STOCHASTIC CONTROL AND THE SECOND LAW OF THERMODYNAMICS

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Abstract

The second law of thermodynamics is studied from the point of view of stochastic control theory. We find that the feedback control laws which are of interest are those which depend only on average values, and not on sample path behavior. We are lead to a criterion which, when satisfied, permits one to assign a temperature to a stochastic system in such a way as to have Carnot cycles be the optimal trajectories of optimal control problems. Entropy is also defined and we are able to prove an equipartition of energy theorem using this definition of temperature. Our formulation allows one to treat irreversibility in a quite natural and completely precise way.

1. Introduction

Stochastic control has been rather successful in providing precise formulations for interesting problems but it has been far less successful in actually solving these problems. Thermodynamics, on the other hand, has been very successful in solving problems but it has a rather shakey foundation -- especially insofar as the statistical theory is concerned. The purpose of this paper is to construct a mathematically consistent theory whose assumptions and conclusions can be put in correspondence with thermodynamic ideas. Our goal, which is partially realized here, is to simultaneously remove the aforementioned shortcomings of each field, i.e. to suggest an axiomatic basis for a mathematical theory of statistical thermodynamics and to discover a new class of stochastic control problems which can be intuitively understood and solved.

Because of its power and subtlety we are mainly interested in the second law of thermodynamics. Of the classical formulations, the one of Maxwell involving a demon controlling a trap door between two gas chambers is perhaps the most suggestive of a stochastic control theoretic interpretation. The Caratheodory statement in the macroscopic theory involving the hypothesis of inaccessible states also has an obvious connection with control theory. However, we do not find either of these to be a useful point of departure; for our present purpose it seems best to start with a very concrete form of the fluctuation - dissipation equality, namely the Nyquist-Johnson model for electrical conductors in thermal equilibrium. Using this model, together with well established facts about lumped element electrical circuits we are able to arrive at an intuitive and reasonably general setting in which to study statistical thermodynamics.

The essential points of this theory may be summarized as follows.

1. The stochastic control formulation of a thermodynamic process involves manipulating a dynamical systems using open loop control laws. More specifically, carrying out a thermodynamic process involves steering a variance equation along a certain path and Carnot cycles turn out to be the solutions to optimal control problems.

2. Equilibrium and nonequilibrium thermodynamics are captured in the same framework. We can, in principle, determine the deviation from Carnot efficiency which is dictated by the necessity of carrying out a thermodynamic process in finite time.

3. Within the linear, quadratic, gaussian context we isolate those conditions which permit one to assign a single temperature to a stochastic system. We use this idea to establish an equipartition of energy theorem.

4. We give a definition of entropy which is consistent with both the macroscopic theory and the statistical theory.

The remainder of the paper is organized as follows. Section 2 presents a detailed analysis of the simplest example. All the intuitive ideas are to be seen here with a minimum of complexity. In section 3 we set up a much more general model and define what we mean by a monotemperaturic system. In section 4 we define entropy and use it to establish a Carnot efficiency. Finally we give an equipartition of energy theorem in section 5. Because of the limitations on space certain of the arguments are only sketched here. We hope to publish a full account shortly.

2. Example and Motivation

In 1929 H. Nyquist [1] made a theoretical analysis of some experimental work of Johnson

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thereby arriving at the so-called Nyquist-Johnson model for resistor noise. This model relates the statistical properties of the current i and voltage v in a resistor to the temperature of the resistor via the equation

$$i = gv + n$$

where g is the conductance and n is white noise with a characteristic variance $\sqrt{2kgT}$. Here k is Boltzmann's constant whose numerical value depends on the units chosen for the other quantities and T is temperature measured on an absolute scale. The fact that the variance depends on $\sqrt{g}$ rather than some other function of g is easily argued from examining the series connection of two resistors. The fact that it depends on $\sqrt{T}$ rather than some other T dependence cannot be interpreted more deeply without discussing the choice of temperature scale itself. Here after we agree to choose a temperature scale so that k = 1.

If we combine the equation of a Nyquist-Johnson resistor with that of a linear capacitor having capacitance c, the result is an Ito equation

$$dcv = -gvdt + \sqrt{2gT}\, dw$$

The steady state value of $\mathcal{E}(v^2)$ is easily seen to be

$$\mathcal{E}v^2 = T/c$$

and so the expected value of the energy stored in the capacitor in steady state, $\frac{1}{2}\dot{c}v^2$, is just $\frac{1}{2}$ T. The key point is that this is independent of both g and c. This is, a very special form of an equipartition of energy theorem we will prove later.

