisher information theory [12,13], graph theory [14,15] and geometry [16,17] are some branches of mathematics that are applied to modelize chemi-physical phenomena.

The study of differential geometry in statistical mechanics and thermodynamics began with the seminal works of [18,19]. Since then, numerous papers have explored the connection between geometric structure and critical phenomena in these models. Building on techniques from [20], Tsallis [21] pioneered the study of deformed canonical ensembles. Further details can be found in the book [22].

Here we attempt to apply information geometry techniques in modeling *n*-state systems [20]. We assign a Riemannian manifold to any *n*-state system and develop the necessary mathematical tools and concepts. To this end, we define a typical distance between

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two equilibrium temperatures of $n$-state systems using the Riemannian metric on the corresponding manifold. We have also specified a lower bound for the error estimation of the equilibrium temperature in $n$-state systems. This investigation can develop connections between geometry and information theory.

In Section 2, we review $n$-state systems using statistical mechanics. In Section 3, statistical manifolds are introduced. In Section 4, we assign a Riemannian manifold to an $n$-state system. In Section 5, we give an uncertainty inequality by presenting a lower bound for the error estimation of the equilibrium temperature. Section 6 is a summary and discussion.

## 2. $n$-state systems and Boltzmann distribution

In this section, we review an $n$-state system using the canonical ensemble approach. One should note that, there are some useful articles addressing a similar problem. In [23], the information geometry of the quantum mechanic oscillator is studied. However, that study is done in the continuous approximation while the current manuscript is in a discrete energy space. The difficulties in creating a temperature estimator are studied in [24]. However, unlike our current manuscript, [24] assumes a distribution for $T$.

The probability of finding the system in a microstate $k$ with energy $\epsilon_k$ in thermal equilibrium with the environment is given by

$$p_k = \frac{e^{-\beta\epsilon_k}}{Z}, \tag{2.1}$$

where $\beta = 1/k_B T$, $T$ is the temperature and $k_B$ is the Boltzmann constant. Also, $e^{-\beta\epsilon_k}$ is called a Boltzmann factor. Since $p_k$ has a normal probability distribution, then

$$Z = \sum_k e^{-\beta\epsilon_k} \tag{2.2}$$

is known as the partition function. For an $n$-state system with equal energy intervals between the states of non-interacting particles, the partition function is given by

$$\begin{aligned} Z &= \sum_{k=1}^{n} e^{-(k-1)\beta\Delta} \\ &= 1 + e^{-\beta\Delta} + e^{-2\beta\Delta} + \cdots + e^{-(n-1)\beta\Delta} \end{aligned}, \tag{2.3}$$

where $\epsilon_1 = 0$ and $\epsilon_k - \epsilon_{k-1} = \Delta$ $(k = 2, 3, \ldots, n)$. For $\beta\Delta \ll 1$ and using the sum of the first $n$ terms of a geometric series, we can obtain the partition function as

$$Z = \frac{1 - e^{-n\beta\Delta}}{1 - e^{-\beta\Delta}}. \tag{2.4}$$

We can consider the $n$-state system for a variety of physical problems, such as the binary states with two-level states ($n = 2$) and the infinity-level states for the ideal quantum harmonic oscillators [25].

## 3. Statistical manifold

Let $S = \{p_\xi\}_{\xi\in\Theta}$ be a family of probability distributions on $\Omega = \{x_1, x_2, \ldots, x_n\}$. In other words, for any $\xi \in \Theta$, $p_\xi : \Omega \to [0, 1]$ is a probability distribution function and

$$S = \{p_\xi = p(x, \xi) : \quad \xi = (\xi_1, \xi_2, \ldots, \xi_m) \in \Theta\}.$$

Note that, the mapping $\xi \longmapsto p_\xi$ is an injection. It is also assumed that $p_\xi$ $(\xi = (\xi_1, \xi_2, \ldots, \xi_m))$ is smooth with respect to the components $\xi_i$ $(i = 1, 2, \ldots, m)$, i.e., the function $\xi \longmapsto p_\xi$ is $C^\infty$. Let also $\Theta \subset \mathbb{R}^m$ be an open set. So, all the terms of the form $\frac{\partial p_\xi}{\partial \xi_i}$ and $\frac{\partial^2 p_\xi}{\partial \xi_i \partial \xi_j}$ are well-defined on $\Theta$ and we have

$$\sum_{l=1}^{n} \frac{\partial p_\xi}{\partial \xi_i}(x_l) = \frac{\partial}{\partial \xi_i} \sum_{i=1}^{n} p_\xi(x_l) = \frac{\partial}{\partial \xi_i}(1) = 0.$$

