

Xiaoyu's thermostat interpreted as targeting an space or time average

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In Xiaoyu's version of the thermostat the ζ equation reads:

$$\dot{\zeta} = \frac{1}{d} p^T M^{-2}(p) p - \text{tr} \left(\frac{d}{dp} \left(\frac{1}{d} M^{-1}(p) p \right) \right) \quad (1)$$

$$= \frac{1}{d} \sum_i^d \left((M^{-1}(p)_{ii} p_i)^2 - \frac{d}{dp_i} (M^{-1}(p)_{ii} p_i) \right) \quad (2)$$

Note that $\frac{dK}{dp_i} = M^{-1}(p)_{ii} p_i$. Hence we have

$$\dot{\zeta} = \frac{1}{d} \sum_i^d \left(\left(\frac{dK}{dp_i} \right)^2 - \frac{d}{dp_i} \frac{dK}{dp_i} \right) \quad (3)$$

Now consider the space average of this quantity:

$$\left\langle \left(\frac{dK}{dp_i} \right)^2 - \frac{d^2 K}{dp_i^2} \right\rangle \quad (4)$$

A simple integration by parts gives:

$$\left\langle \frac{d^2 K}{dp_i^2} \right\rangle = \int \frac{d^2 K}{dp_i^2} \exp(-K(p)) dp \quad (5)$$

$$= \underbrace{\int \left[\frac{dK}{dp_i} \exp(-K(p)) \right]_{p_i=\infty}^{\infty} dp}_{=0} - \int \frac{dK}{dp_i} \left(-\frac{dK}{dp_i} \exp(-K(p)) \right) dp \quad (6)$$

$$= \left\langle \left(\frac{dK}{dp_i} \right)^2 \right\rangle \quad (7)$$

Note that because $K(p) = -\log f_p(p)$, the negative log density of p we can interpret $\left\langle \frac{d^2 K}{dp_i^2} \right\rangle$ as the negative Fisher information of the distribution of the momenta - not entirely sure this helps us but it's nice. In any case this calculation implies that

$$\langle \dot{\zeta} \rangle = 0 \quad (8)$$

I think this makes it clear why this thermostat equation might be expected to work.

Interestingly, the classical thermostat can also be interpreted in this way since $p_i \frac{dK}{dp_i} = \left(\frac{dK}{dp_i} \right)^2$ and $\frac{d^2 K}{dp_i^2} = 1$.