We now consider a thermodynamic cycle constructed by using resistors at two different temperatures and a variable capacitor.

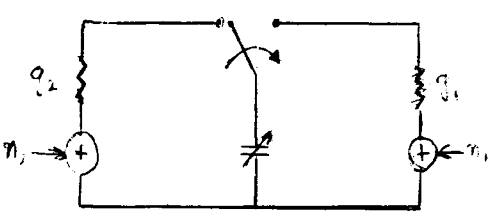

Figure 1: The basic model for this section 2.

We are interested in analyzing the possibility of extracting energy from the system using control laws which depend on average values only and not any properties of sample paths. Now of course one way to get mechanical energy (i.e. work) out of such a system is by changing the capacitance when a charge is present. Since the energy stored in a capacitor is $\frac{1}{2}cv^2$ where v is the voltage we see that when we change the capacitance we extract work e according to

$$\dot{e} = \frac{1}{2}\dot{c}v^2$$

phenomenalogically speaking, this might show up, for example, as the work done in moving the plates of a charged parallel plate capacitor. The equation of motion for the system in figure 1 is

$$dv = -(\dot{c}/c)vdt-(g_i/c)vdt+(\sqrt{2g_iT_i}/c)dw;$$
$$i = 1,\ 2 \text{ or } g_i = 0$$

The expected value of the energy which comes out of the conductance g_i is just

$$q_i = \int I_i(t)g_iv^2dt;$$

$$I_i(t) = \begin{cases} 1 & \text{if } g_i \text{ is connected} \\ 0 & \text{otherwise} \end{cases}$$

This quantity is interpreted as a heat flow because it is energy supplied by the random fluctuations.

From the stochastic equation for the network we get a variance equation

$$\dot{\sigma} = -2(\dot{c}/c)\sigma - 2(g_i/c)\sigma + 2g_iT_i/c^2$$

which implies two important relations

$$\frac{d}{dt}(c\sigma) = -\frac{de}{dt} + 2g_i\left(\frac{T_i}{c} - \sigma\right) \qquad \text{(A)}$$

and

$$\frac{d}{dt}(\ln c^2\sigma) = \frac{\dot{\sigma}}{\sigma} + 2\frac{\dot{c}}{c} = \frac{2g_i}{c}\left(\frac{T_i}{\sigma c} - 1\right) \qquad \text{(B)}$$

The first of these expresses conservation of energy and the second is to be interpreted as defining the flow of entropy. To justify this language it is enough to observe that the right hand side of equation (B) can be though of as dq/T along reversible paths. This will become clearer as we go on.

We now state a control problem which will lead to Carnot cycles. To do so we introduce the special notation

$$[f(t)]_+ = \frac{1}{2}[f(t)+|f(t)|]$$

Problem 1: Given the differential equation

$$\dot{\sigma}(t) = -2\frac{\dot{c}(t)}{c(t)}\sigma(t) - 2\frac{g(t)}{c(t)}\sigma(t) + 2\frac{g(t)T(t)}{c^2(t)}$$

and given the constraints

$$q_+ = 2\int_0^a \left[\frac{g(t)T(t)}{c(t)} - g(t)\sigma(t)\right]_+ dt \leq 1$$

(i) $\sigma(0) = \sigma(a)$, (ii) $c(0) = c(a)$,

(iii) $c(t) > 0$ (iv) $g(t) \geq 0$

(v) $T_2 \leq T(t) \leq T_1$

find $c(\cdot)$, $g(\cdot)$, $T(\cdot)$ on the interval [0,a] such as to maximize

$$e = \int_0^a \dot{c}(t)\sigma(t)dt$$

The interpretation of this problem is, of course, that of maximizing the work for a given quantity of heat inflow.

This problem will have solutions for $a < \infty$ but such solutions correspond to irreversible thermodynamic processes. There is, however an idealized solution corresponding to a particular limit as a goes to infinity which is quite easy to compute and which corresponds to the idea of a quasi-static process in classical thermodynamics. We now develop some ideas which we need to explain this limit. The following lemma is fundamental.