The mapping $\phi : S \to \mathbb{R}^m$ defined by $\phi(p_\xi) = \xi$ gives a coordinate system $\phi = [\xi_i]$ on $S$ which makes it a manifold with one single local chart. On the other hand, if $\psi : \Theta \to \psi(\Theta) \subset \mathbb{R}^m$ is another $C^\infty$-diffeomorphism, then $\eta = \psi(\xi)$ is another coordinate system for $S$, and indeed $S = \{p_{\psi^{-1}(\eta)}\}_{\eta\in\psi(\Theta)}$. Based on the previous discussions, $S$ is a $C^\infty$-manifold, where each parameterization of $S$ is indeed a coordinate system. $S$ is called a *statistical manifold* as shown in Fig. 1. Now, a Riemannian metric is defined on $S = \{p_\xi\}_\xi$, using the Fisher information matrix $G(\xi) = [g_{ij}(\xi)]_{m\times m}$ $(\xi \in \Theta)$ with

$$g_{ij}(\xi) = \sum_{l=1}^{n} p_\xi(x_l) \frac{\partial l}{\partial \xi_i}(x_l) \frac{\partial l}{\partial \xi_j}(x_l), \tag{3.1}$$

where $l = l_\xi(x) = \log p_\xi(x)$ [20].

The functions $g_{ij} : \Theta \to \mathbb{R}$ are $C^\infty$. Note that, using the correspondence $\xi \longmapsto p_\xi$, each $g_{ij}$ may be considered as a function defined on $S$. We have:

1. $G(\xi)$ is a symmetric matrix, since

$$\forall \xi \in \Theta \quad g_{ij}(\xi) = g_{ji}(\xi) \quad (i, j = 1, 2, \ldots, m).$$

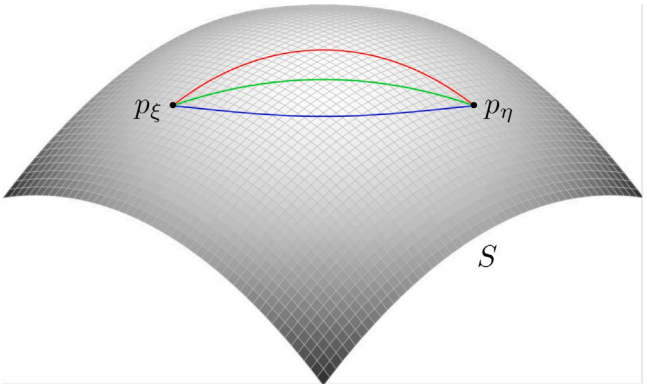



**Fig. 1.** A schematic of statistical manifold and curves between two points on it.

2. $G(\xi)$ is semi positive-definite, since, for every given $V = (v_1, v_2, \dots, v_m)^t$ we have:

$$V^t G(\xi) V = \sum_{i,j} v_i v_j g_{ij}(\xi) = \sum_{l=1}^{n} \left( \sum_{i=1}^{m} v_i \frac{\partial l}{\partial \xi_i}(x_l) \right)^2 \geq 0.$$

Now, the inner product $< \cdot, \cdot >$ on the tangent space $TS$ is defined as follows:

$$g_{ij} =< \partial_i, \partial_j >, \tag{3.2}$$

where $\partial_i = \frac{\partial}{\partial \xi_i}$. Clearly, the Riemannian metric $g =< \cdot, \cdot >$ is uniquely determined by (3.2). So, the pair $(S, g)$ is a Riemannian manifold corresponding to the family of distributions $S$. One may see a comprehensive discussion on statistical manifolds in [20]. In the following, we review some classical concepts which may be used in the sequel.

### 3.1. Fisher distance

Let $S = \{p_\xi\}_{\xi \in \Theta}$ be a statistical manifold. For any $C^1$-curve $\gamma : [0, 1] \to S$, the length of $\gamma$ is given by

$$L(\gamma) := \int_0^1 \sqrt{\sum_{i,j} g_{ij} \dot{\gamma}_i \dot{\gamma}_j} dt. \tag{3.3}$$

Let $\xi, \eta \in \Theta$. The set of all $C^1$-curves $\gamma : [0, 1] \to S$ with $\gamma(0) = p_\xi$ and $\gamma(1) = p_\eta$ is denoted by $\Delta_{\xi\eta}$. The Fisher distance between $\xi$ and $\eta$ is defined by

$$d_F(\xi, \eta) := \inf\{L(\gamma) : \gamma \in \Delta_{\xi\eta}\}. \tag{3.4}$$

Clearly $d_F : \Theta \times \Theta \to [0, +\infty)$ induces a metric on $S$, i.e.,

1. $d_F(\xi, \eta) \geq 0$ for all $\xi, \eta \in \Theta$, and $d_F(\xi, \eta) = 0$ if and only if $\xi = \eta$.
2. $d_F(\xi, \eta) = d_F(\eta, \xi)$ for all $\xi, \eta \in \Theta$.
3. $d_F(\xi, \eta) \leq d_F(\xi, \zeta) + d_F(\zeta, \eta)$ for all $\xi, \eta, \zeta \in \Theta$.

