Preprints of the 21st IFAC World Congress (Virtual)
Berlin, Germany, July 12-17, 2020

Reducing dynamics

Miroslav Grmela * **Michal Pavelka** **

* *École Polytechnique de Montréal, C.P.6079 suc. Centre-ville, Montréal, H3C 3A7, Québec, Canada (email: miroslav.grmela@polymtl.ca)*
** *Mathematical Institute, Faculty of Mathematics, Charles University, Sokolovská 83, 18675 Prague, Czech Republic (email: pavelka@karlin.mff.cuni.cz)*

Abstract: Reduction of a dynamical theory consists of two steps: (i) finding its phase portrait (collection of all trajectories), and (ii) recognizing in it a pattern that is then identified with the phase portrait of the reduced dynamical theory. The original dynamical system becomes split in the reduction into the reduced dynamics representing the recognized pattern and the reducing dynamics representing the process of its emergence. From the experimental point of view, the reducing dynamics represents the process of preparing macroscopic systems for using the reduced description.

Keywords: Dynamical systems, control, reduction, thermodynamics.

1. INTRODUCTION

An effort to combine mechanics with heat gave birth to thermodynamics. Its most significant contribution is the introduction of a new potential called entropy. Features of the microscopic mechanics of $\sim 10^{23}$ particles that are detectable in macroscopic observations emerge in the process of maximizing the entropy subjected to certain constraints. This way of extracting pertinent features from complex and very large data is called Maximum Entropy Principle or, in short, MaxEnt. From the experimental point of view, the macroscopic features are seen in the macroscopic experimental observations only in systems that have been specifically prepared. For example, the preparation process for experimental observations made in the classical equilibrium thermodynamics is to leave the system under investigation sufficiently long time free of external influences and internal constraints. The entropy is a potential generating the time evolution involved in the preparation process. The entropy thus makes its first appearance in the preparation for certain type of experimental observations and is maximized in the course of the process.

We introduce the following terminology and notation. The level of description involving more details is called an upper level. The level of description involving less details is called a lower level. The state space used on the upper level is denoted M, its elements x (i.e. $x \in M$). Similarly N and $y \in N$ denotes the state space and its elements on the lower level. Quantities belonging to the upper respectively the lower level are denoted by the upper index $\uparrow$ and $\downarrow$ respectively. Both levels have an autonomous existence. They have arisen from an experience collected in certain type of experimental observations (different for a different level). If we consider them both simultaneously then we call the lower level also a reduced level and the preparation process from the upper to the lower level is governed by a reducing dynamics. If we assume that the entropy is known and consider only its maximization we call MaxEnt static. If we consider the reducing dynamics that maximizes the entropy we call MaxEnt dynamic.

To give an example, x is a one particle distribution function and y are hydrodynamic fields; the upper level in this example is the Boltzmann level of kinetic theory and the lower level is the level of hydrodynamics. In another example we take y to be the volume, the energy and the number of moles. In this case the lower level is the level of the classical thermodynamics and the reducing (i.e. the preparation) process is governed by the Boltzmann kinetic equation. This latter example is historically the first example Gesamtausgabe (1983) in which the reducing dynamics has been mathematically formulated.

The upper level involves always the time evolution (called the upper time evolution). The lower level can but it does not have to involve the time evolution. For example the level of hydrodynamics does involve the time evolution and thus if we consider hydrodynamics as a lower level it will be the lower level with the lower time evolution. But there are levels without the time evolution. In particular it is the level of equilibrium thermodynamics. If the lower level involves the lower dynamics we shall also consider reductions from the upper level to the vector fields of the lower dynamics (i.e. the mapping $M \to \mathfrak{X}(N)$). We use "rate" to distinguish the concepts and the quantities involved in reductions $M \to \mathfrak{X}(N)$ from the same type of concepts and quantities involved in reductions $M \to N$. We thus have the concept of entropy (denoted S) involved in the analysis $M \to N$ and the rate entropy (denoted Σ) involved in the analysis of $M \to \mathfrak{X}(N)$. The MaxEnt principle becomes the Maximum Rate Entropy Principle (MaxRent).

