Learning Physics from Data: 
an Thermodynamic Interpretation

Francisco Chinesta\textsuperscript{a}, Elías Cueto\textsuperscript{b}, Miroslav Grmela\textsuperscript{c,}\textsuperscript{*}, Beatriz Moya\textsuperscript{b}, Michal Pavelka\textsuperscript{d}

\textsuperscript{a}ESI Group Chair. Arts et Metiers ParisTech. 155 Boulevard de l'Hopital. 75013 Paris, France.
\textsuperscript{b}Aragon Institute of Engineering Research. Universidad de Zaragoza. Maria de Luna, s.n. 50018 Zaragoza, Spain.
\textsuperscript{c}École Polytechnique de Montréal, C.P. 6079 succ. Centre-ville, Montréal, H3C 3A7 Québec, Canada.
\textsuperscript{d}Mathematical Institute, Faculty of Mathematics and Physics, Charles University, Sokolovská 83, 186 75 Prague, Czech Republic.

\textsuperscript{*}Corresponding author: miroslav.grmela@polymtl.ca

Abstract

Experimental data bases are typically very large and high dimensional. To learn from them requires to recognize important features (a pattern), often present at scales different to that of the recorded data. Following the experience collected in statistical mechanics and thermodynamics, the process of recognizing the pattern (the learning process) can be seen as a dissipative time evolution driven by entropy. This is the way thermodynamics enters machine learning. Learning to handle free surface liquids serves as an illustration.

Keywords: Machine learning, GENERIC.

PACS: 05.70.Ln, 05.90.+m

Contents

1 Introduction 2

2 Pattern recognition in statistical physics and thermodynamics 4
  2.1 Reduction and pattern recognition 4
  2.2 Reducing dynamics, thermodynamics 5
  2.3 Reduced dynamics 8

3 Pattern recognition in machine learning 10
  3.1 General scheme 10
  3.2 Reduced manifold recognition by POD 11
    3.2.1 Loss of information 11
1. Introduction

An ideal gas that is left undisturbed reaches a state, called an equilibrium state, at which its behavior is found to be well described by the classical equilibrium thermodynamics. The features of the ideal gas that play an important role in the classical equilibrium thermodynamics are thus revealed in the process that prepares the ideal gas for equilibrium thermodynamics. The equation governing the time evolution describing the preparation process has been introduced at the end of the nineteenth century by Ludwig Boltzmann [1]. The equation is now called the Boltzmann equation. The equilibrium thermodynamics emerges from its solutions as features of the solutions that survive the dissipation eliminating gradually in the course of the time evolution the irrelevant details. The "Natural Intelligence" (NI), c.f. [2], entering the dissipation-driven pattern recognition process is the realization that the binary collisions are the principal culprits of the disorder generation that creates the irrelevant details and makes the pattern to emerge. Due to very fast and very large changes of the gas particle trajectories that occur during the collisions, details of the trajectories are escaping our attention that is specified by choosing only the one particle distribution function as the variable describing states of the ideal gas. Such loss of details enters the Boltzmann equation as a new dissipative term that brakes the time reversibility of mechanics and brings solutions eventually to equilibrium states.
Can we see the dissipation-driven pattern recognition process as a result of a data-driven learning? Let us assume that we have in our disposition trajectories of a large number of gas particles. This is our data base with which we begin our investigation. We now apply to the data base the methods Proper Orthogonal Decomposition (POD), Locally Linear Embedding (LLE), Topological Data Analysis (TDA), etc. developed in [3, 4, 5, 6], for finding a structure in the data base. We conjecture that such analysis would lead to the same structure as the one revealed in the Boltzmann dissipation-driven pattern recognition process. In other words, we conjecture that “Artificial Intelligence” (AI) analysis also reveals the Boltzmann insight that the binary collisions represent the essential physics involved in the possibility to use equilibrium thermodynamics for describing the experimentally observed behavior of ideal gases.

We shall use hereafter the following terminology. NI modeling is the ”natural intelligence’’ modeling that has unfolded from Newton’s formulation of mechanics. An NI model is the time evolution equation (2.1). AI modeling is the “artificial intelligence” modeling that is also referred to as machine learning. Data base plays important but different roles in both NI and AI modeling.

In the NI modeling the data base serves first only as one of the inspirations leading to a physical insight needed to write down the time evolution equation (2.1) that then represents the NI model. Equation (2.1) is subsequently solved and its solutions (i.e. predictions of the NI model) are compared with the data base. The comparison is the process of the validation of the NI model. The real beginning of the NI modeling is the time evolution equation (2.1). The NI modeling is rather insight driven than data driven. The data base however participates in the formulation of Eq.(2.1) and then continues to inspire also the process of solving it (see more in Section 2) and finally it is used to validate the NI model.

In the AI modeling the data base is the principal input. The AI modeling is truly data driven [7] [8] [9]. The objective is to formulate Eq.(2.1) (or an equivalent to it set of instructions for computer that allow to simulate the time evolution) that generates the data base. The beginning of the AI modeling is thus the data base, its final result is the physical insight introduced at the beginning of the NI modeling in the form of Eq.(2.1). In this sense, the AI modeling is a learning process.

In this paper we recall first (in Section 2) some aspects of the NI modeling that, as we show in Section 3, play very likely an important role also in the machine learning. We focus our attention in particular on the passage from the time evolution equation (2.1) to a simple time evolution equation in which the essential overall features (the pattern in solutions of (2.1)) became manifestly displayed and unimportant details were ignored. Such passage is a principal step in getting an insight needed to make predictions based on (2.1). Such passage is also, as we recall in Section 2, a general formulation of thermodynamics. Our principal objective in this paper is thus to contribute to the development of thermodynamics of machine learning. In trying to recognize common features in the NI and AI modeling we follow the spirit of Machine Learning via Dynamical Systems proposed in [10,11].
The analysis presented in Sections 2 and 3 are illustrated in Section 4 on the example of free surface fluid flows discussed already in [12].

Novelty of this paper lies in the following points. Learning is dictated by entropy production, i.e. removing details and capturing first order insights. This is the main aim of dimensionality reduction (linear and nonlinear). When learning physics, thermodynamics is the appropriate framework for accomplishing it safely and precisely. This provides a thermodynamic interpretation of the rather numerical approach from [12]. It is moreover important to recognize both the projection and the inverse embedding between the different detailed and less detailed manifolds (scales), as within the MaxEnt framework. We learn from detailed data, by removing details, etc. Then we predict in the reduced space, in which we created our (reduced) model, but we validate in the rich space, and for that the embedding is needed. At least when addressing physics, both scales are thermodynamically linked and we move from one to the other for coming back later. This thermodynamic link can be exploited in the numerical algorithms.

2. Pattern recognition in statistical physics and thermodynamics

In this section we recall some ideas and methods that have emerged in statistical mechanics and thermodynamics and that, as shown in Section 3, are also pertinent in machine learning.

2.1. Reduction and pattern recognition

Consider a manifold $\mathcal{M}$ with coordinates $x \in \mathcal{M}$, and assume that there is a vector field $X \in \mathfrak{X}(\mathcal{M})$ on the manifold. The vector field determines a flow on the manifold. In other words, components of the vector field are the right hand sides of evolution equations for $x$,

$$\dot{x}^i = X^i(x), \quad (2.1)$$

and the evolution simply follows arrows of the vector field. We note that if the system under investigation is a physical system composed of atoms and molecules, then one possible model in the form of Eq. (2.1) is in principle known. The state variable $x$ consists of the position vectors and momenta of all the particles involved (provided we limit ourselves to the classical mechanics) and the vector field $X$ is the vector field of classical mechanics (right hand side of Hamilton canonical equations). To specify it we need to know (or assume to know) all the forces participating in the time evolution. If the system under investigation is still a physical system, but the data base addresses some macroscopic features (e.g. fluid flows), then $x$ has to address the quantities entering the data base and an additional insight is needed to formulate the vector field $X$.

