On the Thermodynamic Temperature of a General Distribution and Its Relationship to Fisher Information

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Introduction

Brief Description

- N particles and state is given by $[\vec{X}, \vec{P}]$
- $\vec{P} \in R^{3N}$ denotes momenta and $\vec{X} \in R^{3N}$ denotes positions
- $f_{\vec{P}}(\vec{y})$ is the marginal PDF of momenta

Thermal entropy of the distribution S

$$S(f_{\vec{P}}) = -k \int f_{\vec{P}}(\vec{y}) \ln(f_{\vec{P}}(\vec{y}))\, d\vec{y}$$

Kinetic Energy $\mathcal{E}$

$$\mathcal{E}(f_{\vec{P}}) = \frac{E[||\vec{P}||^2]}{2m} = \frac{1}{2m} \int_{-\infty}^{\infty} ||\vec{y}||^2 \; f_{\vec{P}}(\vec{y}) d\vec{y}$$

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System in Equilibrium

- PDF is given by the classical Boltzmann formula

$$f_{\vec{P}}(\vec{y}) \propto e^{-\frac{1}{T}\left(\frac{||\vec{y}||^2}{2m}\right)}$$

Kinetic temperature

Can be obtained from $(3/2)NkT_{kin} = \mathcal{E}(f_{\vec{P}})$

Thermodynamic temperature

$$\frac{1}{\theta} = \frac{dS(f_{\vec{P}})}{d\mathcal{E}(f_{\vec{P}})}$$

- Both definitions lead to same result, $\theta = T_{kin} =$ Variance

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Systems not in Equilibrium

- What about when the PDF $f_{\vec{P}}(\vec{y})$ is not Gaussian?
- Clearly, T_{kin} can be defined for any PDF
- However, it is not possible to directly define $\frac{1}{\theta} = \frac{dS(f_{\vec{P}})}{d\mathcal{E}(f_{\vec{P}})}$
- $S(f_{\vec{P}})$ is not necessarily even a function of $\mathcal{E}(f_{\vec{P}})$!

Main Question

Can we define a thermodynamic temperature for a general (non-equilibrium) distribution?

Some Answers

We propose such a definition

- Main idea is to perturb $f_{\bar{P}}$ and compute $\frac{1}{\theta} = \frac{dS(f_{\bar{P}})/df_{\bar{P}}}{d\mathcal{E}(f_{\bar{P}})/df_{\bar{P}}}$
- Propose a particular form of perturbation
- $\frac{1}{\theta}$ is the Fisher information associated with $f_{\bar{P}}$
- This approach works for discrete momenta also
- Can be used to analyze the dynamics of heat flux and work when a body is immersed in a heat bath

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Perturbation Approach

- Perturb $f_{\vec{P}}$ to $f_{\vec{P}'}$ (i.e. $\vec{P}$ is transformed to $\vec{P}'$)
- Calculate ΔS and $\Delta \mathcal{E}$
- Compute thermodynamic temperature as

$$\frac{1}{\theta} = \lim_{\Delta \mathcal{E} \to 0} \frac{\Delta S}{\Delta \mathcal{E}}$$

Required Properties

- θ must be non-negative
- θ should be equal to the thermodynamic temperature for the Gaussian distribution
- θ should represent "spread" of the kinetic energy, i.e., the more spread out the kinetic energy, the higher temperature
- θ should be a functional of the PDF $f_{\vec{P}}$

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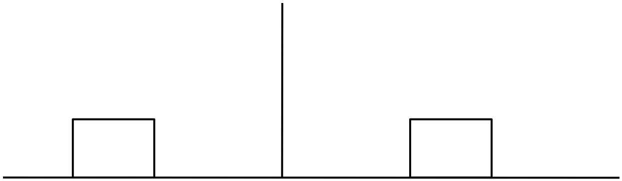
Example of Unacceptable Perturbation



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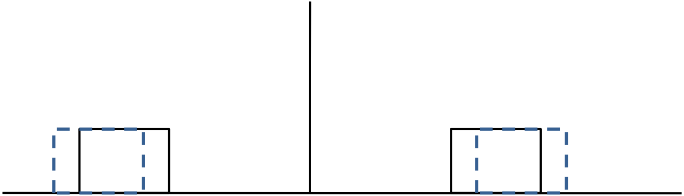

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Additive Perturbation

- Statistical realization of the notion of heating

$$\vec{P}' = \vec{P} + \sqrt{\delta}\vec{Q},$$

where $\vec{Q}$ is any random variable with zero mean and unit variance in each dimension and let the components of $\vec{Q}$ be independent of each other i.e., $E[\vec{Q}\vec{Q}^T] = I_{3N \times 3N}$. Further, let $\vec{Q}$ be independent of $\vec{P}$

$$f_{\vec{P}'}(\vec{y}, \delta) = f_{\vec{P}}(\vec{y}) \otimes f_{\sqrt{\delta}\vec{Q}}(\vec{y})$$

Note that $f_{\vec{P}'}(\vec{y}, \delta)$ is explicitly a function of δ also.

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Properties

It can be shown that this perturbation satisfies the required positivity. I will skip the proof, ask me later if you want to see it.