Formula (3.4) is not suitable for practical and computational aspects, since the infimum is taken over an infinite (even more on an uncountable) set. To resolve this difficulty, we need to have some suitable connection on $S$.

### 3.2. Christoffel symbols and connections

Let $S = \{p_\xi\}_{\xi \in \Theta}$ be a statistical manifold. For $\xi \in \Theta$, let $l_\xi := \log p_\xi$. The functions $\Gamma_{ij,k} : \Theta \to \mathbb{R}$ defined by

$$\left(\Gamma_{ij,k}\right)_\xi := \sum_{l=1}^{n} p_\xi(x_l) \partial_k l_\xi(x_l) \left( \partial_i \partial_j l_\xi(x_l) + \frac{1}{2} \partial_i l_\xi(x_l) \partial_j l_\xi(x_l) \right)$$

are called the Christoffel symbols of first kind of the statistical manifold $S$. Now, the connection $\nabla$ on $S$ is defined as follows:

$$< \nabla^{\partial_i}_{\partial_j}, \partial_k >:= \Gamma_{ij,k},$$

where $g =< \cdot, \cdot >$ is the Fisher metric of the statistical manifold $S$. Clearly, $\nabla$ is a symmetric connection. Also,

$$\begin{aligned}\left(\partial_k g_{ij}\right)_\xi &= \partial_k\left(\sum_{l=1}^{n} p_\xi(x_l)\partial_i l_\xi(x_l)\partial_j l_\xi(x_l)\right)\\ &= \sum_{l=1}^{n}\left(\partial_k p_\xi(x_l)\partial_i l_\xi(x_l)\partial_j l_\xi(x_l) + p_\xi(x_l)\partial_k\partial_i l_\xi(x_l)\partial_j l_\xi(x_l) + p_\xi(x_l)\partial_i l_\xi(x_l)\partial_k\partial_j l_\xi(x_l)\right)\\ &= \left(\Gamma_{ki,j}\right)_\xi + \left(\Gamma_{kj,i}\right)_\xi.\end{aligned}$$

Briefly,

$$\partial_k g_{ij} = \Gamma_{ki,j} + \Gamma_{kj,i}. \tag{3.5}$$

The Christoffel symbols of second kind $\Gamma_{ij}^k$ are also defined using the equality $\Gamma_{ij,k} = \sum_{l=1}^m \Gamma_{ij}^l g_{lk}$. They may be calculated directly, using the following equation:

$$(\Gamma_{ij}^k)_\xi = \frac{1}{2}\sum_{l=1}^{m} g^{kl}(\xi)\left(\partial_j g_{il}(\xi) + \partial_i g_{jl}(\xi) - \partial_l g_{ij}(\xi)\right),$$

where $G(\xi)^{-1} = [g^{ij}(\xi)]_{m\times m}$ $(\xi \in \Theta)$.

In light of (3.5), we will have the following theorem [20]:

**Theorem 3.1.** *The operator $\nabla$ is a Levi-Civita connection with respect to the Fisher metric $g =< \cdot, \cdot >$.*

By the previous discussions, to determine the distance between two points $\xi$ and $\eta$ on $S$, one should solve the following geodesic initial valued problem:

$$\begin{cases} \ddot{\gamma}^k(t) + \sum_{i,j=1}^m \Gamma_{ij}^k(\gamma(t))\dot{\gamma}^i(t)\dot{\gamma}^j(t) = 0 \qquad (1 \le k \le m)\\ \gamma(0) = \xi,\ \gamma(1) = \eta \end{cases} \tag{3.6}$$

The solutions of initial valued problem (3.6) are geodesics passing through $\xi$ and $\eta$. So, the distance between these two points is the minimum length of geodesics passing through them.

## 4. Statistical manifold of an *n*-state system

We first present the motivations and basic ideas behind our approach in the current paper.

### 4.1. Motivations and basic ideas

Differential geometry serves as a fundamental tool in modern science, particularly in mathematical physics and its applications across physics, chemistry, and engineering. In thermodynamics, notable contributions by Gibbs [26], Carathéodory [27], Hermann [28], and Mrugala [29,30] have established a differential geometric framework based on the contact structure of thermodynamic phase space. This space is characterized as a $(2n + 1)$-dimensional manifold comprising $n$ extensive variables, $n$ intensive variables, and one thermodynamic potential.

In an alternative geometric approach to thermodynamic systems, Weinhold [31] introduced an *ad hoc* metric on the space of equilibrium states, defined through the Hessian matrix of the internal thermodynamic energy.