Now we turn to the problem of solving Eq. (2.1), i.e. to the problem of finding the flow generated by (2.1). There are two routes to follow. On the first route we find all details of the trajectories generated by (2.1). This, of course, is in general a very difficult task even for very well performing computers.
Moreover, the result, i.e. the phase portrait generated by (2.1), still needs to be subjected to a pattern recognition process in order to be useful. The complexity of the phase portrait has to be reduced by highlighting important features and ignoring unimportant details. On the second route the objective is not to find all the details of solutions of Eq. (2.1) but only their important qualitative features. We shall follow the second route.

Consider a projection \( \pi : \mathcal{M} \to \mathcal{N} \), range of which determines a reduced manifold \( \mathcal{N} \). An insight (inspired also by the data base in our disposition) is needed to specify the projection \( \pi \). As an example, we take (2.1) to be the Boltzmann kinetic equation (i.e. \( x \) is the one particle distribution function) and \( \pi \) the projection to hydrodynamic fields (that are the first five moments of the distribution function in the velocity variable).

The projection \( \pi \) maps each point \( x \in \mathcal{M} \) to a point \( y \in \mathcal{N} \). To each point \( x \) there is an arrow attached (vector field \( \mathbf{X} \)), and this arrow (an instruction how to proceed in the time evolution in \( \mathcal{M} \)) can be also mapped to the tangent bundle of \( \mathcal{N} \), i.e. to a vector tangent to \( \mathcal{N} \) attached to a point \( y \in \mathcal{N} \). The projected vector field then generates the time evolution in \( \mathcal{N} \). However, in a thermodynamic setting—this is not the case in projection-based model reduction—there are typically many points from \( \mathcal{M} \) projected to single \( y \in \mathcal{N} \), there are many vectors to be attached to \( y \). How to choose the right one (i.e. the one expressing properly the induced flow on \( \mathcal{N} \)) and consequently how to determine the vector field on \( \dot{y}^a = Y^a(y) \) representing the reduced dynamics?

In order to answer this question we need again an insight. Imagine a phase portrait where trajectories of a dynamical system are depicted. For a physical system it is usually possible to find a pattern where typical trajectories are contained, see e.g. [13]. When starting somewhere in the phase space, the point typically evolves towards the pattern. The reduction introduced above takes the phase space (or the vector field generating it) and finds a reduced manifold where typical evolution takes place, i.e. leads to the pattern recognition. It is therefore not surprising to anticipate (see more in Section 3) that dynamic reductions provide inspiration for machine learning and vice versa. Let us now recall several methods of the dynamic reduction.

2.2. Reducing dynamics, thermodynamics

We begin with an example. Let \( \mathcal{M} \) be the state space of kinetic theory (i.e., the physical system under investigation is a gas and \( x \) is the one-particle distribution function) and \( \mathcal{N} \) is the state space of the classical equilibrium thermodynamics (i.e., \( y = (V,N,E) \in \mathbb{R}^3 \), where \( V \) is the volume of the region in \( \mathbb{R}^3 \) in which the gas under investigation is confined, \( N \) is the number of moles, and \( E \) is the total energy of the microscopic particles composing the gas). In this case, no time evolution takes place in \( \mathcal{N} \). The projection \( \pi \) is thus the projection on the fixed points of the time evolution taking place in \( \mathcal{M} \). Let us assume that...
the models in $\mathcal{M}$ and in $\mathcal{N}$ have been validated by their corresponding data bases.

The question that we ask now is of what we have learned by relating the two models, i.e., by reducing the model in $\mathcal{M}$ to the model in $\mathcal{N}$. If the model in $\mathcal{N}$ was a model with the time evolution then we would clearly obtain the time evolution in $\mathcal{N}$ as a reduced dynamics and thus learn how to see the time evolution in $\mathcal{N}$ from the point of view of $\mathcal{M}$. But in the case when the model in $\mathcal{N}$ is the equilibrium thermodynamics (i.e., there is no time evolution in $\mathcal{N}$, there is no reduced dynamics) the question becomes particularly pertinent. Following Boltzmann, we answer the question as follows. A part of the data base corresponding to the kinetic theory is an observation of the process that prepares the gas under investigation to states at which its behavior can be well described by the model in $\mathcal{N}$. According to Boltzmann, the time evolution describing the preparation process is governed by the Boltzmann equation. It is the time evolution generated by the Boltzmann equation that makes the projection $\pi$. We call the dynamics making the projection $\pi$ a reducing dynamics. The dynamics expressed in the Boltzmann equation is thus an example of reducing dynamics. Following solutions to the Boltzmann equation, kinetic theory becomes reduced to equilibrium thermodynamics.

The potential driving the reduction is called an entropy in $\mathcal{M}$. We shall call it an upper entropy $\uparrow S$. This potential, if evaluated at the states in $\mathcal{M}$ reached as $t \to \infty$, becomes the entropy in $\mathcal{N}$, called a lower entropy $\downarrow S$. In the case of $\mathcal{N}$ being the state space of the equilibrium thermodynamics, $\downarrow S$ is the entropy $S(V, N, E)$ entering the model in $\mathcal{N}$. The reduction from $\mathcal{M}$ thus gives us the fundamental thermodynamic relation in $\mathcal{N}$.

Following [14, 15, 16, 17], the reducing dynamics to the equilibrium thermodynamics is expressed mathematically by the General Equation for Non-Equilibrium Reversible-Irreversible Coupling, GENERIC,

$$\dot{x}_i = \uparrow L_{ij} \frac{\partial \uparrow E}{\partial x^j} + \frac{\partial \Xi}{\partial x^i} \bigg|_{x^i = \frac{\partial \uparrow S}{\partial x^i}}. \tag{2.3}$$

The Boltzmann kinetic equation as well as many other equations (e.g., the Navier-Stokes-Fourier of fluid mechanics) expressing dynamics in other state spaces $\mathcal{M}$ (see [14, 15, 16, 17]) are particular examples of Eq. (2.3). We now explain the meaning of the symbols appearing on the right hand side of Eq. (2.3).