2. STATIC MAXENT

The input of MaxEnt is the upper fundamental thermodynamic relation

$$\begin{aligned} &Y^{\uparrow}(x) = y \\ &S^{\uparrow}(x) \end{aligned} \tag{1}$$

Both the mappings $Y^{\uparrow} : M \to N$ and $S^{\uparrow} : M \to \mathbb{R}$ are assumed to be sufficiently regular, the mapping $S^{\uparrow}$ is moreover assumed to be a concave function of x. MaxEnt is formulated as follows. First, we introduce an upper thermodynamic potential

$$\Phi^{\uparrow}(x, y^*) = -S^{\uparrow}(x) + < y^*, Y^{\uparrow}(x) > \tag{2}$$

where y^* are Lagrange multipliers and $<,>$ is a pairing in N. Next, we solve equation

$$\Phi^{\uparrow}_x = 0 \tag{3}$$

(we use hereafter the shorthand notation $\Phi^{\uparrow}_x = \frac{\partial \Phi^{\uparrow}}{\partial x}$). Let its solution, called an upper equilibrium state, be $\hat{x}(y^*)$. In the third step we evaluate the upper thermodynamic potential $\Phi^{\uparrow}(x, y^*)$ at $\hat{x}(y^*)$,

$$S^{\downarrow *}(y^*) = \Phi^{\uparrow}(\hat{x}(y^*), y^*) \tag{4}$$

where $S^{\downarrow *}(y^*)$ is called a lower conjugate entropy implied by the upper fundamental thermodynamic relation (1). In order to obtain the lower entropy $S^{\downarrow}(y)$ implied by the upper fundamental thermodynamic relation (1), we make the standard Legendre transformation $S^{\downarrow *}(y^*) \to S^{\downarrow}(y)$ (i.e. we introduce $\Phi^{\downarrow *}(y^*, y) = -S^{\downarrow *}(y^*) + < y^*, y >$ solve $\Phi^{\downarrow *}_{y^*} = 0$ (let its solution be $\hat{y}^*(y)$) and obtain $S^{\downarrow}(y) = \Phi^{\downarrow *}(\hat{y}^*(y), y)$).

Summing up, we made the MaxEnt reduction of the upper fundamental thermodynamic relation (1) in two stages:

$$(S^{\uparrow}(x), Y^{\uparrow}(x)) \to (S^{\downarrow *}(y^*), y^*) \to (S^{\downarrow}(y), y) \tag{5}$$

The second mapping in (5) is the standard Legendre transformation, the first mapping is the reducing Legendre transformation which is just an alternative viewpoint of the maximization of $S^{\uparrow}(x)$ subjected to constraints $Y^{\uparrow}(x)$ with y^* playing the role of the Lagrange multipliers.

Example

We choose $x = f(\boldsymbol{r}, \boldsymbol{v})$, where $\boldsymbol{r}$ ia the position coordinate and $\boldsymbol{v}$ momentum of one particle; $y = (E, N^{(mol)})$, where E is the energy per unit volume and $N^{(mol)}$ the number of moles per unit volume. The upper fundamental thermodynamic relation: $(E, N^{(mol)}) = (\int d\boldsymbol{r} \int d\boldsymbol{v} f \frac{\boldsymbol{v}^2}{2m}; \; N^{(mol)} = \int d\boldsymbol{r} \int d\boldsymbol{v} f); \; S^{\uparrow} = -\int d\boldsymbol{r} \int d\boldsymbol{v} f \ln f$, m is the mass of one particle;. The MaxEnt reduction (5) leads in this example to the entropy $S^{\downarrow}(E, N^{(mol)})$ that in the classical equilibrium thermodynamics represents the ideal gas (for details see Pavelka et al. (2018)).

