Biomedical Signal Processing and Control 40 (2018) 163–170

Contents lists available at ScienceDirect

Biomedical Signal Processing and Control

journal homepage: www.elsevier.com/locate/bspc

Thermodynamic analogies for the characterization of 3D human coronary arteries

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ARTICLE INFO

Article history:
Received 3 November 2016
Received in revised form 15 June 2017
Accepted 16 September 2017

Keywords:
Thermodynamics of curves
Geometric characterization
Coronary arteries
Classification
Geometrical risk factors

ABSTRACT

The thermodynamics of three-dimensional curves is explored through numerical simulations, providing room for a broader range of applications. Such approach, which makes use of elements of information theory, enables the processing of parametric as well as non-parametric data distributed along the curves. Descriptors inspired in thermodynamic concepts are derived to characterize such three-dimensional curves. The methodology is applied to characterize a sample of 48 human coronary arterial trees and compared with standard geometric descriptors. As an application, the usefulness of the thermodynamic descriptors is tested by assessing statistical associations between arterial shape and diseases. The feature space defined by arterial descriptors is analyzed using multivariate kernel density classification methods. A two-tailed *U*-test with 95% confidence interval showed that some of the proposed thermodynamic descriptors have different mean values for healthy/diseased left anterior descending (LAD) and left circumflex (LCx) arteries. Specifically: in the LAD, the temperatures based on mean number of intersection points and curvature are larger in healthy arteries ($p < 0.05$); in the LCx, the intersection counting pressure is larger in healthy arteries ($p < 0.05$). Moreover, the shape of the right coronary artery is thoroughly characterized by these descriptors. Specifically: intersection count thermodynamics, i.e. entropy, temperature and pressure are larger in Σ-Shape RCAs, in turn curvature based entropy and pressure are larger in C-Shape RCAs ($p < 0.05$).

1. Introduction

The theory known as *thermodynamics of plane curves* was originally proposed by Mendès France [1,2]. The core idea was to characterize planar curves with classical thermodynamics quantities, e.g. entropy, temperature and pressure, preserving analogies to the corresponding physical laws. The very foundation of the theory relies on a theorem from the field of *integral geometry*, known as the Cauchy–Crofton theorem [3], which states that the expected number of intersections ($\bar{n}$) between a random line intersecting a plane curve Γ, is related to the length (ℓ) of Γ and the perimeter (C) of its convex hull. The link to thermodynamics came from an *information-theory* based analysis of the discrete probability distribution (p_n) of the intersection count function.

Over the years the ideas behind the theory of *thermodynamics of plane curves* were further explored in close relation to fractal theory, with strong theoretical flavors and a modest number of applications. For example, [4] revisited the theory for planar curves and related the entropy to the notion of dimension of curves. In [5] used the rationale behind thermodynamics analogies to define the temperature of non-random maps. In [6] adapted the concept of entropy for application in time/spatial series, showing practical examples in geological data processing. The same research group used entropy of time/spatial series to the identification of functional relationships between carbon dioxide concentration and atmospheric pressure in caves [7]. More recently, [8,9] adapted the entropy of curves, generalizing it to an arbitrary number of dimensions, with application to analysis and classification of dynamical systems. In [10] recently presented applications of the $\bar{n}$, also known as inconstancy, to numerical sequences and proposed

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http://dx.doi.org/10.1016/j.bspc.2017.09.015
1746-8094/

some practical applications. More recent contributions in the area focused on the use of a variety of generalized entropy definitions, like Rényi's [11].

It is worth to remark that neither the entropy adaptations for time/spatial series [6], nor the one proposed by [8] for curves in $\mathbb{R}^n$, are linked to the expected number of intersection ($\bar{n}$) between a curve and hyperplanes, which is a cornerstone of the original theory. In fact, both works proposed a new definition of the entropy function based on the series/curve characteristics, without considering any probability distribution. This strays those contributions from the original notion: an information-theory-based entropy with analogy to statistical mechanics.

In this work, we present a natural extension of the thermodynamic descriptors to curves in three-dimensional (3D) space. In order to do that, we use directly the probability distribution p_n instead of the Cauchy–Crofton theorem. A computational approximation of p_n allows the numerical estimation of the entropy, temperature and pressure descriptors of a 3D curve. The use of probability distributions also inspired a generalization of these thermodynamic descriptors for characterizing curves using spatially distributed information, e.g. curvature, torsion.

There are several applications fields in which the characterization of 2D or 3D curves are valuable, i.e. spatio-temporal trajectory, numerical series, signal processing, handwriting and shape analysis (from contours or skeletons). To use the proposed framework in such fields, a representation of input data in the form of a curve, is required. In this work, as application examples, we use thermodynamic descriptors for the characterization of human coronary arteries, extracted from patient-specific medical images. The motivation and context for the use of such dataset are stated in Section 3.