Lemma 1: Consider Problem 1. Along any path for which T is constant we have

$$c\sigma\Big|_0^a + \int_0^a \dot{e}\,dt + T\ell n(c^2\sigma)\Big|_0^a \leq 0$$

Proof: From equations (A) and (B) we have

$$c\sigma\Big|_0^a + \int_0^a \dot{e}\,dt = \int_0^a (T-c\sigma)\,2\,\frac{g}{c}\,dt$$

$$\ell n(c^2\sigma)\Big|_0^a = \int_0^a (T-c\sigma)\,\frac{1}{c\sigma}\,2\,\frac{g}{c}\,dt$$

Multiplying the second equation by T and subtracting it from the first we see that, in an obvious notation,

$$\sigma c\Big|_0^a + \int_0^a \dot{e}\,dt - T\ell n c^2\sigma\Big|_0^a = T\int_0^a [(1-\rho)+(1-\rho^{-1})]\frac{2g}{c}dt$$

But since $\rho > 0$, $(2-\rho-\rho^{-1}) \leq 0$ we see that the inequality holds.

If we look at the special case where the initial conditions and the final conditions are the same this statement carries the force of the Kelvin-Planck statement of the second law. That is, it shows that it is impossible to remove work from a single heat bath using a cycle which begins and ends at the same state. The usual thermodynamic reasoning from this point on is to construct a reversable cycle which uses two heat sources, one at T_1 and one at T_2 and which produces work according to the Carnot efficiency. This is easy to do here. However one then shows that if there exists any heat engine with efficiency greater than the Carnot efficiency it could be used, together with the original one, to violate the Kelvin-Planck statement. We find it more convenient to proceed differentially since to define mathematically some of these terms would be cumbersome.

Theorem 1: Consider Problem 1. For any closed path in (c,σ)-space along which T takes on only the values T_1 and T_2 with $T_1 > T_2$ we have

$$e \leq \left(\frac{T_1-T_2}{T_1}\right)q_+$$

Proof: Suppose we break the path up into segments along which the temperature is T_1 and segments along which it is T_2. We can put the $g = 0$ segments in either part. Then by the lemma

$$\Sigma(c\sigma)\Big|_{a_i}^{b_i} + e_i - T_i\ell n\, c^2\Big|_{a_i}^{b_i} \leq 0; \quad i = 1,2$$

Adding this inequality for T_1 to that for T_2 and using the fact that $b_1 = a_2$ etc. we get

$$e + \Sigma(T_1-T_2)\ell n\, e^2\sigma\Big|_{a_i}^{b_i} \leq 0$$

But we have

$$q_+ = \Sigma T_1\,\ell n\, c^2\sigma\Big|_{a_i}^{b_i}$$

Thus

$$e \leq \left(\frac{T_1-T_2}{T_1}\right)q_+$$

This result gives an answer to problem 1 in the following sense. If $\varepsilon > 0$ is given then we can find a time $a(\varepsilon)$ and a choice of control policy on $[0,a]$ for which the energy is within ε of the value $(T_1-T_2)/T_1$. To do this we construct a finite time approximation to the cycle shown in figure 2. The line AB corresponds to the system being connected to the hot resistor and c varying in such a way as to keep $c\sigma = T$. This takes

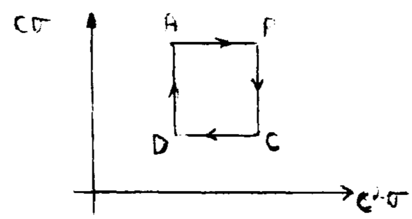

Figure 2: A Carnot Cycle

infinite time. The line from B to C corresponds to setting the conductance to zero and changing c to reduce $c\sigma$ to T_2. This can be done any positive time interval. The line C to D corresponds to the system being connected to the cold resistor and c being changed to keep $c\sigma = T_2$. This also takes infinite time. And finally along DA we reverse the BC process. A glance at the proof of Theorem 1 shows that for this process we have equality for all inequalities which appear there and so this is a Carnot cycle.

Finite time versions involve letting $c\sigma$ be slightly less than T_1 (greater than T_2). This will enable the variance equations to reach near the end point in finite time but at some small loss of efficiency. It would be interesting to make a detailed comparison with the recent results in the literature on finite time Carnot cycles [2].

3. Linear Stochastic Systems

We now turn to a more general situation which illustrates the much broader scope of the previous somewhat special reasoning. For a more detailed account of the background ideas involved here see [3] and [4], on the deterministic side, and [5] for the stochastic.