Proposed Definition of Temperature

$$\frac{1}{\theta} = \lim_{\delta \to 0} \frac{S(f_{\vec{P}'}) - S(f_{\vec{P}})}{\mathcal{E}(f_{\vec{P}'}) - \mathcal{E}(f_{\vec{P}})} = \frac{2m}{3N} \lim_{\delta \to 0} \frac{S(f_{\vec{P}'}) - S(f_{\vec{P}})}{\delta} = \frac{2m}{3N} \frac{\partial}{\partial \delta} S(f_{\vec{P}'})|_{\delta=0}$$

We can show that $\frac{1}{\theta}$

- is independent of the perturbation $f_{\vec{Q}}$ (notice $\delta \to 0$)
- depends only on $f_{\vec{P}}$, which is intuitively pleasing.
- is the trace of the Fisher information matrix corresponding to the distribution of $f_{\vec{P}}$ with respect to the location family, scaled by $mk/3N$

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Fisher Information w.r.t location family

- For a scalar random variable P with PDF $f_P(y)$, Fisher Information w.r.t location family is

$$J(f_P) = \int_{-\infty}^{\infty} f_P(y) \left[\frac{\partial}{\partial y} \ln f_P(y)\right]^2 dy = \int_{-\infty}^{\infty} f_P(y) \left[\frac{\frac{\partial}{\partial y} f_P(y)}{f_P(y)}\right]^2 dy.$$

- For a vector valued random variable $\vec{P}$ with $3N$ components, the i,jth entry of the Fisher information matrix is given by

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de Bruijn Identity

Let P' be the random variable given by

$$P' = P + \sqrt{\delta} Q, \quad \text{where,} \quad f_Q(y) = f_Q(-y)$$

Gaussian perturbation

If Q is a Gaussian random variable,

$$\frac{\partial S(f_{P'})}{\partial \delta} = \frac{k}{2} J(f_{P'})$$

Arbitrary perturbation

For *any* f_Q

$$\frac{\partial S(f_P')}{\partial \delta}|_{\delta=0} = \frac{k}{2} J(f_{P'})|_{\delta=0} = \frac{k}{2} J(f_P).$$

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Heat Equation

- On the way to the proof, we show that

$$\frac{\partial f_{P'}(y,\delta)}{\partial \delta}|_{\delta=0} = \frac{1}{2}\frac{\partial^2 f_P(y)}{\partial y^2} = \frac{1}{2}\frac{\partial^2 f_{P'}(y)}{\partial y^2}|_{\delta=0}.$$

- Additive perturbation results in PDF's that satisfy the heat (diffusion) equation which is intuitively pleasing
- It is precisely for the additive perturbation that we are able to connect $\frac{\partial S}{\partial \mathcal{E}}$ to Fisher information via the de Bruijn identity

Main Theorem

Connection between Temperature and Fisher Info

$$\frac{1}{\theta} = \frac{2m}{3N}\frac{\partial S(f_{\vec{P}'})}{\partial \delta}|_{\delta=0} = \frac{mk}{3N}\sum_i J_{i,i}(f_{\vec{P}})$$

Apply the de Bruijn identity to each dimension separately

Scalar Version

$$\frac{1}{\theta} = mkJ(f_{\vec{P}})$$

Clearly θ is measure of spread of the distribution of the momenta. But it is not the same as variance

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Example

$$f_P(y) = \frac{1}{\sqrt{2\pi\sigma^2}} \frac{1}{2} \{ e^{-\frac{1}{2\sigma^2}(y-\mu)^2} + e^{-\frac{1}{2\sigma^2}(y+\mu)^2} \}$$

- $f_P(y)$ is the mixture of two Gaussian distributions
- $\mathcal{E} = \mu^2 + \sigma^2$ and, hence,

$$T_{kin}(\mu, \sigma^2) = \frac{1}{mk}(\mu^2 + \sigma^2)$$

- The thermodynamic temperature is

$$\theta(\mu, \sigma^2) = \frac{1}{mk} \frac{1}{J(f_P)}$$

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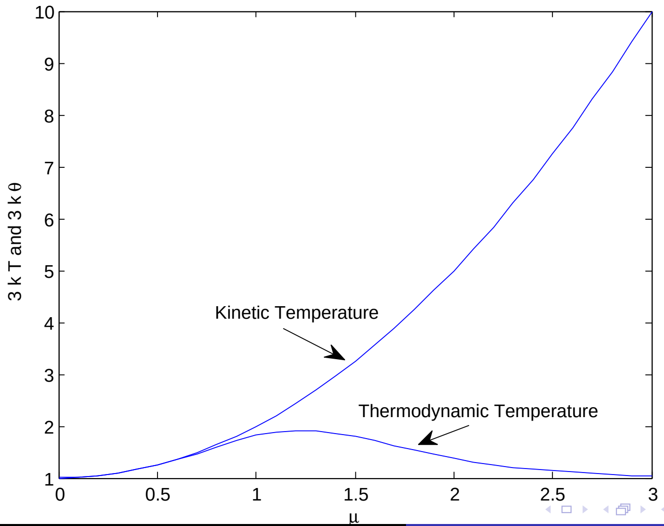
Kinetic and Thermodynamic Temperature