Remark 1

The MaxEnt reduction (5) gives the lower entropy as a function of the upper fundamental thermodynamic relation (1) and the Lagrange multipliers y^* (that at the end of the reduction appear as conjugates of the lower state variables y). The question of how can we find the upper fundamental relation is discussed in Section 4. If the lower level involves the time evolution then the only information about the lower vector field that is implied by the MaxEnt reduction (5) is that it is the upper vector field restricted to the submanifold of equilibrium states $\hat{x}(y^*)$ and projected (in a way that remains to be determined)) on its tangent space. Various extensions of MaxEnt that aim at the lower entropy as well as the lower vector field are discussed in Klika et al. (2019); Grmela et al. (2020).

Remark 2

The fundamental thermodynamic relation can be formulated on the level of the classical equilibrium thermodynamics in two equivalent representations: (i) the entropy representation $(E, N^{(mol)}, S(E, N^{(mol)}))$ and (ii) the energy representation $(S, N^{(mol)}, E(S, N^{(mol)}))$. The exchange of the roles between the energy E and the entropy S is possible because $S_E = E^* = \frac{1}{T} > 0$, where T is the absolute temperature. Moreover, because of the ubiquity in the nature of the walls that freely pass or stop the passage of the internal energy, the temperature T can be easily measured by thermometers.

Both the double view of the fundamental representation as well as the easy way to measure the temperature do not extend to the general mesoscopic formulation (1). With the classical equilibrium thermodynamics as the lower level, the general upper fundamental thermodynamic relation (1) takes the form $(E(x), N^{(mol)}(x), S^{\uparrow}(x))$ together with the Lagrange multipliers $(E^*, N^{(mol)*})$. In such general mesoscopic setting the roles of the entropy and the energy cannot be exchanged and the quantity E^* plays only the role of the Lagrange multiplier (it becomes the conjugate of the energy only after the reduction has been completed). This is the reason for the well known difficulty with an appropriate definition of (and an appropriate way to measure) the temperature on mesoscopic levels. How can we express the temperature T in terms of the upper state variables x? The main problem is that there does not seem to be a single answer to this question. For example, T can be seen as an appropriately chosen moment of $\hat{x}(E^*, N^{(mol)})$.

Remark 3

From the mathematical point of view, MaxEnt is a sequence of, broadly speaking, Legendre transformations. We can then ask the question of what is the geometrical environment in which Legendre transformations appear as natural transformations. The contact structure geometry answers this question since the contact structure is preserved in Legendre transformations (see more Hermann (1984), Grmela (2018))

3. STATIC MAXRENT

The reduction discussed in the previous section is based on the fact that both the upper and the lower levels are autonomous. This means that the lower phase portrait (collection of all trajectories in N) has to be visible aa a pattern in the upper phase portrait (collection of all trajectories in M). Moreover, we have also used the experimental observation according to which the system under consideration has to be prepared before the lower level can be applied. The preparation process is governed by the reducing dynamics. Both of these features of the reduction are independent of the presence or absence of the lower dynamics. However, there is an important difference. In the former case the main interest is to obtain the lower dynamics as a reduced upper dynamics (for example the famous and the extensively studied problem of reducing the Boltzmann kinetic equations to hydrodynamic equations). How can we combine the reduction presented in the previous section with the search for the reduced upper dynamics? What does such combination bring new to the lower dynamics seen as a reduced upper dynamics?

The approach to equilibrium states investigated in MaxEnt is replaced in MaxRent with the approach to the lower vector field that is seen as a reduced upper vector field. The input of MaxRent is the upper rate fundamental thermodynamic relation (compare with (1))

$$\begin{aligned} J(y) &= J^{\uparrow}(x,y) \\ \Sigma^{\downarrow} &= \Sigma^{\uparrow}(x) \end{aligned} \tag{6}$$

where $J(y) \in \mathfrak{X}(N)$. With (6) replacing (1) we now follow all the steps made in the previous section. The lower rate entropy $\Sigma^{\downarrow}(J(y))$ implied by upper rate fundamental relation (6) arises, as in (5)), in two stages:

$$(\Sigma^{\uparrow}(x), J^{\uparrow}(x,y)) \to (\Sigma^{\downarrow *}(J^*(y)), J^*(y)) \to \\ \to (\Sigma^{\downarrow}(J(y)), J(y)). \tag{7}$$

In the first stage we are making the Legendre transformation in which the upper rate entropy is maximized subjected to the constraints $J^{\uparrow}(x,y)$ with $J^*(y)$ playing the role of the Lagrange multiplier. The second stage is the regular Legendre transformation.