The first part of the right hand side is the Hamiltonian evolution, constructed from the Poisson bivector $\uparrow \mathbf{L}$ and the gradient of energy $\uparrow \mathbf{E}$. Hamiltonian dynamics conserves energy (due to the antisymmetry of $\uparrow \mathbf{L}$) and entropy (due to the requirement that $\uparrow \mathbf{S}$ is the Casimir of Poisson bracket, i.e., the requirement

---

Footnote 1: The Poisson bracket corresponding to the Poisson bivector $\uparrow \mathbf{L}$ and the gradient of energy $\uparrow \mathbf{E}$. Hamiltonian dynamics conserves energy (due to the antisymmetry of $\uparrow \mathbf{L}$) and entropy (due to the requirement that $\uparrow \mathbf{S}$ is the Casimir of Poisson bracket, i.e., the requirement
that
\[ \overset{\dagger}{L}^{ij} \frac{\partial \overset{\dagger}{S}}{\partial x_i^j} = 0 \quad \forall i. \quad (2.4) \]

The second term in Eq. (2.3) is a gradient dynamics, where \( x_i^* \) are conjugate variables and \( \Xi(x, x^*) \) is a dissipation potential with convex dependence on them (see more in \([17]\)). From the convexity it follows that
\[
\overset{\dagger}{S} = \left( x_i^* \frac{\partial \Xi}{\partial x_i^*} \right) \bigg|_{x_i^* = \frac{\partial \overset{\dagger}{S}}{\partial x_i}} \geq 0,
\]
Moreover, the dissipation potential \( \Xi \) and entropy \( \overset{\dagger}{S} \) have to be such that energy \( \overset{\dagger}{E} \) is conserved in the gradient dynamics. These properties of \( \overset{\dagger}{E}, \overset{\dagger}{S}, \overset{\dagger}{L}, \Xi \), together with the convexity of \( \overset{\dagger}{S} \) and the requirement that \( \Xi \) reaches its minimum at \( x^* = 0 \), makes it possible to regard \( -\overset{\dagger}{S} \) as a Lyapunov function displaying the approach, as \( t \to \infty \), to the equilibrium states at which the entropy \( \overset{\dagger}{S} \) reaches its maximum. Such states then form \( \mathcal{N} \subset \mathcal{M} \) (in the sense that \( \mathcal{N} \) be isomorphic to a submanifold of \( \mathcal{M} \)). The Hamiltonian mechanics is moreover reversible with respect to time-reversal transformation while gradient dynamics is irreversible \([18]\), and generalized Onsager reciprocal relations \([19, 21, 22]\) are automatically fulfilled, see \([16, 17, 23]\).

Let us assume now that we are projecting from \( \mathcal{M} \) to \( \mathcal{N} \) on which the time evolution still takes place. In the next subsection we shall discuss the reduced dynamics, i.e. the projection of the vector field \( X \in \mathfrak{X} \) on the the vector field \( Y \in \mathfrak{X}(\mathcal{N}) \). For a moment, we assume that the reduced dynamics is known. It has been conjectured in \([24, 25]\) that \( \overset{\dagger}{L}^{ij} \frac{\partial \overset{\dagger}{S}}{\partial x_i^j} = 0 \) with an appropriate modifications of the properties required from \( \overset{\dagger}{E}, \overset{\dagger}{S}, \overset{\dagger}{L}, \Xi \), expresses also reducing dynamics to \( \mathcal{N} \) on which the time evolution takes place. In such case, the result of the dynamic reduction is the reduced dynamics (that we discuss in more detail in the next subsection) and thermodynamics in \( \mathcal{N} \) that is inherited from the entropy \( \overset{\dagger}{S} \) generating the reducing time evolution leading from \( \mathcal{M} \) to \( \mathcal{N} \).

Summing up, we see that the dynamical reduction from \( \mathcal{M} \) to \( \mathcal{N} \), that can be seen as a process of learning the model in \( \mathcal{N} \) from the model in \( \mathcal{M} \), makes possible to see the dynamics in \( \mathcal{N} \) as a reduced dynamics from \( \mathcal{M} \) and, in addition, introduces into \( \mathcal{N} \) a new element that has been absent in the original model in \( \mathcal{N} \). The new element is thermodynamics. It is the fundamental thermodynamic relation in \( \mathcal{N} \) expressed in the entropy \( \overset{\dagger}{S} \). If the model in \( \mathcal{N} \) is the equilibrium thermodynamics, then the fundamental thermodynamic relation arising in the dynamical reduction is the fundamental thermodynamic relation constituting the model in \( \mathcal{N} \) (i.e. the equilibrium thermodynamics). If, on the other hand, the model in \( \mathcal{N} \) involves the time evolution, then such model does not (at least in general) involve any thermodynamic relation and thus the fundamental thermodynamic relation arising in the dynamic reduction is a new information obtained from seeing the model in \( \mathcal{N} \) from the point of view of the more detailed model in \( \mathcal{M} \).

Still another thermodynamics in \( \mathcal{N} \) arises if we regard the model in \( \mathcal{N} \) as a more detailed than another model in \( \mathfrak{N} \). The upper entropy \( \overset{\dagger}{S} \) appearing
in (2.3) with $x$ replaced by $y$, i.e. the upper entropy $S^\uparrow$ generating the time evolution from $\mathcal{N}$ to $\mathcal{M}$, introduces thermodynamics in $\mathcal{N}$ (that is different from the thermodynamics introduced by $S^\downarrow$) obtained from seeing the model in $\mathcal{N}$ as a basis for reduction to a less detailed model in $\mathcal{M}$.

Finally, we note that if we are interested only in the result of the time evolution generated by (2.3), then we can replace (2.3) by simply a MaxEnt reduction which consists of the maximization of the upper entropy $S^\uparrow$ subjected to the constraints $\pi(x)$, as shown in the appendix of [23]. The Lagrange multipliers in this maximization are $y^\ast$. This is indeed the principle of maximum entropy (MaxEnt) formulated by Shannon [26] and Jaynes [27]. The question that arises in this static viewpoint of the reduction is of what is the entropy $S^\uparrow$, how shall we find it. In the dynamical viewpoint the upper entropy $S^\uparrow$ is the potential generating the reducing time evolution (that is, in general, a part of the data base associated with the model in $\mathcal{M}$). In the static viewpoint of the reduction one has to turn to other insights (see [26] and [27] for more details).

2.3. Reduced dynamics

We turn our attention now to the reduced dynamics, i.e., to the projection of $X \in \mathfrak{X}$ to $Y \in \mathfrak{X}(\mathcal{N})$.

Perhaps the simplest method of projecting $X \in \mathfrak{X}$ on $Y \in \mathfrak{X}(\mathcal{N})$ is provided by MaxEnt. Pick one point $y \in \mathcal{N}$. Due to the MaxEnt embedding there is an associated point $\pi^\ast(y) \in \mathcal{M}$. Take the vector attached to that point and project it to $y$. The vector field $Y \in \mathfrak{X}(\mathcal{N})$ obtained by repeating this for each $y \in \mathcal{N}$ is the MaxEnt projection of $X$ onto $\mathcal{N}$.

$$ Y^a(y) = \left. \frac{\partial \pi^a}{\partial x^i} \right|_{x(y)} X^i(x(y)). $$

But this vector field has a drawback. The trajectories obtained by solving evolution equations $\dot{y} = Y$ approximate poorly the trajectories on the $\mathcal{M}$ manifold. This is because the approach towards states with higher entropy is not explicitly contained in $Y$. Therefore, a more precise approximation is needed, see [28], [29].