Cramer-Rao Bound

- Family of distributions $f_{\vec{P}}(y;\alpha) = f_{\vec{P}}(y-\alpha)$ s.t. $E[\vec{P}] = 0$
- Suppose we wish to estimate α from a single observation of y
- Consider the estimator $\hat{\alpha} = y$
  - Unbiased
  - Var(Estimation error) $= Var(f_{\vec{P}}) = mkT_{kin}$

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Var(Est. error) $\geq \frac{1}{J(f_{\vec{P}})} = mk\theta$

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Discrete Case

- Momentum P is a discrete scalar random variable
- P can take values nh, for any integer n and a real constant h
- $f_P[n] = Pr(P = nh)$ is the PMF

Why extension is not trivial

- One cannot define an additive perturbation, since for arbitrary values of δ, the perturbed random variable P' will in general not be restricted to the set $\{nh\}$
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Relative Entropy or Kullback-Leibler Divergence

$$D(f||g) = \int f(y) \log \frac{f(y)}{g(y)} \, dy$$

- Can be roughly thought of as a distance between two distributions f and g
- Tells us how different two distributions are

Fisher Information and Relative Entropy

Consider two distributions $f_P(y+t)$ and $f_P(y-t)$ which are shifted versions of $f_P(y)$, shifted by t to the left and right. Let $D(\cdot||\cdot)$ is the relative entropy between them. Then,

$$J(f_P) = \lim_{t \to 0} \frac{1}{t^2} \left(D(f_P(y+t)||f_P) + D(f_P(y-t)||f_P) \right)$$

Main Result

$$\frac{1}{\theta} = \lim_{\delta \to 0} \frac{H(f_{P'}) - H(f_P)}{\mathcal{E}(f_{P'}) - \mathcal{E}(f_P)} = \frac{mk}{h^2} D(f_P[n+1]||f_P) + D(f_P[n-1]||f_P)$$

Notice the similarity!

Fisher Information and Relative Entropy

Consider two distributions $f_P(y+t)$ and $f_P(y-t)$ which are shifted versions of $f_P(y)$, shifted by t to the left and right. Let $D(\cdot||\cdot)$ is the relative entropy between them. Then,

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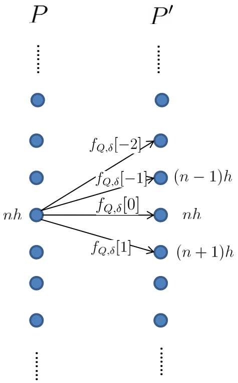
Proposed Perturbation



$$f_{Q,\delta}[i-j] = Pr(P' = ih | P = jh)$$

Body Immersed in a Heat Bath at Temperature T

Langevin Equation

- The velocity v is given by

$$m\frac{dv(t)}{dt} = -m\gamma v(t) + \eta(t), \quad E[\eta(t)^2] = 2m\gamma kT$$

- If we write $\frac{dv(t)}{dt} = \frac{v(t+\epsilon)-v(t)}{\epsilon}$

$$v(t+\epsilon) = (1-\epsilon\gamma)v(t) + \frac{\epsilon}{m}\eta(t)$$

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Fokker-Planck Equation

$$\frac{\partial f_P}{\partial t} = \gamma \frac{\partial (y f_P)}{\partial y} + \frac{\gamma k T}{m} \frac{\partial^2 f_P}{\partial y^2}$$

- Using this we can compute various quantities such as $\frac{d\mathcal{E}}{dt}$, $\frac{dS}{dt}$

Heat flux rate and Work

$$\frac{d\mathcal{E}}{dt} = \gamma k[T - T_{kin}]$$

$$\frac{dS}{dt} = \gamma k \frac{T - \theta}{\theta} = \frac{dQ}{\theta}$$

$dQ = \gamma k(T - \theta)$ - is the heat flux rate

$$\frac{d\mathcal{E}}{dt} = \gamma k(T - \theta) + \gamma k(\theta - T_{kin})$$

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$$\frac{dS_{body}}{dt} = \frac{\gamma k(T-\theta)}{\theta}$$

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Net entropy gain

$$\frac{dS_{body}}{dt} + \frac{dS_{bath}}{dt} = \gamma k\frac{(T-\theta)^2}{\theta T} + \gamma k\frac{T_{kin}-\theta}{T}$$

- Using the Cramer-Rao bound it is positive!
- $k(T_{kin}-\theta)$ is called Mechanical dissipation!

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Conclusions

- Thermodynamical temperature can be extended to non-equilibrium distributions in a relatively straightforward way for both the discrete and continuous cases.
- In each situation, we introduce a "diffusive" perturbation
- This definition retains all the features of the classical temperature without the need for any hypothesis of equilibrium
- Can be used to identify heat flux rate, work and mechanical dissipation when used to analyze the dynamics of a body immersed in a heat bath
- We can define a temperature field by using the condition distribution of the momentum given the position of the particle, i.e., $f_{\vec{P}|\vec{X}}$

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