Remark

The output of the MaxRent reduction (7) is the lower vector field $J(y)$ and the lower rate entropy $\Sigma^{\downarrow}(J(y))$. The input is the upper fundamental thermodynamic relation (6) and the Lagrange multipliers $J^*(y) = \Sigma^{\downarrow}_{J(y)}$. In comparison with MaxEnt, the lower vector field in the output $J(y)$ is new. The provenance of the upper rate fundamental relation (6) is discussed in Section 5.

4. DYNAMIC MAXENT (REDUCING DYNAMICS)

Both reductions presented in the two previous sections emerge in the process of trying to recognize a pattern in the upper time evolution. After the pattern has been recognized, the upper dynamics becomes split into the reduced dynamics representing the recognized pattern and the reducing dynamics representing the process of its emergence. From the experimental point of view, the reducing dynamics represents the process of preparing macroscopic systems for using the lower level description. Instead of engaging in the complex investigation of the upper time evolution that is necessary for revealing such split, we shall only attempt to identify the time evolution during which the first transformation in (5) is made.

We begin with the maximization of $S^{\uparrow}(x)$ without constraints. There are two obvious candidates for the time evolution maximizing $S^{\uparrow}(x)$. First, it is the gradient time evolution

$$\dot{x} = \Lambda S^{\uparrow}_x \tag{8}$$

where Λ is a positive operator. The second candidate is

$$\dot{x} = \left[\Xi^{\uparrow}(x^*, x)_{x^*}\right]_{x^* = S^{\uparrow}_x} \tag{9}$$

that generalizes (8). The quantity $\Xi^{\uparrow}$, called a dissipation potential, is a real valued function of (x, x^*) such that: (i) $\Xi^{\uparrow}(x,0) = 0$, (ii) $\Xi^{\uparrow}$ reaches its minimum at $x^* = 0$, (ii) $\Xi^{\uparrow}$ is convex in a neighborhood of $x^* = 0$. In the particular case of $\Xi^{\uparrow} = \frac{1}{2} < x^*, \Lambda^{\uparrow} x^* >$ the right hand side of (9) becomes the same as the right hand side of (8).

Indeed, solutions to both (8) and (9) approach, as the time $t \to \infty$, to $\hat{x}(y^*)$. This is because (8) and (9) imply $\dot{S}^{\uparrow} > 0$ so that $-S^{\uparrow}(x)$ plays the role of the Lyapunov function for the approach $x \to \hat{x}(y^*)$.

Now we take into account the constraints. In the static maximization this is done by the Lagrange multiplier method. In the dynamic maximization the problem is more complex. One type of the modification of (8) or of (9) that takes into account the constraints is made in the following two steps. First, we require that the operator Λ in (8) (and a corresponding to it requirement in (9)) is degenerate in the sense that $\Lambda Y^{\uparrow}_x = 0$. Second, in the nullspace of Λ we introduce a new time evolution that leaves $S^{\uparrow}$ unchanged. We call this new time evolution a non-dissipative time evolution. Next,we construct a new vector field on M as a sum of the gradient vector field (the right hand side of (8) or (9)) and the non-dissipative vector field. If, in addition, the non-dissipative time evolution leaves the constraints unchanged then the time evolution generated by the combined vector field leaves the constraints unchanged and the upper thermodynamic potential $\Pi^{\uparrow}(x, y^*) = -S^{\uparrow}(x) + < y^*, Y^{\uparrow} >$, plays the role of the (weak) Lyapunov function for the approach $x \to \hat{x}(y^*)$. The Lyapunov function is weak since $\dot{\Phi}^{\uparrow} \leq 0$. The weak inequality implies that solutions approach the non-dissipative submanifold $\{x \in M | \dot{\Phi}^{\uparrow} = 0\}$. The equilibrium submanifold composed of $\hat{x}(y^*)$ is a submanifold of the non-dissipative submanifold. In order to prove the approach $x \to \hat{x}(y^*)$ we need to prove that the non-dissipative submanifold is approached only when the equilibrium manifold is approached. An example of a proof of this kind is in Desvillettes and Villani (2005). An example of the reducing dynamics that makes the maximization described in the example in Section 2 is the Boltzmann kinetic equation. An abstract Boltzmann equation whose solutions make the MaxEnt reduction with the level of the classical equilibrium thermodynamics being the lower level is called GENERIC (see Pavelka et al. (2018) and references cited therein).