A classical example of reduction beyond MaxEnt is the Chapman-Enskog expansion [30]. Let $\mathcal{M}$ be the state space of kinetic theory (i.e., the physical system under investigation is a gas and $x$ is the one-particle distribution function) and $\mathcal{N}$ is the state space of the hydrodynamics (i.e., hydrodynamic fields of density, momentum density and energy density, $y = (\rho, \mathbf{u}, e)$). In this case, the time evolution takes place in $\mathcal{N}$ is often well described by the Navier-Stokes-Fourier system of equations, see e.g. [22], obtained by the Chapman-Enskog expansion. The projection $\pi$ is the projection on the first 5 moments of the distribution function, and the detailed Boltzmann equation (vector field $X$) is reduced to less detailed Navier-Stokes-Fourier equations (vector field $Y$). The upper entropy $S^\uparrow$ is the Boltzmann entropy and it generates a lower-level entropy $S^\downarrow$, expressed by the Sackur-Tetrode relation for ideal gases [31], [17]. The embedding $\pi^\ast$ is the MaxEnt mapping from hydrodynamic fields to the locally
Maxwellian distribution functions. The locally Maxwellian distribution functions form the local equilibrium submanifold of $\mathcal{M}$, which is isomorphic to $\mathcal{N}$. When the evolution in $\mathcal{M}$ takes place close to the local equilibrium submanifold, the evolution in $\mathcal{N}$ is close to the detailed evolution in $\mathcal{M}$. The Chapman-Enskog expansion, however, also has a few drawbacks. Firstly, it relies on the a priori unknown form of asymptotic expansion and, secondly, it requires the presence of dissipative terms in vector field $\mathbf{X}$.

Another robust method of projecting the vector field $\mathbf{X}$ on $\mathcal{Y}$ was formulated by Bruce Turkington in [32]. The reduction consists of the following steps. Consider a manifold $\mathcal{M}$. Liouville equation for the probability distribution function on the manifold is formulated, and linear projection from the distribution function is defined, range of which determines a manifold $\mathcal{N}$. Shannon entropy is assumed for the distribution function, which forms and embedding $\pi^*$ of $\mathcal{N}$ onto $\mathcal{M}$.

Let us first project Hamiltonian mechanics on $\mathcal{M}$ (the Liouville equation) to Hamiltonian mechanics on $\mathcal{N}$. The upper Poisson bivector $^\dagger L$ is projected as a twice contravariant tensor field on the space of state variables and, if necessary, evaluated at the MaxEnt embedding,

$$ ^\dagger L^{ab} = \left( \frac{\partial \pi^a}{\partial x^i} \right)^\dagger_i L^{ij}(x) \frac{\partial \pi^a}{\partial x^j} \bigg|_{x=\pi^*(y)}. $$

To construct the Hamiltonian vector field on the lower level one further needs a Hamiltonian, energy on the lower level.

Let energy on $\mathcal{M}$ be $^\dagger E(x)$. Energy on the lower level $\mathcal{N}$ is inherited from the higher level through the MaxEnt mapping $^\dagger E(y) = ^\dagger E(\pi^*(y))$. However, since some energy modes present on the higher level have already been damped on the lower level, typically $^\dagger E(\pi(x)) \neq ^\dagger E(x)$. If the latter relation were an equality, one could project the higher-level evolution to the lower-level easily as one would obtain that time derivative of $\pi(x)$ be equal to $^\dagger L \cdot d^\dagger E$, which would be the lower-level purely Hamiltonian vector field. Since, however, the equality typically does not hold, simple projection does not give the desired result.

Instead, a lack-of-fit Lagrangian is defined which compares projections of the exact trajectories on $\mathcal{M}$ with trajectories on $\mathcal{N}$. Minimization of the Lagrangian then leads to a GENERIC evolution on $\mathcal{N}$ and gives a dissipation potential driving thermodynamic evolution on $\mathcal{N}$.

Still another method of constructing the reduced vector field is the Ehrenfest method developed in [33, 34, 35] and [28]. The method has the following ingredients: detailed manifold $\mathcal{M}$ equipped with entropy and with a vector field (evolution equations), manifold $\mathcal{N}$ and projection $\pi$ from $\mathcal{M}$ to $\mathcal{N}$. MaxEnt then provides the embedding of $\mathcal{N}$ into $\mathcal{M}$ as usually. The vector field on $\mathcal{M}$ does not need to have the GENERIC structure, but it is advantageous as shown in [36].

---

2 The more detailed level is referred to as the upper while the less detailed (reduced) as lower.
The vector field $X \in \mathfrak{X}(\mathcal{M})$ is first projected to a vector field $Y_0 \in \mathfrak{X}(\mathcal{N})$ by the MaxEnt projection. This vector field, however, needs to be corrected. Therefore, the vector field $X$ is lifted to the tangent bundle $T\mathcal{M}$ and subsequently projected back to $\mathcal{M}$, which results in a smoothed vector field on $\mathcal{M}$, $ER(X(\mathcal{M}))$, which expresses a sort of overall motion on $\mathcal{M}$, called Ehrenfest regularization in [37]. The same is done with vector field $Y_0$, which results in vector field $ER(Y_0) \in \mathfrak{X}(\mathcal{N})$. Finally, vector field $ER(X)$ is MaxEnt-projected to $\mathcal{N}$ and compared with $ER(Y_0)$. A correction term is then added to $Y_0$, forming a new vector field $Y_1 \in \mathfrak{X}(\mathcal{N})$, which makes $ER(X)$ equal to $ER(Y_1)$ (to a given order of relaxation time parameter). Vector field $Y_1$ then represents the evolution on $\mathcal{N}$, its components are right hand sides of evolution equations for $y \in \mathcal{N}$. This is the Ehrenfest reduction of detailed evolution on $\mathcal{M}$.

Another method of dynamic reduction is the Dynamic MaxEnt developed in [38, 23, 29]. The main idea is to first promote the conjugate variables $x^*$ in the GENERIC framework (2.3) to independent variables, which is natural from the point of view of contact geometry [39, 17]. The goal is to reduce a GENERIC model for state variables on manifold $\mathcal{M}$ so that a fast variables relaxes and becomes enslaved by the remaining slower variables, $\mathcal{N}$ being the manifold of slow variables.

The fast variable is first evaluated at the MaxEnt value determined by the remaining state variables. But since the conjugate fast variable is still present in the evolution equations for the slow variables, we need to express the conjugate variable in terms of the remaining state and conjugate variables. The fast conjugate variable is found as the solution to the evolution equation of the fast state variable evaluated at the MaxEnt value of the state variable. The conjugate fast variable is thus determined by compatibility of the MaxEnt value of the fast variable and the evolution equation for the fast variable. This way we end up with a vector field for the slow variables (on manifold $\mathcal{N}$) compatible with the MaxEnt embedding of the slow manifold into the original manifold.

### 3. Pattern recognition in machine learning

Imagine now a robot [40] that is, for instance, supposed to perform a mechanical task with a physical system, as e.g. in [12], while learning by itself how to operate the system. The robot has as the input a set of discrete trajectories on $\mathcal{M}$, $G(\mathcal{M})$. It should give as output an approximation of them by a low dimensional vector field which can be used to predict future evolution of the system approximately (so that it can be operated in a reasonable way).

#### 3.1. General scheme

For simplicity we shall illustrate the machine learning using the Proper Orthogonal Decomposition (POD), but the general picture will be applicable also to other methods. The problem is that the robot has discrete trajectories on a high-dimensional manifold $\mathcal{M}$, and it would be too costly to reconstruct the vector field $X \in \mathfrak{X}(\mathcal{M})$ from them; the vector field would have too many dimensions. Moreover, such high dimensional model would not provide the insight
we look for. The trajectories must be approximated by trajectories on a low dimensional manifold $\mathcal{N}$. Therefore, the task consists of the following steps:

1. **Manifold recognition**: Find a low-dimensional manifold $\mathcal{N}$ such that a projection of trajectories $G(\mathcal{M})$ to $\mathcal{N}$ well approximates the original set $G(\mathcal{M})$ of trajectories on $\mathcal{M}$. To accomplish this task, the robot needs the following:

   a. To measure distances and define orthogonality, the robot needs a **metric** on $\mathcal{M}$, $g(\bullet, \bullet)$, e.g. the $l^2$ scalar product with or without weights.

   b. Find a **projection** operator $\pi : \mathcal{M} \to \mathcal{N}$.

   c. To compare in $\mathcal{M}$ the trajectories $G(\mathcal{M})$ with their projections to $\mathcal{N}$, which is the means of assessing “goodness” of the approximative manifold $\mathcal{N}$, the robot needs an **embedding** mapping $\pi^* : \mathcal{N} \times \cdots \times \mathcal{N} \to \mathcal{M} \times \cdots \times \mathcal{M}$, mapping trajectories on $\mathcal{N}$ to trajectories on $\mathcal{M}$. The embedding is typically determined by MaxEnt in thermodynamics, but it is often difficult to construct it outside thermodynamics. Alternatively, the robot can compare the trajectories on the reduced manifold $\mathcal{N}$, for which the embedding is not needed. On the other hand, the embedding will be needed in the last step below anyway.