By a linear, finite dimensional, gaussian system (FDLGS) we understand a pair

$$dx = Axdt + Budt + Gdw$$

$$dy = C\dot{x}dt + D\dot{u}dt + Hdf$$

where dw and df are independent vector valued Wiener processes, and x, u, y are all finite dimensional. This system is said to be minimal if (A,B) is a controllable pair and (A,C) is an observable pair.

We call

$$G(s) = C(Is-A)^{-1}B+D$$

the transfer function associated with the system and we call

$$\Phi(s) = (H+C(-Is-A)^{-1}G)'(H+C(Is-A)^{-1}G)$$

the power spectrum of the system. We say that the system is externally reciprocal if $G(s) = G'(s)$. The system is said to be determinately passive if G(s) is a matrix valued positive real function. A conservative system is one for which G(s) is positive real and $G(i\omega)+G'(-i\omega) = 0$.

We now introduce a key idea. A deterministically passive FDLGS is said to be monotemperaturic if there exists a proportionality factor $\beta \geq 0$ such that

$$(C(-Is-A)^{-1}G+H)'(C(Is-A)^{-1}G+H) =$$
$$\beta[C(-Is+A)^{-1}B)'+H'+C(Is-A)^{-1}B)+H] \qquad (*)$$

In the language of thermodynamics, what this equation expresses is a fluctuation-dissipation proportionality. In the language of system theory it expresses a proportionality between the power spectrum and the parahermetian part of the transfer function. If equality (*) holds we call β the temperature of the system.

Several justifications for this definition can be given. One is that (*) expresses a property of electrical networks constructed from linear constant inductors, capacitors and resistors in Nyquist-Johnson form. The theorems of the next two sections provide a more intrinsic justification.

We conclude this section with a canonical form for monotemperaturic systems. This theorem might be thought of as a generalization of the Darlington normal form of [5].

Theorem 2: If S is a minimal, externally reciprocal, monotemperaturic system then we can make a linear change of coordinates on x such that it takes the form ($\Omega = -\Omega'$)

$$dx = (\Omega - \frac{1}{2\beta}GG')xdt + Budt + Gdw$$
$$dy = B\dot{x}dt + D\dot{u}dt + \sqrt{2\beta D}\,df$$

Conversely, any system of this form is monotemperaturic.

Proof: That systems of this form are monotemperaturic is just a calculation.

Consider the deterministic system

$$\dot{x} = (A-GG')x+Bu_1+Gu_2;\quad y_1 = Bu;\quad y_2 = G'x$$

Adopt the notation

$$\begin{bmatrix}\hat{y}_1\\ \hat{y}_2\end{bmatrix} = \begin{bmatrix}G_{11}(s) & G_{12}(s)\\ G_{21}(s) & G_{22}(s)\end{bmatrix}\begin{bmatrix}\hat{u}_1\\ \hat{u}_2\end{bmatrix}$$

The characterization of monotemperaturic implies that this system is convervative and hence by [5] it can be realized with $A-\frac{1}{2\beta}G'G$ skew symmetric.

4. A More General Kelvin Planck Statement

Corresponding to the general monotemperaturic system we have a generalization of lemma 1 enabling us to conclude in a wider setting that one cannot get work from a single heat bath.

Theorem 3: Consider a minimal, monotemperaturic (FDLGS) with scalar input and scalar output

$$dx = Axdt + budt + Gdw$$
$$dy = b'\dot{x}dt + \dot{u}dt + \sqrt{2d\beta}\,df$$

If we adjoin the equation

$$dcv = dy;\quad u = -v$$

then for any choice of c(·) which is differentiable, which starts and ends with the variance of these combined equations in the same, equilibrium, state we have

$$\int_0^a \dot{c}(\mathcal{E}\,v^2) \leq 0$$

Proof: The equations of motion for the combined system can be written in terms of the variables $\sqrt{c}\,v = z$ and x. They are

$$d\begin{bmatrix}x\\ z\end{bmatrix} = \begin{bmatrix}A & -c^{-1/2}b\\ c^{-1/2}b' & -d-\dot{c}/c\end{bmatrix}\begin{bmatrix}x\\ z\end{bmatrix}dt + \begin{bmatrix}Gdw\\ \sqrt{2d\beta}c^{-1/2}df\end{bmatrix}$$