Remark

The fundamental thermodynamic relations (1) and (6) arise in the pattern recognition process in the phase portrait of the upper dynamics. This realization shows, of course, only a direction for further investigations leading eventually to the fundamental thermodynamic relations representing specific macroscopic systems. The viewpoints and methods developed in stochastic dynamics provide another complementary avenue leading to the fundamental thermodynamic relations Feynman (1972), Jizba and Korbel (2019).

5. DYNAMIC MAXRENT (REDUCING RATE DYNAMICS)

The same steps that led us in the previous section to the split of the upper time evolution into the reducing and the reduced time evolution lead us also to another split into reducing rate time evolution and the reduced rate time evolution. The latter is the time evolution of the lower vector fields and thus it is no time evolution. The reducing rate time evolution results in the lower rate entropy $\Sigma^{\downarrow *}(J^*(y))$, and, via the relation $J(y) = \Sigma^{\downarrow *}_{J^*(y)}$, to the lower vector field $J(y)$. Both the lower rate entropy $\Sigma^{\downarrow}(J(y)$ and the Lagrange multipliers $J^*(y)$ arise in the process of the pattern-recognition type analysis of the upper dynamics.

6. CONCLUDING REMARK

Let our goal be to simplify (to reduce) a complex dynamical system. We argue that it is useful to pay an equal attention to the result of the simplification (i.e. to the simpler dynamical system) as well as to the process leading to it. The latter process (reducing dynamics) brings to the reduction a extra information of the thermodynamical nature. From the experimental point of view, the reducing dynamics represents the process of preparing the system under observations to the observations made in the reduced setting.

ACKNOWLEDGEMENTS

MP was supported by Czech Grant Agency, grant no. 20-22092S.

REFERENCES

Desvillettes, L. and Villani, C. (2005). On the trend to global equilibrium for spatially inhomogeneous kinetic systems: The Boltzmann equation. *Inventiones mathematicae*, 159, 245–316.

Feynman, R. (1972). *Statistical Mechanics: A Set of Lectures*. Advanced Book Classics. Basic Books.

Gesamtausgabe, L. (1983). *Ludwig Boltzmann Gesamtausgabe - Collected Works*.

Grmela, M. (2018). GENERIC guide to the multiscale dynamics and thermodynamics. *J. Phys. Commun.*, 2(032001).

Grmela, M., Klika, V., and Pavelka, M. (2020). Gradient and GENERIC evolution towards reduced dynamics. *Phil. Trans.R.Soc.A*, 378(20190472).

Hermann, R. (1984). *Geometry, Physics and Systems*. Marcel Dekker, New York.

Jizba, P. and Korbel, J. (2019). Maximum entropy principle in statistical inference: Case for non-shannonian entropies. *Phys. Rev. Lett.*, 122, 120601. doi:10.1103/PhysRevLett.122.120601. URL `https://link.aps.org/doi/10.1103/PhysRevLett.122.120601`.

Klika, V., Pavelka, M., Vágner, P., and Grmela, M. (2019). Dynamic maximum entropy reduction. *Entropy*, 21(715). doi:doi:10.3390/e21070715.

Pavelka, M., Klika, V., and Grmela, M. (2018). *Multiscale Thermo-Dynamics*. de Gruyter (Berlin).