Thermostats in Kac's Model

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Kac's Model

In 1956 Mark Kac invented an N-particle, stochastic model in an effort to study Boltzmann's equation.

In Kac's model, we take

1. In N indistinguishable particles moving in 1-dimension.
2. The distribution of the particles is space-homogeneous (no x-coordinates in the picture)
3. Particle i has velocity v_i.
4. Particles interact via collisions. There is 1 collision at a time, during which only 2 particles collide.
5. Time between collisions are independent and exponentially distributed (rate $= N\lambda$)

Kac's Collision Operator

When particles i and j collide, we obtain

$$\begin{aligned}
(v_i, v_j) &\mapsto (v_i', v_j'), \\
v_i'^2 + v_j'^2 &= v_i^2 + v_j^2 \quad \text{E is conserved} \\
\begin{cases} v_i' \\ v_j' \end{cases} &= \begin{matrix} v_i \cos\alpha + v_j \sin\alpha \\ v_i \sin\alpha - v_j \cos\alpha \end{matrix}
\end{aligned}$$

α uniformly distributed in $[0, 2\pi)$. Equivalently,

$$f(v_1, \dots, v_N) \mapsto Q_{i,j}[f] = \frac{1}{2\pi} \int_0^{2\pi} f(v_1, \dots, v_i'(\alpha), \dots, v_j'(\alpha), \dots, v_N)\, d\alpha.$$

Kac's Master Equation

(Maxwellian-molecule-assumption) All pairs of particles are equally likely to collide.

$$k \text{ collisions} \Rightarrow \mathbb{P} = e^{-Nt}\frac{(Nt)^k}{k!}$$

$$f(v,t) = \sum_{k=0}^{\infty} e^{-Nt}\frac{(Nt)^k}{k!} Q^k[f] \tag{1}$$

$$\frac{\partial f}{\partial t} = N\lambda(Q - I)f \tag{2}$$

where

$$Q[f] = \binom{N}{2}^{-1} \sum_{i<j} Q_{i,j}[f] \tag{3}$$

Ergodicity and Spectral Gap

Kac's model is ergodic on $S^{N-1}(\sqrt{N})$ to the uniform distribution.

Kac (1956) conjectured that there is a spectral gap γ_N in $L^2(S^{N-1}(\sqrt{N}))$ controlled independently of N.

This conjecture was proven by E. Janvrésse 2001, and the gap was computed explicitly by Carlen-Carvalho-Loss explicitly.

Carlen-Carvalho-Loss 2003

Let $f \in L^2(S^{N-1}(\sqrt{N}), \text{unif.})$ be a probability density, and be symmetric in its variables. Then

$$||f(t,.) - 1||_{L^2(S^{N-1}(\sqrt{N}))} \leq e^{-\frac{1}{2}t} ||f(0,.) - 1||_{L^2(S^{N-1}(\sqrt{N}))} \tag{4}$$

Maxwellian (or Strong) Thermostat

The Maxwellian thermostat acting on the particle j is represented by R_j:

$$R_j[f](v) = \int_{-\infty}^{\infty} f(v_1, \dots, v_{j-1}, w, \dots, v_N)\, dw \sqrt{\frac{\beta}{2\pi}} e^{-\frac{\beta}{2} v_j^2} \tag{5}$$

The partially-thermostated Kac model has Master equation

$$\frac{\partial f}{\partial t} = N\lambda \binom{N}{2}^{-1} \sum_{i<j} (Q_{i,j} - I) f + \mu \sum_{k=1}^{m<N} (R_j - I)[f] \tag{6}$$

The Partialy Thermostated Kac Model

When $\mu > 0$, energy is no longer conserved

$$f \in L^1(\mathbb{R}^N),$$

$$\lim_{t\to\infty} e^{tL_{m=0,N}} f = \left(\begin{array}{c} \text{angular} \\ \text{average of } f \end{array} \right).$$

All radial functions are invariant under Kac evolution.

$$\lim_{t\to\infty} e^{tL_{m\geq 1,N}} f = \left(\frac{\beta}{2\pi}\right)^{\frac{N}{2}} e^{-\frac{\beta}{2}|v|^2} =: \Gamma_\beta(v)$$

Remark The case $m = N$ was studied by Bonetto, Loss, Vaidyanathan with a more physical thermostat (weak thermostat).