In developing the concept of thermodynamic length, Ruppeiner [32] introduced a metric defined as the Hessian of the entropy. This metric is conformally equivalent to Weinhold's metric, with the inverse temperature serving as the conformal factor. The Ruppeiner metric has found significant applications in black hole thermodynamics [33–36].

In this work, we employ an alternative approach within classical statistical mechanics to examine the geometry of thermodynamic systems. Our formulation begins with the probability density distribution incorporating the system's partition function. This framework naturally incorporates the Fisher information metric [37–39], which arises from information-theoretic considerations. While conceptually distinct from previous geometric formulations, we note that both the Weinhold and Ruppeiner metrics can be related to the Fisher metric through Legendre transformations of the relevant thermodynamic variables [40].

The central objective of this paper is to establish a Riemannian manifold $(S, g)$ for $n$-state systems, where: 1. Each point in $S$ represents an $n$-state system in thermal equilibrium at temperature $T$, characterized by its corresponding probability distribution $p_T$ 2. The metric $g$ is precisely the Fisher information metric. This geometric framework naturally induces a distance measure between distinct $n$-state systems with different equilibrium temperatures. Building upon this structure, we derive an uncertainty inequality that provides a fundamental lower bound for temperature estimation error. Furthermore, we demonstrate a consistent relationship between the Fisher metric $g$ (of information-theoretic origin) and the heat capacity $C_V$, revealing a connection between information geometry and thermodynamic quantities.

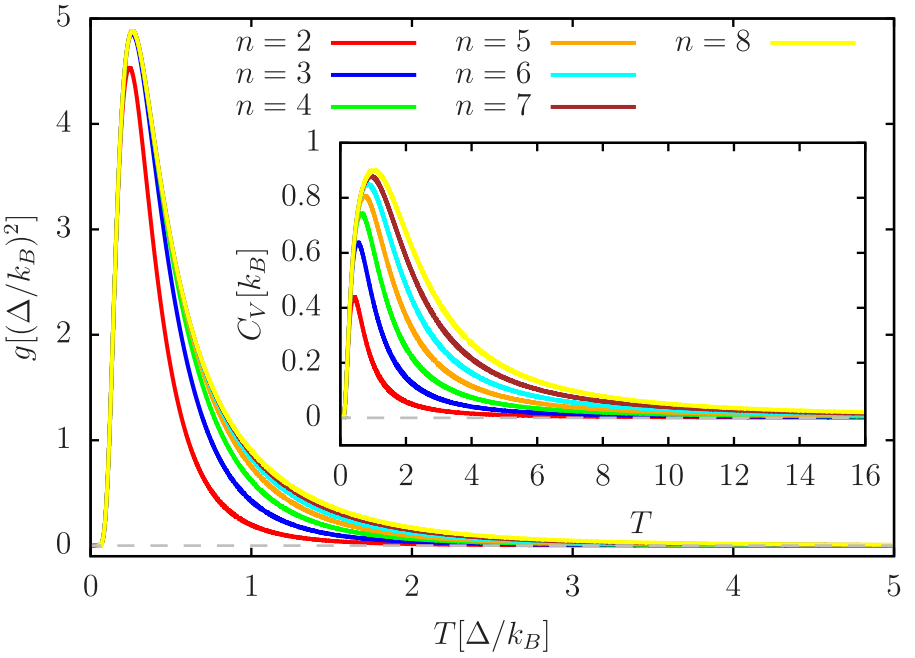



**Fig. 2.** The graphs of $g$ and $C_V$ as functions of $T$ for $n = 2, 3, \ldots, 8$.

### 4.2. Riemannian metric of n-states

In this subsection, we return to $n$-state systems and will apply the mathematical framework mentioned in Section 3, for $n$-state systems. Consider an $n$-state system with energy levels $\Omega = \{\epsilon_1, \epsilon_2, \ldots, \epsilon_n\}$. Given any temperature $T > 0$, the probability of finding the system in a microstate $k$ with energy $\epsilon_k$ in thermal equilibrium with the environment is given by

$$p_T(\epsilon_k) = \frac{1}{Z} e^{-\epsilon_k / k_B T}, \tag{4.1}$$

where $k_B$ is the Boltzmann constant and

$$Z = \sum_k e^{-\epsilon_k / k_B T} \tag{4.2}$$

is the partition function. So, we have a family of probability distributions $S = \{p_T\}_{T>0}$ on $\Omega = \{\epsilon_1, \epsilon_2, \ldots, \epsilon_n\}$, parameterized by temperature $T$. The mapping $T \longmapsto p_T$ is a smooth injection. The mapping $\phi : S \to \mathbb{R}$ defined by $\phi(p_T) := T$ gives a coordinate system $\phi = [T]$ on $S$ which makes it a one dimensional smooth manifold with one single local chart.