2. **Recognition of the reduced vector field**: Once having the low-dimensional manifold and projected trajectories $\pi(G(\mathcal{M}))$, the goal is to find a vector field $Y \in \mathfrak{X}(\mathcal{N})$ approximating the trajectories on $\mathcal{N}$. This is done by choosing an Ansatz on the form of the vector field, e.g. GENERIC, and fitting the unknown parameter so that the trajectories on $\mathcal{M}$ and $\mathcal{N}$ coincide in a sense. Once this step is successfully finished, the robot has recognized how the typical trajectories are created, he has learned how the system works.

3. To use this acquired knowledge, the robot is then supposed to integrate the vector field $Y$ to future times in order to **predict** future states on the $\mathcal{N}$ manifold. These states are then embedded into the $\mathcal{M}$ manifold of experimental data by mapping $\pi^*$ to obtain prediction of future states of on manifold $\mathcal{M}$.

Note that steps 1 and 2 can be seen as pattern recognition (manifold recognition and vector field recognition).

### 3.2. Reduced manifold recognition by POD

Let us now demonstrate the first step (manifold recognition) on a standard reduction method—the proper orthogonal decomposition (POD) or principal component analysis (PCA), see e.g. [41, 4].

#### 3.2.1. Loss of information

Let us have $N$ time snapshots of $m$-dimensional experimental data, assuming that $m >> N$, ordered to a $N \times m$ matrix $Z$. This matrix represents the high dimensional trajectories on manifold of the data $\mathcal{M}$. This matrix is now to be
approximated by POD. The core of POD is the singular value decomposition of matrix $Z$,

$$Z = U \Sigma V^T,$$

(3.1)

where $U$ is an orthogonal $N \times N$ matrix, $V$ is an $m \times m$ orthogonal matrix and $\Sigma$ is an $N \times m$ matrix with entries only on the diagonal. The entries are the called singular values, they are non-negative and ordered, $\sigma_1 \geq \sigma_2 \geq \ldots \sigma_N$. Note that there no information has been lost so far. The singular values are calculated as square roots of eigenvalues of the symmetric positive definite $N \times N$ matrix

$$Q = ZZ^T = U \Sigma \Sigma^T U^T.$$

(3.2)

In this way we also obtain the matrix $U$, which consists of the eigenvectors of $Q$. Now only $k$ first singular values are taken into account while setting $\sigma_l = 0$ for all $l > k$, which turns $\Sigma$ to a new matrix $\Sigma$. This is the crucial point where reduction takes place. The advantage of SVD is that it gives the best possible $k$-dimensional approximation of $Z$ provided the $l^2$ metric is used.

3.2.2. Projection

Finally—look at Eq. (3.1)—, the relevant part (first $k$ rows, since other are multiplied by zeroes) of matrix $V$ is calculated from $U^T Z = \tilde{\Sigma} V^T \overset{\text{def}}{=} B$. There are $k$ non-zero rows of this $N \times m$ matrix $B$, and these rows, denoted as $v_j \in \mathbb{R}^m$, form a basis of the $k$-dimensional submanifold $N \subset M$. Step (a) in the above abstract procedure is given made by choosing the usual $l^2$ scalar product and corresponding Frobenius norm. Step (b) is made by orthogonal projection $\pi$ to the basis of $N$,

$$N \ni y = \sum_{j=1}^{k} \langle x, v_j \rangle v_j \quad \forall x \in M.$$

(3.3)

3.2.3. Embedding

Consider now a trajectory $(y_1, \ldots, y_N)$ on $N$. We construct an $N \times m$ matrix $Y(y_1, \ldots, y_N)$ rows of which correspond to $y_i = \sum_{j=1}^{k} c_{ij} v_j$. The embedding $\pi^*$ is then given by

$$\pi^*(y) = U Y(y),$$

(3.4)

which is a trajectory on $M$. Step (c) has been finished. The POD method took the set of trajectories on $M$, encoded it into matrix $Z$, and identified a $k$-dimensional submanifold $N \subset M$ that approximates the trajectories $Z$. Moreover, there is an orthogonal projector $\pi$ onto the basis of $N$ and an embedding $\pi^*$ mapping trajectories on $N$ to trajectories on $M$. Step 1, manifold recognition, is thus finished.

3.2.4. Thermodynamics

We shall now look at the reduction described above through the eyes of thermodynamics recalled in Sec. 2.2. We regard the embedding of the projected
manifold $N$ to the original $M$ as a result of a learning time evolution which has revealed the important features in the data base collected in $M$. We thus interpret the reducing time evolution as the learning time evolution. This dissipative evolution is generated by an entropy. Having the entropy and focusing our interest only on the final outcome of the learning time evolution, we can also see the passage from $M$ to $N$ as maximization of the entropy (MaxEnt principle). We now proceed to identify the entropy associated with POD.

The crucial step in POD where information is lost is the dropping of eigenvalues. We shall seek its thermodynamic interpretation. A way to calculate eigenvalues is based on minimization of the Rayleigh quotient in a dynamical system, see [44]. Let us interpret the Rayleigh quotient as entropy of a vector related to a matrix $A$,

$$S(x) = \frac{x^T \cdot A \cdot x}{x^T \cdot x}.$$  \hspace{2cm} (3.5)

Gradient dynamics of $x$ is then prescribed as

$$\dot{x} = \frac{\partial \Xi}{\partial x^*} \bigg|_{x^* = S_x} = \tau \frac{\partial}{\partial x} \frac{x^T \cdot A \cdot x}{x^T \cdot x},$$  \hspace{2cm} (3.6)

for $\Xi = \frac{1}{2} \tau (x^*)^2$. The magnitude of $x$ is conserved by the dynamical system, so we can regard $x$ to be normalized to unity. This dynamical system has stationary points corresponding to eigenvectors of matrix $A$, and as it converges to the stationary values, it converges to the eigenvectors. From the eigenvectors, the eigenvalues can be recovered as the Rayleigh quotients, i.e. as the values of entropy in the stationary states. Eigendecomposition can be seen as result of a thermodynamic evolution.

However, as the matrix has typically more eigenvectors, the dynamical system has more stationary points. Typically it converges to the eigenvector corresponding to the dominant eigenvalue (highest entropy), but there are other lower eigenvalues (lower entropy) that also represent stationary solutions of the system. By being restricted only to some region around the global maximum of entropy, we obtain the information loss from POD.

