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Extensive Lyapounov functionals for moment-preserving evolution equations

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Abstract We consider a certain class of moment-preserving equations from the point of view of their stationary solutions. Starting from a given stationary distribution, we construct a convex entropy functional which is (in a class of functions with prescribed moments) minimal precisely at this point. Under general assumptions, we show that the entropy which is canonically associated to a stationary distribution is, up to a polynomial change of variables, its Legendre–Fenchel transform. We then show that, if this entropy is extensive, necessarily the stationary distribution is a Gibbs state. Such a state being given by the exponential of the energy density, this clarifies the duality relationship between energy and entropy. ***To cite this article: J.F. Collet, C. R. Acad. Sci. Paris, Ser. I 334 (2002) 429–434.*** © 2002 Académie des sciences/Éditions scientifiques et médicales Elsevier SAS

Fonctions de Lyapounov extensives pour des problèmes d'évolution preservant certains moments

Résumé Nous considérons des solutions stationnaires pour des classes d'équations d'évolution préservant certains moments. Etant donnée une solution stationnaire, nous construisons une fonctionnelle convexe (l'entropie) qui est (dans une classe de fonctions de moments fixés) minimale en ce point. Sous des hypothèses générales, nous montrons qu'une telle entropie canoniquement associée à une distribution stationnaire est, à un changement de variable polynomial près, sa transformée de Legendre. On montre ensuite que, si la fonctionnelle ainsi obtenue est extensive, la solution stationnaire de départ est nécessairement une distribution de Gibbs. Une telle distribution étant donnée par l'exponentielle de la densité d'énergie, ceci clarifie la relation de dualité entre énergie et entropie. ***Pour citer cet article : J.F. Collet, C. R. Acad. Sci. Paris, Ser. I 334 (2002) 429–434.*** © 2002 Académie des sciences/Éditions scientifiques et médicales Elsevier SAS

Version française abrégée

1. Introduction

Cette Note est motivée, à l'origine, par un travail de Giuseppe Toscani [5] sur la construction de fonctionnelles d'entropie pour une classe de problèmes d'évolution préservant un certain nombre de

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moments. Plus précisément, le problème considéré par Toscani est le suivant : soit F_m une classe de fonctions d'intégrale fixée :

$$F_m = \left\{ f \geqslant 0 : \int_\Omega f(x)\,\mathrm{d}x = m \right\},$$

où Ω est un intervalle de $\mathbb{R}$ et m est une constante positive fixée, et soit f_∞ un élement de F_m de la forme :

$$f_\infty(x) = g_\infty\big(\big|\psi(x)\big|^2\big), \tag{1}$$

où ψ est une fonction affine, et g_∞ est une fonction monotone. Cherchant à définir une fonctionnelle convexe H sur F_m qui soit minimale au point g_∞ et qui soit de la forme :

$$H(f) = \int_\Omega \big[\big|\psi(x)\big|^2 f(x) + \Phi\big(f(x)\big)\big]\,\mathrm{d}x, \tag{2}$$

Toscani [5] montre que nécessairement la fonction Φ vérifie la relation :

$$\Phi'(r) = -g_\infty^{-1}(r) + \lambda r,$$

pour une certaine constante λ. Si la forme particulière (1) choisie pour l'optimum est motivée par l'application aux états Maxwelliens de la physique statistique, en revanche la forme particulière (2) choisie pour la fonctionnelle H ne semble pas particulièrement canonique. Le but de cette Note est donc de reconsidérer ce même problème de construction de fonctionnelle convexe qui soit optimale en un point précis, d'une part en autorisant des contraintes sur un nombre quelconque de moments, d'autre part en cherchant la fonctionnelle H sous une forme plus générale que (2).