Now, we may define a Riemannian metric $g$ on $S = \{p_T\}_{T>0}$ as follows:

$$g(T) := \sum_{i=1}^{n} p_T(\epsilon_i) \frac{\partial}{\partial T} \left(l_T(\epsilon_i)\right)^2 = \sum_{i=1}^{n} \frac{1}{p_T(\epsilon_i)} \left(\frac{\partial p_T(\epsilon_i)}{\partial T}\right)^2, \tag{4.3}$$

where $l_T(\epsilon_i) = \log p_T(\epsilon_i)$.

An easy calculation shows that

$$\begin{aligned} \frac{\partial}{\partial T} \log p_T(\epsilon_i) &= \frac{\epsilon_i}{k_B T^2} - \frac{1}{Z} \frac{\partial Z}{\partial T} \\ &= \frac{\epsilon_i}{k_B T^2} - \frac{1}{k_B T^2} \frac{1}{Z} \sum_{j=1}^{n} \epsilon_j e^{-\epsilon_j / k_B T} \\ &= \frac{1}{k_B T^2} (\epsilon_i - \langle \epsilon \rangle_T), \end{aligned}$$

where $\langle \epsilon \rangle_T = \sum_{j=1}^{n} \epsilon_j p_T(\epsilon_j)$ denotes the mean value of energy at temperature $T$. So,

$$g(T) = \frac{1}{k_B^2 T^4} \sum_{i=1}^{n} (\epsilon_i - \langle \epsilon \rangle)^2 p_T(\epsilon_i) = \frac{1}{k_B^2 T^4} \sigma_T^2,$$

where $\sigma_T^2 = \sum_{j=1}^{n} (\epsilon_j - \langle \epsilon \rangle_T)^2 p_T(\epsilon_i)$ denotes the variance of energy at temperature $T$.

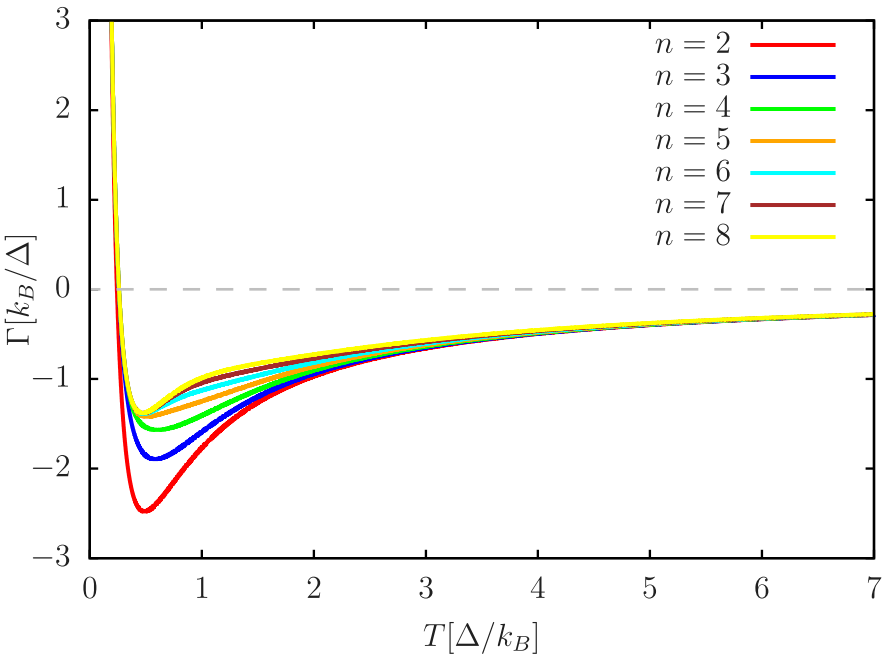



**Fig. 3.** The graph of $\Gamma(T)$ for $n = 2, 3, \ldots, 8$.

Generally, the variance can be written in terms of the special heat capacity in constant volume $C_V$ as $\sigma_T^2 = k_B T^2 C_V$ [20]. Therefore, the metric $g(T)$ may be written in terms of the special heat capacity by

$$g(T) = \frac{C_V}{k_B T^2}. \tag{4.4}$$

As one may see in (4.4), the Riemannian metric $g(T)$ given in (4.3) is nearly related to the heat special capacity in constant volume $C_V$. In Fig. 2, one can compare the graphs of $g$ and $C_V$ as functions of $T$ at different states [25].

**Remark 4.1.** In general, it is possible to define an infinite number of distinct Riemannian metrics on a manifold. This is of course also true for the manifolds which are formed by statistical models, as our model $S = \{p_T\}_{T>0}$. So the Fisher metric (4.3) is simply an instance among all possible metrics. This naturally arises the question, whether there is anything which distinguishes the Fisher metric from the others. The answer is indeed affirmative. The fact that a statistical manifold, like $S$, has the property that "each point in $S$ is a probability distribution" results in some natural structural conditions which are uniquely met by the Fisher metric.