Spectral Gap

Consider the ground state transformation $f(v) = \Gamma_\beta(v)(1 + h(v))$; then $L_{m,N} f = (\bar{L}_{m,N}[h] + 1)\Gamma_\beta(v)$. Let

$$\Delta_{m,N} = \inf \left\{ -\langle h \bar{L}_{m,N} h \rangle : \int h(v)^2 \Gamma_\beta(v)\, dv = 1, \int h(v)\Gamma_\beta(v) = 0 \right\}.$$

Theorem 1 (H. Tossounian, R. Vaidyanathan)

For all $N \geq 2$ and $1 \leq m < N$, we have $C(\lambda, \mu)\frac{m}{N-1} \geq \Delta_{m,N} \geq c(\lambda, \mu)\frac{m}{N-1}$

This inequality is sharp when $N = 2$ and $m = 1$.

Relative Entropy and an Open Problem

Let $S(f|\phi) = \int f \ln \frac{f}{\phi}\, dv$. Then $S(e^{tL_{m,N}} f|\Gamma_\beta) \searrow$.
Can one improve the result:

Theorem 2 H. T., Vaidyanathan (2015)

Let $1 \leq m < N$, then we have

$$S(e^{tL_{m,N}} f|\Gamma_\beta) \leq D(t) S(f|\Gamma_\beta(v))$$

where

- $D(t) \geq 0, D(t) \searrow, D(0) = 1, D'(0) = 0,$
- $\log D(t) \sim -\frac{m}{N^2}$ when t is away from zero.

to results involving $\frac{m}{N}$?
The case $m = N$ has been achieved by Bonetto-Loss-Vaidyanathan (2014).

Thank You!

Connection: The Kac-Boltzmann equation

Kac's model is connected with the following Boltzmann-like equation, through a mechanism now known as propagation of chaos.

$$
\begin{aligned}
\frac{\partial f}{\partial t} &= \lambda \int_{\alpha \in [0,2\pi)} \int_{w \in \mathbb{R}} \left[f(v'(\alpha)) f(w'(\alpha)) - f(v) f(w) \right] \, dw \, d\alpha, \\
f &= f(v,t) \; v \in \mathbb{R}
\end{aligned}
$$

known as the Kac-Boltzmann equation.

The "Weak" Thermostat

The thermostat at temperature $\frac{1}{\beta}$ used in Bonetto-Loss-Vaidyanathan and acting on particle i is represented by T_i:

$$T_i[f](v) = \int_{-\infty}^{\infty} \int_0^{2\pi} f(v_1, \dots, v'_{i-1}(\theta), v_{i+1}, \dots, v_N) \sqrt{\frac{\beta}{2\pi}} e^{-\beta w'(\theta)^2/2} \, \frac{d\theta}{2\pi} \, dw \tag{7}$$

where

$$\begin{aligned} v'_i(\theta) &= v_i \cos\theta - w \sin\theta \\ w'(\theta) &= v_i \sin\theta + w \cos\theta \end{aligned}$$

Propagation of Chaos

Chaotic Sequence

A sequence of probability densities
$\{f_N : S^{N-1}(\sqrt{N}) \mapsto [0, \infty), f_N$ symmetric$\}$ is said to be "chaotic" if

$$\int_{S^{N-1}(\sqrt{N})} f_N(v)\phi(v_1, \ldots, v_k) d\sigma_N \to_{N\to\infty} \int_{\mathbb{R}^k} g(v_1)\ldots g(v_k)\phi(v_1, \ldots, v_k) \tag{8}$$

for some g fixed in $L^1(\mathbb{R})$ and all bounded continuous functions ϕ depending on finitely many variables.

Kac 1956

If $\{f_N\}$ is chaotic sequence, so is $\{e^{tL_N} f_N\}$. The "limit" $\phi(t)$ satisfies

$$\frac{\partial f}{\partial t} = \lambda \int_{\alpha\in[0,2\pi)} \int_{w\in\mathbb{R}} \left[f(v'(\alpha))f(w'(\alpha)) - f(v)f(w)\right] dw\, d\alpha.$$

References

1. M. Kac. Foundations of kinetic theory. In Proceedings of the Third Berkeley Symposium on Mathematical Statistics and Probability, 1954–1955, vol. III, pages 171–197, Berkeley and Los Angeles, 1956. University of California Press.
2. E. Janvrésse. Spectral gap for Kac's model of Boltzmann equation. Ann. Probab., 29(1) : 288–304, 2001.
3. E. A. Carlen, M. C. Carvalho, and M. Loss. Many-body aspects of approach to equilibrium. In Journees "Equations aux Dérivées Partielles" (La Chapelle sur Erdre, 2000), pages Exp. No. XI, 12. Univ. Nantes, Nantes, 2000.
4. F. Bonetto, M. Loss, and R. Vaidyanathan. The Kac model coupled to a thermostat. J. Stat. Phys., 156(4) : 647–667, 2014.
5. H. Tossounian, R. Vaidyanathan. Partially thermostated Kac model. J. Math. Phys. 56 (2015), no. 8, 083301, 16 pp. 80A10 (82C22).