2. L'entropie comme transformée de Legendre de la solution stationnaire

Commençons par préciser les notations : étant donnés un entier n et $2n+2$ constantes $r = (r_0, \ldots, r_n) \in \mathbb{R}^{n+1}$, $m = (m_0, \ldots, m_n) \in \mathbb{R}^{n+1}$ avec $r_n \neq 0$, posons :

$$\mathcal{M}_{r,m} := \left\{ f : \mathbb{R} \to \mathbb{R} \;\middle|\; r_0 \int_\mathbb{R} f(x)\,\mathrm{d}x = m_0, \ldots, r_n \int_\mathbb{R} x^n f(x)\,\mathrm{d}x = m_n \right\}. \tag{3}$$

Autrement dit, $\mathcal{M}_{r,m}$ est un espace de fonctions dont le n-ième moment, et certains moments d'ordre inférieur, sont prescrits. Les coefficients r_k sont utilisés ici pour permettre de ne pas contraindre certains moments, la contrainte d'ordre k étant vide si $r_k = m_k = 0$. Etant donnée une fonction $f_\infty \in \mathcal{M}_{r,m}$, on cherche à construire une fonctionnelle convexe sur $\mathcal{M}_{r,m}$ qui soit minimale en f_∞. Le résultat (constructif) d'existence d'une telle fonctionnelle est le suivant :

THÉORÈME 2.1. – *Soit $g_\infty : \mathbb{R} \to \mathbb{R}$ une fonction de classe $\mathcal{C}^1$ vérifiant $g'_\infty(x) < 0$ pour tout x, et $g_\infty(+\infty) = 0$. Etant donné P un polynôme fixé de degré n, posons $f_\infty(x) = g_\infty(P(x))$ pour tout x. Supposons P et g_∞ tels que $f_\infty \in \mathcal{M}_{r,m}$. Enfin, soit $\Phi : \mathbb{R} \to \mathbb{R}$ une fonction convexe de classe $\mathcal{C}^1$ vérifiant $\Phi''(x) > 0$ pour tout x. Définissons une fonctionnelle convexe H sur $\mathcal{M}_{r,m}$ par :*

$$H(f) = \int_\mathbb{R} \Phi\big(f(x)\big)\,\mathrm{d}x.$$

Si f_∞ est le minimiseur de H sur $\mathcal{M}_{r,m}$, alors il existe deux constantes a et b, avec $a < 0$, telles que pour tout $s \in f_\infty(\mathbb{R})$ on ait :

$$\Phi'(s) = a g_\infty^{-1}(s) + b.$$

Si tous les coefficients r_k sont non nuls, il en résulte qu'on a :

$$H(f) - H(f_\infty) = a \iint_{f_\infty(x)}^{f(x)} \big[g_\infty^{-1}(s) - g_\infty^{-1}\big(f_\infty(x)\big)\big]\,\mathrm{d}s\,\mathrm{d}x. \tag{4}$$

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3. Fonctionnelles de Lyapounov extensives et états de Gibbs

La deuxième question que nous abordons ici concerne le caractère extensif de la fonctionnelle H ainsi construite : en effet si dans les applications à la physique statistique la quantité H doit jouer le rôle d'un potentiel thermodynamique, il est naturel d'exiger que celle-ci soit extensive, c'est-à-dire en termes mathématiques, homogène de degré 1. Le résultat, obtenu ici, montre que si la fonctionnelle H canoniquement associée par cette construction à une fonction f_∞ est extensive de degré un (modulo une constante additive), alors nécessairement f_∞ est un état de Gibbs :

THÉORÈME 3.1. – *En retenant toutes les hypothèses et notations du théorème précédent, supposons de plus que l'entier n soit pair, que le coefficient du polynôme P soit positif, que P ait un zéro réel, et finalement que $g_\infty(0)=1$. Si pour tout $\lambda>0$ la fonction λf_∞ minimise H sur l'ensemble $\lambda\mathcal{M}_{r,m}$, alors il existe trois constantes α, β, γ telles que g_∞ soit donnée par l'une des deux formules suivantes* :

$$g_\infty(x)=\left(1+\frac{\alpha x+\beta}{\gamma}\right)^{\gamma}\quad \forall x, \tag{5}$$

ou :

$$g_\infty(x)=\exp(\alpha x+\beta)\quad \forall x. \tag{6}$$

Enfin si on fait sur H l'hypothèse d'homogénéité suivante :

$$\forall\lambda>0,\ f\in\mathcal{M}_{r,m}:\quad H(\lambda f)-H(\lambda f_\infty)=\lambda\big(H(f)-H(f_\infty)\big),$$

alors g_∞ est donné par la relation (6).