Finally, the projection from all vectors normalized to unity (manifold $M$) to the chosen eigenvectors (manifold $N$, also represented by the eigenvalues) is simply the usual orthogonal projection to the span of the eigenvectors. Since the eigenvectors are contained in the original manifold $M$, the embedding is trivial (identity).

The reduction by POD, where only part of spectrum is considered while the remaining eigenspaces being ignored, can be seen as a dynamic reduction driven by entropy and implying a maximum entropy principle.

---

\*\*Another dynamical system converging to eigenvalues of a matrix was found in [42], where the double bracket dissipation, geometrized in [43], was found.\*\*
3.2.5. Comparison with Locally Linear Embedding

Locally linear embedding (LLE) typically provides better approximation of the low-dimensional manifold than POD. Let us therefore briefly mention the method. Starting with points \( x \in \mathcal{M} \), a weight matrix \( W_{ij} \) is found, which provides local interpolation of points on \( \mathcal{M} \) by their chosen number of neighbors. Then points \( y \in \mathcal{N} \) are found as the points that are best interpolated by weights \( W_{ij} \). This provides the projection \( \pi : \mathcal{M} \rightarrow \mathcal{N} \).

How to construct the embedding \( \pi^* : \mathcal{N} \rightarrow \mathcal{M} \)? We see three possible routes: (i) One can use a crude interpolation between \( y \) and \( x \), as e.g. in [12]. (ii) One can reverse the LLE procedure. Starting with points on \( \mathcal{N} \), constructing new weights \( \bar{W}_{ij} \) and finding \( x \in \mathcal{M} \) that are best interpolated by the new weights, as suggested in [5]. (iii) Finally, one can reformulate the LLE projection as gradient dynamics maximizing an entropy. The embedding could be then constructed by the MaxEnt procedure with respect to that entropy. Let us comment on this possibility in more detail.

The LLE algorithm consists of two steps, namely finding the weights \( W_{ij} \) and subsequently finding the projection \( \pi \). Both the steps are formulated as minimizations of certain cost functions. It can be therefore anticipated that LLE can be reformulated as gradient dynamics. The first step stands for minimization of cost functions

\[
e_i(W) = (x_i - \sum_j W_{ij} \eta_j)^2, \tag{3.7}
\]

where \( x_i \) is the \( i \)-th vector from \( \mathcal{M} \) and \( \eta_j \) is the \( j \)-th, \( j = 1, \ldots, K \), neighbor of \( x_i \). Note that the choice of \( K \) and the notion of distance (metric on \( \mathcal{M} \)) are needed. Moreover, the weights are supposed to sum to one for each \( i \), \( \sum_j W_{ij} = 1 \), since this is the gauge freedom of the cost function. By minimization subject to the sum-to-one constraint one obtains

\[
W_{ij} = -\lambda_i \sum_k C_{jk}^{-1(i)} + \sum_l x_i \cdot \eta_l C_{jl}^{-1(i)} \tag{3.8}
\]

with \( C_{jk}^{(i)} = \eta_j \cdot \eta_k \) being the correlation matrix, \( C_{ij}^{-1(i)} \) is its inverse, and \( \lambda_i = \frac{x_i \sum_j \eta_j \sum_k C_{jk}^{-1(i)}}{\sum_k C_{jk}^{-1(i)}} \) being the Lagrange multiplier.

The second step is minimization of cost function

\[
\phi(y) = \sum_i \left(y_i - \sum_j W_{ij} y_j \right)^2 \tag{3.9}
\]

subject to the constraints that \( \sum_i y_i = 0 \) and \( y_i \otimes y_j \propto I \), \( I \) being the \( d \times d \) identity matrix on the low-dimensional manifold. This step can be seen as eigenvalue decomposition, and \( d \) eigenvectors are then the sought vectors \( y_i \), see [5] for more details.

Therefore the LLE projection can be seen as eigendecomposition of matrix \( W_{ij} \) given by equation (3.8). It has already been noted in Sec. 3.2.4 that eigendecomposition can be seen as gradient dynamics, which means that LLE
3.3. Reduced vector field

In Step 2 a vector field $\mathbf{Y}$ on $\mathcal{N}$ is sought. We shall now regard the process of identifying $\mathbf{Y}$ through the eyes of Section 2.3. The vector field $\mathbf{Y}$ is found in such a way that the trajectories on $\mathcal{N}$ corresponding to the vector field are as close as possible to the measured trajectories. The comparison can be made either on $\mathcal{M}$ (embedding trajectories on $\mathcal{N}$ into $\mathcal{M}$), or on $\mathcal{N}$ (projecting trajectories from $\mathcal{M}$ onto $\mathcal{N}$).

3.3.1. Prediction

Finally, Eq. (4.1) can be solved to obtain future trajectories on $\mathcal{N}$. The embedding then lifts the trajectories to future trajectories on $\mathcal{M}$, which is a prediction of future trajectories on $\mathcal{M}$.

4. Illustration

Let us now illustrate the foregoing theoretical construction on a recent successful method of machine learning in dynamical systems [12]. The physical system under investigation is a free-surface fluid, the objective is to teach a robot how to handle it. First, we address the NI modeling of such a system. The standard modeling based on the classical fluid mechanics with the Navier-Stokes equation serving as the governing equation leads to a very complex mathematical formulation. In order to avoid the difficulties associated with numerical solutions of partial differential equations, we choose the Lagrange formulation of fluid flows (the fluid is seen as composed of fluid particles) and then still a simpler formulation known as the method of Smoothed Particle Hydrodynamics (SPH), see [45], and the method of Smoothed Dissipative Particle Dynamics (SDPD), see [46, 47]. The data base DB presented to the robot thus consists of pseudo-experimental data. These are the fluid particle trajectories calculated as solutions to the system of ordinary differential equations serving as the governing equations in the SPH and SDPD formulations of fluid flows.

4.1. Smoothed particle hydrodynamics

First, we briefly recall the SPH and SDPD methods. Imagine a fluid motion. Instead of the usual way based on partial differential equations (e.g., Navier-Stokes equations), the fluid can be described as composed of fluid quasi-particles. Dynamics of these particles is governed by Hamilton canonical equations, which are ordinary differential equations. The particles are also equipped with their
energy or entropy, which makes it possible to address the thermodynamic behavior, see e.g. [45, 46].

Apart from the Hamiltonian part, the evolution equations also contain irreversible terms. These terms can be constructed by direct discretization of the continuous viscous terms (as in SPH) or by including fluctuations compatible with the continuous terms through the fluctuation-dissipation theorem (SDPD), see e.g. [47].

4.2. Reduced manifold

Let us now recall a recent successful approach to machine learning taking advantage of the GENERIC framework [12]. In this approach a pseudo-experimental data of fluid motion are first acquired from an SPH simulation, having a few thousand particles, \( n \) being the number of particles. The detailed manifold \( \mathcal{M} \) is thus \( 7n \)-dimensional, since each particle has its position (3), velocity (3) and energy (1). The measured states of the particles represent trajectories on \( \mathcal{M}, G(\mathcal{M}) \).

Then three different methods searching for a suitable lower-dimensional sub-manifold are employed, namely POD (see above), locally linear embedding (LLE) and topological data analysis (TDA). Each of the methods leads to a different manifold \( \mathcal{N} \). The best performance was given by TDA, where the manifold \( \mathcal{N} \) was consisting of a few particles (instead of a few thousand) while still giving reasonable approximation of the pseudo-experimental data. In all the three approaches, however, the reduced manifold \( \mathcal{N} \) was similar to the original high-dimensional manifold \( \mathcal{M} \) in the sense that it also described pseudo-particle states (although much lower number of them). The methods provided a projection \( \pi \) from \( \mathcal{M} \) to \( \mathcal{N} \) as well as the embedding of \( \mathcal{N} \) into \( \mathcal{M} \). This is the manifold recognition.