Chenstov's theorem states that, the Fisher metric is the unique Riemannian metric, up to rescaling, on a statistical manifold that is invariant under sufficient statistics. See [22,41,42] for comprehensive discussions on uniqueness of Fisher metric.

### *4.3. Cristoffel symbol and geodesies of n-states*

The Cristoffel symbol of the Riemannian statistical manifold $(S, g)$, corresponding to an $n$-state system, is given by

$$\begin{aligned}\Gamma(T) &= \frac{1}{2g}\frac{\partial}{\partial T} g(T) = \frac{1}{2g}\frac{\partial}{\partial T}\left(\frac{C_V}{k_B T^2}\right)\\ &= \frac{1}{T}\left(\frac{1}{2}\frac{1}{C_V}\frac{\partial C_V}{\partial T} - 1\right) = \frac{1}{2}\frac{\partial}{\partial T}\log C_V - \frac{1}{T}\end{aligned}$$

where

$$C_V = \frac{\partial E}{\partial T} = k_B\left(\frac{\Delta}{k_B T}\right)^2\left[-\frac{n^2 e^{-n\Delta/k_B T}}{(1-e^{-n\Delta/k_B T})^2} + \frac{e^{-\Delta/k_B T}}{(1-e^{-\Delta/k_B T})^2}\right].$$

In Fig. 3, one can see that, the Christoffel symbole shows the same treatment at larger states.

In light of (3.6), the geodesics corresponding to an $n$-state system may be attained by the solutions of the following geodesic differential equation:

$$\ddot{\gamma}(t) + \Gamma(\gamma(t))\,(\dot{\gamma}(t))^2 = 0. \tag{4.5}$$

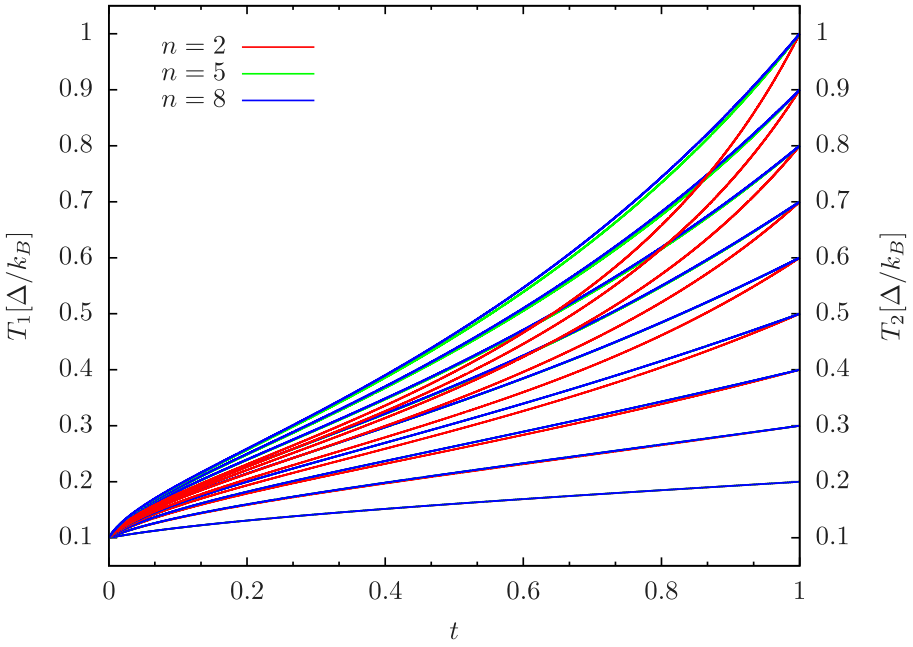



**Fig. 4.** The graphs of geodesics passing through $T_1$ and $T_2$ for $n = 2, 5, 8$.

Note that, given two $n$-state systems with temperatures $T_1$ and $T_2$, the distance between these $n$-state systems are given by

$$d(T_1, T_2) = \int_0^1 \sqrt{g(\gamma(t))}|\dot{\gamma}(t)|dt, \tag{4.6}$$

where $\gamma = \gamma(t)$ is the solution of the following boundary valued problem:

$$\begin{cases} \ddot{\gamma}(t) + \Gamma(\gamma(t))(\dot{\gamma}(t))^2 = 0 \\ \gamma(0) = T_1,\ \gamma(1) = T_2 \end{cases} \tag{4.7}$$

Fig. 4 represents the geodesics for $n$-state systems passing through the temperatures $T_1 = 0.1$ and $T_2 = 0.2, 0.3, \ldots, 1$ for $n = 2, 5, 8$.