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1. Introduction

This Note is motivated by previous work by Toscani [5] on the construction of entropy functionals for a class of moment-preserving evolution equations. More specifically, the issue addressed by Toscani is the following: consider a class F_m of functions with prescribed integral:

$$F_m=\left\{f\geqslant 0:\int_\Omega f(x)\,\mathrm{d}x=m\right\},$$

where Ω is an interval of $\mathbb{R}$ and m is a fixed constant. Let f_∞ be a fixed element of F_m of the form:

$$f_\infty(x)=g_\infty\big(\left|\psi(x)\right|^2\big), \tag{7}$$

where ψ is an affine function, and g_∞ is monotonous. Consider now functionals H which are defined on F_m and are of the form:

$$H(f)=\int_\Omega\left[\left|\psi(x)\right|^2 f(x)+\Phi\big(f(x)\big)\right]\mathrm{d}x, \tag{8}$$

for some convex function Φ. Toscani [5] then shows that, if such a functional H is minimal at f_∞, then the function Φ necessarily satisfies:

$$\Phi'(r)=-g_\infty^{-1}(r)+\lambda r,$$

for some constant λ.

While the specific form (7) chosen for the optimum is motivated by applications to Maxwell states in statistical physics, the form (8) chosen for the functional H does not seem canonical. The quadratic term in the integrand is somewhat reminiscent of entropies found in kinetic equations for massless particles (in which $k^2\,\mathrm{d}k$ is the natural measure, k denoting the wave number) [1]. One may also remark that entropies of this form arise (with one supplementary variable) in the theory of polyatomic gases [4]. However in these cases, the presence of the quadratic term has a very different physical reason.

Therefore, the aim of this Note is to revisit this problem by simultaneously including more constraints, and seeking for H in a more general form.

Let us conclude this introductory section with one word of caution: we are only interested here in the *algebra* relating the equilibrium state to the entropy; the issue of attainability is not addressed here. In this connection, a very interesting discussion may be found in [2,3].

2. The entropy as Legendre–Fenchel transform of the stationary distribution

Let us begin by defining the constraints: given any integer n and $2n+2$ constants $r=(r_0,\dots,r_n)\in\mathbb{R}^{n+1}$, $m=(m_0,\dots,m_n)\in\mathbb{R}^{n+1}$ with $r_n\neq 0$, let:

$$\mathcal{M}_{r,m} := \left\{ f:\mathbb{R}\to\mathbb{R} \;\middle|\; r_0\int_{\mathbb{R}} f(x)\,\mathrm{d}x = m_0,\dots,r_n\int_{\mathbb{R}} x^n f(x)\,\mathrm{d}x = m_n \right\}. \tag{9}$$

The given coefficients r_k are used here in order to allow some moments to not be constrained: the k-th constraint is indeed vacuous if $r_k=m_k=0$. The fact that r_n is nonzero then implies that the n-th moment is indeed prescribed: in short, $\mathcal{M}_{r,m}$ is a manifold of functions whose n-th moment, and some lower moments, are prescribed. Suppose we are given a function $f_\infty\in\mathcal{M}_{r,m}$, we want to construct a convex functional H on $\mathcal{M}_{r,m}$ such that the minimum of H on $\mathcal{M}_{r,m}$ is attained precisely at f_∞. The existence result for such a functional H is as follows:

THEOREM 2.1. – *Let $g_\infty:\mathbb{R}\to\mathbb{R}$ be a $\mathcal{C}^1$ function satisfying $g'_\infty(x)<0$ for all x, and $g_\infty(+\infty)=0$. Let P be a fixed polynomial of degree n, and put $f_\infty(x)=g_\infty(P(x))$ for all x. Assume that P and g_∞ are such that $f_\infty\in\mathcal{M}_{r,m}$. Finally, let $\Phi:\mathbb{R}\to\mathbb{R}$ be a $\mathcal{C}^1$ convex function satisfying $\Phi''(x)>0$ for all x. We define a convex functional H on $\mathcal{M}_{r,m}$ by the prescription*:

$$H(f)=\int_{\mathbb{R}}\Phi\bigl(f(x)\bigr)\,\mathrm{d}x.$$

If the point f_∞ is the minimizer of H in $\mathcal{M}_{r,m}$, then necessarily for any $s\in f_\infty(\mathbb{R})$ we have:

$$\Phi'(s)=a g_\infty^{-1}(s)+b, \tag{10}$$

for some constants a and b, with $a<0$. If all r_k's are non zero this implies the following relation:

$$H(f)-H(f_\infty)=a\iint_{f_\infty(x)}^{f(x)}\bigl[g_\infty^{-1}(s)-g_\infty^{-1}\bigl(f_\infty(x)\bigr)\bigr]\,\mathrm{d}s\,\mathrm{d}x. \tag{11}$$

Proof. – Since the minimum of H on $\mathcal{M}_{r,m}$ is attained at f_∞, by Lagrange multipliers we must have:

$$\bigl\langle H'(f_\infty),g\bigr\rangle=\int_{\mathbb{R}}\Phi'\bigl(f_\infty(x)\bigr)g(x)\,\mathrm{d}x=m_0b_0\int_{\mathbb{R}}g(x)\,\mathrm{d}x+\cdots+m_nb_n\int_{\mathbb{R}}x^n g(x)\,\mathrm{d}x,$$

for some constants $m_0,\dots,m_n$, and any g in the tangent space to $\mathcal{M}_{r,m}$. Defining a polynomial Q by:

$$Q(x)=q_0+\cdots+q_nx^n,$$

where $q_k=b_km_k$, we deduce:

$$\Phi'\bigl(g_\infty\bigl(P(x)\bigr)\bigr)=Q(x). \tag{12}$$

Differentiating this expression with respect to x, we see that the polynomials P' and Q' have exactly the same zeroes. Since these two polynomials have the same degree we must have $Q'=aP'$ for some constant a, thus $Q=aP+b$. Setting $s=g_\infty(P(x))=f_\infty(x)$ in (12) now gives (10). The relation (11) now follows upon remarking that from conservation of the moments, the term $g_\infty^{-1}(f_\infty(x))$ in the integrand gives a zero contribution.

Finally, let us remark that for a given evolution equation which has f_∞ as a stationary solution, the quantity $H(f(t))$ may or may not vary in a monotonic fashion as time increases. It is however the case that for the Boltzmann equation, or any Fokker–Planck equation, the quantity H turns out to be a Lyapounov functional.

3. Extensive Lyapounov functionals and Gibbs states

The second issue we address here is extensivity of the functional H. Indeed, thinking of applications to statistical physics, if H is to play the role of a thermodynamic potential, then it should in some sense be homogeneous of degree 1. Our next result roughly says that if the functional H canonically associated to f_∞ via the previous construction has this property, then necessarily f_∞ is a Gibbs state:

THEOREM 3.1. – *Using all the assumptions and notations of the previous theorem, assume moreover that n is even, that the leading coefficient of the polynomial P is positive, that P has a real root, and finally that $g_\infty(0) = 1$. If for any $\lambda > 0$, the point λf_∞ is the minimizer of H on the class $\lambda\mathcal{M}_{r,m}$, then there exists three constants α, β, γ such that g_∞ is either of the form*:

$$g_\infty(x) = \left(1 + \frac{\alpha x + \beta}{\gamma}\right)^\gamma \quad \forall x, \tag{13}$$

or of the form:

$$g_\infty(x) = \exp(\alpha x + \beta)\ \forall x. \tag{14}$$

If we assume the following stronger homogeneity assumption:

$$\forall\lambda > 0, \quad f \in \mathcal{M}_{r,m}: \quad H(\lambda f) - H(\lambda f_\infty) = \lambda\big(H(f) - H(f_\infty)\big),$$

then g_∞ is given by relation (14).