4.3. Reduced vector field

In step 2 a vector field \( \mathbf{Y} \) on \( \mathcal{N} \) is sought. It is assumed that the vector field on \( \mathcal{N} \) has the GENERIC structure

\[
\dot{y}^a = \mathbb{L}^{ab} \dot{y}^b + \mathbb{M}^{ab} \dot{S} y^b,
\]

where \( \mathbb{L} \) is a Poisson bivector, \( \mathbb{E} \) is an energy on \( \mathcal{N} \), \( \mathbb{M} \) is a dissipative matrix on \( \mathcal{N} \) and \( \mathbb{S} \) is an entropy on \( \mathcal{N} \).

Energy \( \mathbb{E} \) is assumed to be quadratic in \( y \) so that its gradient is linear operator on \( y \) (a matrix), and the same is assumed for entropy \( \mathbb{S} \). The dissipative matrix \( \mathbb{M} \) is assumed to be piecewise constant—data are fitted by regions.

\[\text{It is often assumed that the reduced manifold keeps the structure of a cotangent bundle, such that a reversible evolution is generated by the canonical Poisson bivector (equipped with entropy) as on the original manifold. Therefore, the reduced dynamics can be interpreted as dynamics of a lower number of (quasi-)particles, since otherwise another Poisson bivector would have to be sought. This is not, however, strictly necessary nor a limitation of the method, see for instance [43, 49].}\]

\[\text{corresponding to dissipation potential } \Xi = \frac{1}{2} y^a \mathbb{M}^{ab} y^b,\]
not necessarily monolithically—symmetric and positive definite. The unknown matrices \( \uparrow E_{y^b} \), \( \uparrow S_{y^b} \), and \( \uparrow M \) are then fitted by least squares so that the trajectories given by integration of Eqs. (4.1) coincide with projection of the measured trajectories as much as possible. Least squares can also be interpreted as a result of gradient dynamics [50], which means that reduction takes place in that step.

Note that Eq. (4.1) can be simplified to
\[
\dot{y}^a = \uparrow L^{ab} \downarrow F_{y^b} - T \uparrow M^{ab} \downarrow F_{y^b} \tag{4.2}
\]
for isothermal systems. Here \( \downarrow F = \uparrow E - T \downarrow S \) is the Helmholtz free energy. In this case only two matrices would be necessary.

4.4. Prediction

Finally, Eq. (4.1) are solved to obtain future trajectories on \( N \). The embedding then lifts the trajectories to future trajectories on \( M \), which is a prediction of future trajectories on \( M \), showing remarkable precision in [12].

5. Conclusion

Learning is a process of getting an insight that allows to make quick predictions. If the input of learning is a dynamical system, then the insight is an information about important qualitative features (about a pattern) in the phase portrait (i.e. in the collection of trajectories). One way to get such information is to reduce the dynamical system under investigation to a simpler dynamical system whose phase portrait is the pattern in the phase portrait corresponding to the original dynamical system. The reduction process in which the pattern is recognized can be interpreted as the learning process. This process can also be regarded as a time evolution generated by a dynamics that we call a reducing dynamics or also a learning dynamics. In the reducing time evolution the pattern in the phase portrait of the original dynamical system emerges. The reducing dynamics is dissipative and is driven by a potential called entropy. We can use this terminology, since in the particular case of reductions investigated in statistical mechanics such potentials are indeed physical entropies arising in thermodynamics.

In the machine learning the input of learning is the phase portrait (data base). In this paper we suggest that the approach to learning via reducing dynamics and associated thermodynamics, that has been developed in the context of the dynamical system theory, can also be applied and can be useful in the machine learning. We illustrate the suggestion on the example worked out in [12].

Within the thermodynamic framework, an inverse mapping can be also defined, ensuring scale bridges and the connection between data, fine and reduced models, patterns, etc., which is a crucial point for efficient data-assimilation. In the future we intend to explore new routes opened by the connection with thermodynamics. For instance, thermodynamics provides a close connection of
entropy to fluctuations. We are suggesting that the entropy drives the learning dynamics. This means that an appropriate analysis of fluctuations involved in the data base can serve as a complementary tool in machine learning.

Acknowledgments

F.Ch. thanks ESI Group through its research chair at “Arts et Métiers ParisTech”, whose first invited position was Prof. M. Grmela, for performing the researches here addressed. F. Ch. also knowledges Dr. Alain de Rouvray by the rich and inspiring discussions on pattern recognition as the first step towards machine learning and artificial intelligence, motivating the preset work. The support from ANR (Agence Nationale de la Recherche, France) through its grant AAPG2018 DataBEST is also gratefully acknowledged.

E.C. also acknowledges the financial support of ESI Group through the project “Simulated Reality”. The support given by the Spanish Ministry of Economy and Competitiveness through Grant number DPI2017-85139-C2-1-R, and by the Regional Government of Aragon and the European Social Fund, research group T88, is also greatly acknowledged.

M.G. was supported by the Natural Sciences and Engineering Research Council of Canada, Grants 3100319 and 3100735.

B.M. acknowledges the support of the Spanish Ministry of Science, Innovation and Universities through grant number PRE2018-083211.

M.P. was supported by Czech Science Foundation, Project No. 17-15498Y, and by Charles University Research Program No. UNCE/SCI/023.

Bibliography

References

[1] Gesamtausgabe, L.. Ludwig Boltzmann Gesamtausgabe - Collected Works. 1983. ISBN 9789904000071.

[2] Gorban, A.N., Grechuk, B., Tyukin, I.Y.. Augmented artificial intelligence: a conceptual framework. 2018. arXiv:1802.02172.

[3] Kosambi, D.D.. J Indian Math Soc 1943;7:76–88.

[4] Golub, G., Van Loan, C.. Matrix Computations. Johns Hopkins Studies in the Mathematical Sciences; Johns Hopkins University Press; 2013. ISBN 9781421407944. URL: https://books.google.cz/books?id=X5YfsuCwpzNC

[5] Roweis, S.T., Saul, L.K.. Nonlinear dimensionality reduction by locally linear embedding. Science 2000;290(5500):2323–2326.

[6] Wasserman, L.. Topological data analysis. Annual Review of Statistics and Its Application 2018:5(1):501–532.
[7] Brunton, S., Proctor, J., Kutz, J.. Discovering governing equations from data by sparse identification of nonlinear dynamical systems. Proceedings of the National Academy of Sciences 2016; doi:10.1073/pnas.1517384113

[8] Kaiser, E., Kutz, J., Brunton, S.. Discovering conservation laws from data for control. 2018.

[9] Kevrekidis, Y., Samaey, G.. Equation-free modeling. Scholarpedia 2010;5(9):4847.

[10] E, W.. A proposal on machine learning via dynamical systems. Commun Math Stat 2017;5:1–11. doi:10.1007/s40304-017-0103-z

[11] E, W., Han, J., Li, Q.. A mean-field optimal control formulation of deep learning. Research in the Mathematical Sciences 2018;6(1):10. URL: https://doi.org/10.1007/s40687-018-0172-y

[12] Moya, B., Gonzalez, D., Alfaro, I., Chinesta, F., Cueto, E.. Learning slosh dynamics by means of data. Computational Mechanics 2019;64(2):511–523. URL: https://doi.org/10.1007/s00466-019-01705-3

[13] Maes, C., Netočný, K.. Time-reversal and entropy. eprint arXiv:cond-mat/0202501 2002.