We have numerically used module `integrate.solve_bvp` of `SciPy` package to solve geodesic differential equation (4.7) [43]. It uses more effective Runge–Kutta method (`RK45`) and continuous extensions [44].

Also, Fig. 5 provides the distance between $n$-state systems with different values of $T_1$ and $T_2$. A spacial graph for distance is also shown in Fig. 6.

**Remark 4.2.** A geodesic connecting a system at temperature $T_1$ to a system at temperature $T_2$ with respect to the metric $g$ represents the optimal temperature variation path when the system transitions from $T_1$ to $T_2$. This suggests that one could design an effective thermometer for the statistical manifold $S = \{p_T\}_{T>0}$ based on this geometric structure.

## 5. An uncertainty inequality

Suppose that $S = \{p_T\}_{T>0}$ is the one-dimensional statistical manifold corresponding to an $n$-state system. Suppose that a data is randomly generated subject to probability distribution $p_T$ in $S$. Consider the problem of estimating the unknown temperature $T$ by a function $\hat{T} : \Omega \to \mathbb{R}$ which is called an estimator. $\hat{T}$ is called an unbiased estimator if

$$E_T(\hat{T}) = T \qquad \forall T > 0,$$

where

$$E_T(\hat{T}) = \sum_{j=1}^{n} \hat{T}(\epsilon_j) p_T(\epsilon_j).$$

For a temperature $T > 0$, the mean square error of an unbiased estimator $\hat{T}$ is defined by

$$v(T) := E_T\left[(\hat{T} - T)^2\right].$$

A better estimation of a temperature $T$ occurs if $v(T)$ is as small as possible. The well-known Cramer–Rao inequality states that the mean square error cannot be as small as we like. Equivalently, there is a lower bound for it which is related to the Fisher metric.

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| 1.000 | 1.117 | 1.045 | 0.937 | 0.829 | 0.723 | 0.615 | 0.484 | 0.304 | 0.087 | 0.000 |
| 0.900 | 1.077 | 1.001 | 0.886 | 0.768 | 0.647 | 0.506 | 0.318 | 0.092 | 0.000 | 0.087 |
| 0.800 | 1.027 | 0.945 | 0.819 | 0.685 | 0.533 | 0.335 | 0.097 | 0.000 | 0.092 | 0.304 |
| 0.700 | 0.960 | 0.870 | 0.728 | 0.563 | 0.354 | 0.105 | 0.000 | 0.097 | 0.318 | 0.484 |
| 0.600 | 0.875 | 0.769 | 0.598 | 0.376 | 0.114 | 0.000 | 0.105 | 0.335 | 0.506 | 0.615 |
| 0.500 | 0.762 | 0.629 | 0.401 | 0.126 | 0.000 | 0.114 | 0.345 | 0.533 | 0.647 | 0.723 |
| 0.400 | 0.604 | 0.419 | 0.138 | 0.000 | 0.126 | 0.376 | 0.563 | 0.685 | 0.768 | 0.829 |
| 0.300 | 0.378 | 0.143 | 0.000 | 0.138 | 0.401 | 0.598 | 0.728 | 0.819 | 0.886 | 0.937 |
| 0.200 | 0.116 | 0.000 | 0.143 | 0.419 | 0.629 | 0.769 | 0.870 | 0.945 | 1.001 | 1.045 |
| 0.100 | 0.000 | 0.116 | 0.378 | 0.604 | 0.762 | 0.875 | 0.960 | 1.027 | 1.077 | 1.117 |
| $T_2$ / $T_1$ | 0.100 | 0.200 | 0.300 | 0.400 | 0.500 | 0.600 | 0.700 | 0.800 | 0.900 | 1.000 |

**Fig. 5.** Table distances for various values of temperatures for $n = 5$.

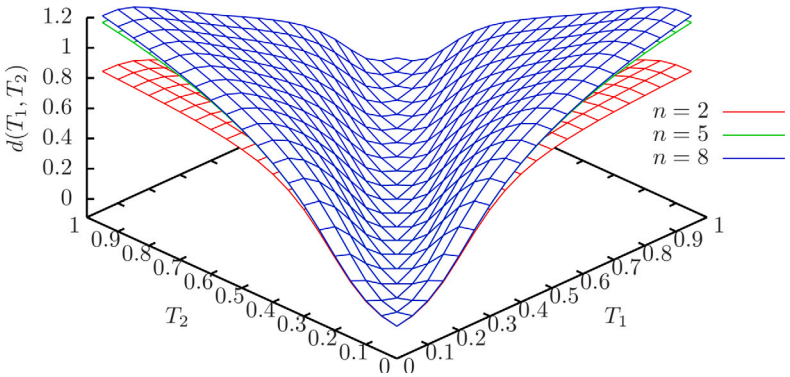



**Fig. 6.** The Spacial graph of distances for $n = 2, 5, 8$.

**Theorem 5.1** (*Cramer–Rao Inequality [20]*). *Let $\hat{\xi}$ be an unbiased estimator and $V(\xi) = \left(v_{ij}(\xi)\right)_{n\times n}$ be the mean square error matrix. Then $V(\xi) \geq G(\xi)^{-1}$ in the sense that $V(\xi) - G(\xi)^{-1}$ is a positive semi-definite matrix.*