Before we indicate how the proof works, let us note that this result provides a new justification for the Boltzmann formula familiar from equilibrium statistical physics: out of all equilibrium states of the form $f_\infty(x) = g_\infty(P(x))$, the only ones that give rise to extensive entropies are Gibbs states. This point of view is in a sense converse to the classical point of view adopted in statistical physics textbooks, in which the Boltzmann formula is obtained by a coarse-graining and optimizing procedure, and extensivity of the associated entropy then follows.

In the extensive case, (10) gives the following expression for Φ:

$$\Phi(r) = c_1 r \ln r + c_2 r + c_3,$$

for three constants c_1, c_2, c_3. This shows that (if we assume for instance $r_1 \neq 0$) the quantity $H(f) - H(f_\infty)$ is, within a multiplicative constant, the Kullback–Leibler distance between f and f_∞.

Stationary states of the form (13) on the other hand are not unphysical, a well-known example being the Barenblatt–Pattle profile for the p-heat equation, as noted by Toscani [5].

Let us now sketch the proof of the theorem: for any $\lambda > 0$, since the minimizer of H on $\lambda\mathcal{M}_{r,m} = \mathcal{M}_{r,\lambda m}$ is λf_∞, we may apply the conclusion of Theorem 1 with λf_∞ in place of f_∞, i.e., with λg_∞ in place of g_∞. Thus, we obtain for all $s \in \lambda f_\infty(\mathbb{R})$:

$$\Phi'(s) = a_\lambda(\lambda g_\infty)^{-1}(s) + b_\lambda = a_\lambda (g_\infty)^{-1}\left(\frac{s}{\lambda}\right) + b_\lambda,$$

for some constants a_λ, b_λ. Now for any $s \in f_\infty(\mathbb{R})$ we have $\lambda s \in \lambda f_\infty(\mathbb{R})$, so that

$$\Phi'(\lambda s) = a_\lambda (g_\infty)^{-1}(s) + b_\lambda.$$

Comparing to (10) we obtain the following relation:

$$\frac{\Phi'(\lambda s) - b_\lambda}{a_\lambda} = \frac{\Phi'(s) - b_1}{a_1}. \tag{15}$$

To obtain a functional equation, let us now introduce some convenient notation. Defining

$$u(\lambda) := \frac{a_\lambda}{a_1} > 0, \qquad v(\lambda) := b_\lambda - b_1 u(\lambda)$$

and setting $x = \lambda$, $y = s$ in (15), we obtain for any $y \in f_\infty(\mathbb{R})$ and $x > 0$:

$$\Phi'(xy) = u(x)\Phi'(y) + v(x).$$

Since P has a real root and $g_\infty(0) = 1$ we may take $y = 1$ in this relation. Subtracting and writing $\chi(x) = \Phi'(x) - \Phi'(1)$ we obtain:

$$\chi(xy) = u(x)\chi(y) + \chi(x). \tag{16}$$

This obviously is the functional equation for the logarithm function if $u(x) \equiv 1$. More precisely, in this case, we obtain $\Phi'(x) = a \ln x + b$ for some constants a and b, and (14) follows from (10). If $u(x)$ is not always equal to 1, by symmetrizing (16) it can be easily shown that χ has to satisfy the following functional equation:

$$\chi(xy) = \chi(x) + \chi(y) - k\chi(x)\chi(y)$$

for some constant k. One can show that the solution to this equation is given by:

$$\chi(x) = \frac{1 - y^{-k}}{k}.$$

Coming back to g_∞ via (10) we obtain (13) with $\gamma = -1/k$.

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