The resulting variance equation is expressed in terms of

$$\tilde{\Sigma} = \begin{bmatrix}\Sigma & \eta\\ \eta & \sigma\end{bmatrix} = \begin{bmatrix}xx' & x\sqrt{c}v\\ x'\sqrt{c}v & c^2v^2\end{bmatrix}$$

$$\dot{\tilde{\Sigma}} = \begin{bmatrix}A & -b\\ b' & -d-\dot{c}/c\end{bmatrix}\tilde{\Sigma} + \tilde{\Sigma}\begin{bmatrix}A' & b'\\ -b'c & -d-\dot{c}/c\end{bmatrix} + \begin{bmatrix}GG' & 0\\ 0 & 2\beta d/c\end{bmatrix}$$

Now conservation of energy is just (note σ does not have the same meaning here as in section 2. Here work is the integral of $\dot{c}\sigma/c$.)

$$\frac{1}{2}\frac{d}{dt}(\mathrm{tr}\,\Sigma + \frac{\sigma}{c}) + \frac{\dot{c}}{c}\sigma = \mathrm{tr}(A\Sigma) + \mathrm{tr}\,GG' - 2(d/c)(\beta-\sigma) \qquad (A')$$

The flow of entropy is given by

$$\frac{d}{dt}(\mathrm{tr}\,\ln\Sigma + \ln c\sigma) = 2[\mathrm{tr}\,A + GG'\Sigma^{-1} + (2d/c\sigma)(\beta-\sigma)] \qquad (B')$$

This last calculation may call for some comment. First of all, because Σ is symmetric and positive definite it has a logarithm and tr $\ell n\ \Sigma$ is the natural vector version of entropy as defined in section 2. Now tr $\ell n\ \Sigma = \ell n \det \Sigma$. (Think about the eigenvalues!) We can easily see that the derivative of $\ell n \det \Sigma$ is just tr $\Sigma^{-1}\dot{\Sigma}$ since the derivative of det M is tr((Adj M)·$\dot{M}$).

We now use theorem 2 to assume that

$$A = \Omega - \frac{1}{2\beta} GG'; \quad \Omega = -\Omega'$$

combining A' and B' in some way as in the proof of theorem 1 we get

$$\frac{d}{dt}[\mathrm{tr}(\Sigma)+ \frac{\sigma}{c}]-2\beta\frac{d}{dt}[\mathrm{tr}\ \ell n(\Sigma)+\ell n\ \sigma] + \frac{\dot{c}}{c}\ \sigma =$$
$$-\mathrm{tr}(G'G- \frac{1}{2\beta}G'\Sigma G) + \mathrm{tr}[G'G-2\beta G'\Sigma^{-1}G]-(1-\rho)+(1-\rho^{-1})$$

Reasoning as before, the trace term is upper bounded by zero and the remaining terms are upper bounded by zero.

5. Equipartition of Energy

One of the beautiful facts about the linear theory of equilibrium thermodynamics is the equipartition of energy theorem which states that the expected value of the energy of each mode of a system in equilibrium is the same. For example, a balloon in still air can be expected to have as much kinnectic energy as an O_2 molecule. This idea finds its expression here in terms of the interconnection of lossless systems with monotemperaturic systems.

Let S be a (LFDGS) with inputs u, outputs y and transfer function G(s). We will say that it has the equipartition property if there exists a positive number β such that whenever it is connected to a conservative system with impedance Z(s) the resulting system has a unique invariant measure and for this measure

$$\mathcal{E}yy' = \beta G_o; \quad G(s) = G_o s^{-1}+G_1 s^{-2}+\ldots$$

$$\mathcal{E}uu' = \beta Z_o; \quad Z(s) = Z_o s^{-1}+Z_1 s^{-2}+\ldots$$

regardless of the impedance Z(s) of the conservative system.

The explanation of this definition is that if one chooses normal coordinates for the lossless system then it appears as

$$\dot{x} = \Omega x+Bu; \quad y = B'x$$

Equipartition means that $\mathcal{E}xx' = \beta I$ for some β and thus $\mathcal{E}yy' = \beta B'B$. However $Z(s) = B'BS^{-1}+B'ABS^{-2}+\ldots$ Similar but more involved calculations apply to $\mathcal{E}uu'$. The following theorem is easily verified.

Theorem 4: A (FDLBS) has the equipartition property if and only if it is monotemperaturic.

6. Conclusions

In this paper we have constructed a linear quadratic gaussian theory which embraces many of the important aspects of thermodynamics. The original motivation came from an attempt to understand in what sense the concept of a dissipative dynamical system could be useful in a statistical setting. The translation of thermodynamics ideas into this setting proved to be remarkably faithful. It would be interesting to study these models further to see if there are problems from other fields, such as economics, which they may be applied to.

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