Now, we apply the Cramer–Rao inequality for the one-dimensional manifold of an $n$-state system. Clearly, in this case, the mean square error matrix has only one array $v(T) = v_{11}(T)$, and is given by

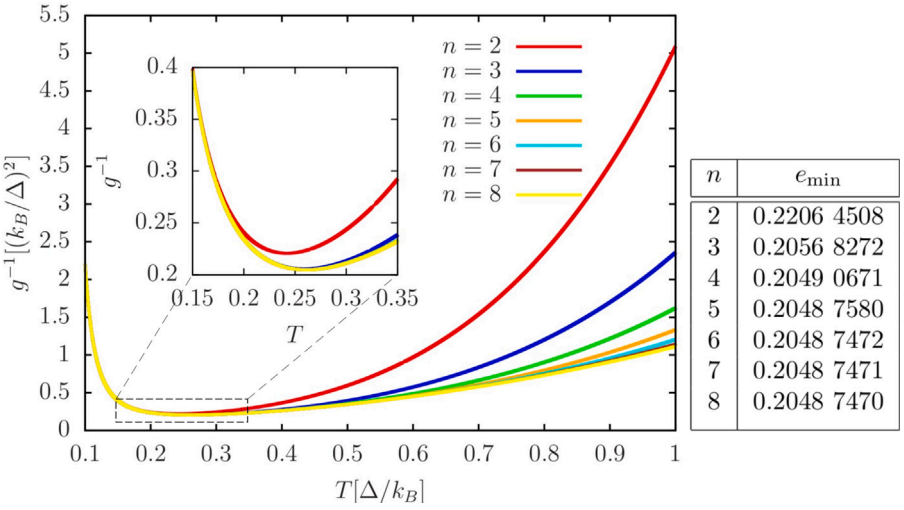
$$v(T) = E_T\left[(\hat{T} - T)^2\right]$$

and the Cramer–Rao inequality will be as follows:

$$v(T) \geq g(T)^{-1} = \frac{k_B T^2}{C_V}.$$

Note that, as shown in Fig. 7, $g(T)^{-1} = \frac{k_B T^2}{C_V}$ has a minimum which gives a lower bound for estimation error of the temperature of system. Fig. 7 shows the minimum error $e_{\min} = \min g(T)^{-1}$ of temperature estimation of an $n$-state system with an accuracy of $10^{-8}$ for $n = 1, 2, \ldots, 8$. It can be seen that, as $n$ increases, the minimum estimation error of the temperature of an $n$-state system approaches a common lower bound (see Fig. 3).

In physics, measurements inherently involve some degree of error. We propose that the universal lower bound presented in this manuscript reflects a fundamental uncertainty in temperature measurement. This is supported by numerical evidence demonstrating




| $n$ | $e_{\min}$ |
|---|---|
| 2 | 0.2206 4508 |
| 3 | 0.2056 8272 |
| 4 | 0.2049 0671 |
| 5 | 0.2048 7580 |
| 6 | 0.2048 7472 |
| 7 | 0.2048 7471 |
| 8 | 0.2048 7470 |

**Fig. 7.** The graph of $g^{-1}$ and its minimum as the lower bound of error estimation of temperature for $n = 2, 3, \ldots, 8$.

the independence of this lower bound from $n$ (see Fig. 7 and its accompanying table). Importantly, this common lower bound establishes the minimum achievable scale for system temperature measurement.

## 6. Summary and discussion

In this paper, a mathematical modeling of an $n$-state system with equal energy intervals is presented, by using information geometry techniques. In this regard, we have assigned a Riemannian manifold to an $n$-state system which made us capable to define a metric on the family of distributions of an $n$-state system, parameterized by temperature. Numerical methods are also applied to calculate the distance between different equilibrium statistical states of an $n$-state system. Finally, using Cramer–Rao inequality, we gave a lower bound for the mean square error of any unbiased estimator of the temperature. The procedure described for $n$-state systems can be generalized to any system characterized by a family of parameterized probability distributions. In equilibrium statistical mechanics, this approach is applicable to both canonical and grand canonical ensembles.

## CRediT authorship contribution statement

**M. Rahimi:** Writing – original draft, Project administration. **M.R. Mozaffari:** Writing – review & editing, Software. **A. Tayebi:** Writing – review & editing, Investigation.

## Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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## Data availability

No data was used for the research described in the article.

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