[14] Grmela, M., Öttinger, H.C.. Dynamics and thermodynamics of complex fluids. i. development of a general formalism. Phys Rev E 1997;56:6620–6632. URL: http://link.aps.org/doi/10.1103/PhysRevE.56.6620

[15] Öttinger, H.C., Grmela, M.. Dynamics and thermodynamics of complex fluids. ii. illustrations of a general formalism. Phys Rev E 1997;56:6633–6655. doi:10.1103/PhysRevE.56.6633

[16] Öttinger, H.. Beyond Equilibrium Thermodynamics. Wiley; 2005. ISBN 9780471727910.

[17] Pavelka, M., Klika, V., Grmela, M.. Multiscale Thermo-Dynamics. Berlin, Boston: De Gruyter; 2018. ISBN 9783110350951. URL: http://www.degruyter.com/view/books/9783110350951/9783110350951/9783110350951.xml

[18] Pavelka, M., Klika, V., Grmela, M.. Time reversal in nonequilibrium thermodynamics. Phys Rev E 2014;90(062131).

[19] Onsager, L.. Reciprocal relations in irreversible processes. I. Phys Rev 1931;37:405–426. URL: http://link.aps.org/doi/10.1103/PhysRev.37.405

[20] Onsager, L.. Reciprocal relations in irreversible processes. ii. Phys Rev 1931;38:2265–2279. doi:10.1103/PhysRev.38.2265

[21] Casimir, H.B.G.. On onsager’s principle of microscopic reversibility. Rev Mod Phys 1945;17:343–350. doi:10.1103/RevModPhys.17.343

[22] de Groot, S.R., Mazur, P.. Non-equilibrium Thermodynamics. New York: Dover Publications; 1984.

[23] Grmela, M., Klika, V., Pavelka, M.. Reductions and extensions in mesoscopic dynamics. Phys Rev E 2015;92(032111).

[24] Grmela, M.. Externally driven macroscopic systems: Dynamics versus thermodynamics. Journal of Statistical Physics 2017;166(2):282–316. URL: http://dx.doi.org/10.1007/s10955-016-1694-6 doi:10.1007/s10955-016-1694-6

[25] Grmela, M.. Generic guide to the multiscale dynamics and thermodynamics. Journal of Physics Communications 2018;2(032001).

[26] Shannon, C.E.. A mathematical theory of communication. Bell System Technical Journal 1948;27:379–423,623–656.

[27] Jaynes, E.T.. Information theory and statistical mechanics. Physical Review 1957;106(4):620–630.

[28] Gorban, A., Karlin, I.. Invariant Manifolds for Physical and Chemical Kinetics. Lecture Notes in Physics; Springer; 2005. ISBN 9783540226840. URL: http://books.google.cz/books?id=hjvjPmL5rPwC

[29] Klika, V., Pavelka, M., Váňer, P., Grmela, M.. Dynamic maximum entropy reduction. Entropy 2019;21(715). doi:10.3390/e21070715

[30] Chapman, S., Cowling, T., Burnett, D., Cercignani, C.. The Mathematical Theory of Non-uniform Gases: An Account of the Kinetic Theory of Viscosity, Thermal Conduction and Diffusion in Gases. Cambridge Mathematical Library; Cambridge University Press; 1990. ISBN 9780521408448. URL: https://books.google.cz/books?id=Cbp5JP20TrwC

[31] Callen, H.. Thermodynamics: an introduction to the physical theories of equilibrium thermostatistics and irreversible thermodynamics. Wiley; 1960. URL: http://books.google.cz/books?id=mf5QAAAAAAAJ

[32] Turkington, B.. An optimization principle for deriving nonequilibrium statistical models of hamiltonian dynamics. J Stat Phys 2013;152:569–597.

[33] Ehrenfest, P., Ehrenfest, T.. The Conceptual Foundations of the Statistical Approach in Mechanics. Dover Books on Physics; Dover Publications; 1990. ISBN 9780486662503.
[34] Gorban, A.N., Karlin, I.V., Öttinger, H.C., Tatarinova, L.L.. Ehrenfest’s argument extended to a formalism of nonequilibrium thermodynamics. Physical Review E 2001;63(066124).

[35] Karlin, I.V., Tatarinova, L.L., Gorban, A.N., Öttinger, H.C.. Irreversibility in the short memory approximation. Physica A: Statistical Mechanics and its Applications 2003;327(3-4):399–424.

[36] Pavelka, M., Klika, V., Grmela, M.. Thermodynamic explanation of landau damping by reduction to hydrodynamics. Entropy 2018;20.

[37] Pavelka, M., Klika, V., Grmela, M.. Ehrenfest regularization of hamiltonian systems. Physica D: Nonlinear phenomena 2019;Accepted.

[38] Grmela, M.. Role of thermodynamics in multiscale physics. Computers and Mathematics with Applications 2013;65(10):1457 – 1470. URL: http://www.sciencedirect.com/science/article/pii/S0898122112006803. doi: http://dx.doi.org/10.1016/j.camwa.2012.11.019.

[39] Grmela, M.. Contact Geometry of Mesoscopic Thermodynamics and Dynamics. Entropy 2014;16(3):1652–1686. doi:10.3390/e16031652.

[40] Čapek, K.. R.U.R. (Rossum’s Universal Robots). London ; New York :Penguin Books; 2004.

[41] Chatterjee, A.. An introduction to the proper orthogonal decomposotion. Current Science 2000;78(7).

[42] Brockett, R.. Dynamic-systems that sort lists, diagonalize matrices, and solve linear-programming problems. Linear algebra and its applications 1991;146:79–91. doi:10.1016/0024-3795(91)90021-N.

[43] Bloch, A.M., Krishnaprasad, P.S., Marsden, J.E., Ratiu, T.S.. Dissipation induced instabilities. Annales de l’IHP Analyse non linéaire 1994;11(1):37–90.

[44] Absil, A.. Continuous-time systems that solve computational problems. International Journal of Unconventional Computing 2006;2(4):291–304.

[45] Gingold, R., Monaghan, J.. Smoothed particle hydrodynamics: theory and application to non-spherical stars. Mon Not R Astron Soc 1977;181(3):375–389.

[46] Español, P., Revenga, M.. Smoothed dissipative particle dynamics. Phys Rev E 2003;67:026705. URL: https://link.aps.org/doi/10.1103/PhysRevE.67.026705. doi:10.1103/PhysRevE.67.026705.

[47] Ellero, M., Español, P.. Everything you always wanted to know about sdpd ”(but were afraid to ask) “. Appl Math Mech 2018;39(1):103–124.
[48] González, D., Chinesta, F., Cueto, E.. Thermodynamically consistent
data-driven computational mechanics. Continuum Mechanics and Thermodynamics 2018;doi:10.1007/s00161-018-0677-z

[49] González, D., Chinesta, F., Cueto, E.. Learning corrections for hyperelastic models from data. Frontiers Materials 2019;6(14).

[50] Brockett, R.. Least squares matching problems. Linear Algebra and its Applications 1989;122-124:761 – 777. URL:
http://www.sciencedirect.com/science/article/pii/0024379589906757
doi:https://doi.org/10.1016/0024-3795(89)90675-7 special Issue on Linear Systems and Control.