2. Thermodynamics of curves in 3D space

Consider a curve Γ in 3D space. We define p_n as the probability of a random plane intersecting Γ at n points. Therefore, the mean number of intersection points of a random plane is $\bar{n} = \sum np_n$. Then, we introduce the Shannon's measure of entropy from information theory [12],

$$H = -\sum_{n=1}^{\infty} p_n \log \quad p_n. \tag{1}$$

In physics, finding the probability distribution p that maximizes H, is the basis of the so called MaxEnt thermodynamics principle [13,14], which explains statistical mechanics and equilibrium thermodynamics as inference processes. Maximization of H subjected to a restriction on the mean value was first tackled by [15]. The classical solution, known as Gibbs algorithm, makes use of Lagrange multipliers to find the roots of the functional

$$\mathcal{L}(p) = -\sum_{n=1}^{\infty} p_n \log \quad p_n - \beta\left(\bar{n} - \sum_{n=1}^{\infty} np_n\right) - \lambda\left(1 - \sum_{n=1}^{\infty} p_n\right). \tag{2}$$

Solving the equation $\mathcal{L}' = 0$ yields

$$p_n = (e^{\beta} - 1)e^{-\beta n}, \ \beta = \log \quad \left(\frac{\bar{n}}{\bar{n}-1}\right), \ e^{-1-\lambda} = e^{\beta} - 1, \tag{3}$$

then, the maximum entropy corresponds to a curve in "thermodynamic equilibrium", and can be written in terms of $\bar{n}$ as

$$H_{\max} = \log \quad (\bar{n}) + \frac{\beta}{e^{\beta}-1} = \bar{n}\log \quad (\bar{n}) - (\bar{n}-1)\log \quad (\bar{n}-1). \tag{4}$$

In quantum thermodynamics, p_n usually represents the probability that a system of particles (e.g., atoms or molecules) is in the discrete energy level E_n. Furthermore, the classical definition of temperature results $T = k\beta^{-1}$, where k is the Boltzmann constant (hereafter taken equal to one). In the present context the temperature of a curve can be defined using this analogy, that is

$$T = \frac{1}{\beta} = \left[\log\left(\frac{\bar{n}}{\bar{n}-1}\right)\right]^{-1}. \tag{5}$$

When the temperature vanishes ($T = 0$), the curve freezes to a straight line $\bar{n} = 1$. Furthermore, the entropy also vanishes ($H = H_{max} = 0$), which agrees with classical thermodynamics, for which, at zero temperature the entropy of the system vanishes.

In an attempt to push further the analogy with physics, we define the pressure (P) of a curve in terms of its entropy, Eq. (1), and its temperature, Eq. (5), in analogy with the thermodynamics of ideal gases, that is:

$$H = \frac{\gamma}{1-\gamma}\log \quad T + \log \quad P, \tag{6}$$

where γ is the ratio of specific heats, and the universal gas constant is set to unity. The motivation of Eq. (6) is that the spatial configuration of random intersections are analogous to spatial configurations of point particles. P and γ will be taken as parameters that, hopefully, remain the same for a given class of curves (e.g., with similar shape). Note that $\gamma(1-\gamma)^{-1}$ is the slope of the linear approximation in a ($\log T$ vs. H) plot.

Particularly, the original theory of *thermodynamics of plane curves*, as presented by Mendès France [1], relies on the Cauchy–Crofton theorem [3], which states that, for a planar curve Γ, the expected number of intersections between Γ and a random line, is given by

$$\bar{n} = \sum_{n=1}^{\infty} np_n = \frac{2\ell}{C}, \tag{7}$$

where ℓ is the length of Γ and C is the perimeter of the convex hull of Γ. Expression (7) allows analytical computation of H_{max} and T for a given planar curve Γ. Unfortunately, the lack of an extension of the Cauchy–Crofton theorem to higher dimensions has limited the theory to the plane. Nonetheless, observe that given p_n, for example obtained from numerical simulations, the thermodynamics can be defined for any curve in any dimension, which is the matter of this work.

2.1. An extended framework for the thermodynamics of curves

The most abstract setting of the curve thermodynamics framework depends merely on a discrete probability distribution function (DPDF). In Section 2, the DPDF accounts for the number of intersections between a 3D curve and a random plane. The procedure to obtain a generalized thermodynamic characterization for a given curve Γ is as follows:

i. Choose a random variable (X) associated to the geometry of the curve, e.g. the number of intersection points of Γ with random planes. Note that in the context of the thermodynamics analogy, $X \in \mathcal{G} \subset \mathbb{R}$ represents the "energy levels" of the curve. Here, $\mathcal{G}$ represents the subset of admissible energy levels.
ii. Compute the probability distribution, $p(X, \Gamma) = p$, for the given curve Γ.
iii. Calculate curve descriptors based on the probability function, for example
    i. Statistical moments of p, such as the mean.
    ii. Entropy (H) of p. In this work Shannon's entropy is used, but other definitions like [16] or [17] entropies may be used as well.
    iii. Using the mean, thermodynamic descriptors can be calculated through equations (1), (5) and (6).