Entropy Production Inequalities for the Kac Walk

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Based in joint work with E. Carlen and A. Einav

[1] E. A. Carlen, C. and A. Einav, *Entropy production inequalities for the Kac Walk,* Kinetic Theory and Related Models , **11** (2018) 219-238.

[2] E. A. Carlen, C. and M. Loss, *Spectral gap for the Kac model with hard sphere collisions*, Journal of Functional Analysis, **266** (2014) 1787-1832

[3] E. Carlen, C., J. Le Roux, M. Loss and C. Villani *Entropy and chaos in the Kac model.*, Kinet. Relat. Models **3** (2010) 85-122 .

The Kac Walk on the N-sphere

The Kac walk was introduced by Mark Kac in 1956 as a model for particles undergoing binary collisions. He was interested in the rate of equilibration.

In its simplest form, the model concerns N particles with one dimensional velocities

$$v_1, \ldots, v_N \ .$$

The state of the system will change due to a random process in which 2 of the velocities are changed at a time. This is intended to model binary collisions, and it is required that the total energy $E = \sum_{j=1}^{N} v_j^2$ is conserved.

Then for an N particle system with total energy N, the state space $\mathcal{S}_N$ is the set of all vectors

$$(v_1, v_2, \ldots, v_N)$$

on the sphere of radius $\sqrt{N}$.

In the *Kac walk* on $\mathcal{S}_N$, at each step one picks a pair i, j at random (*depending on the energies, not uniformly*), and then an angle θ uniformly in $[0, 2\pi)$, and then moves from $\vec{v} = (v_1, v_2, \ldots, v_N)$ to

$$(v_1, \ldots, v_i', \ldots, v_j', \ldots, v_N) =: R_{i,j,\theta}\vec{v}$$

where

$$v_i' = \cos\theta v_i + \sin\theta v_j \quad \text{and} \quad v_j' = -\sin\theta v_i + \cos\theta v_j \ .$$

The jumps arrive in a Poisson stream, one for each pair. Associated to each pair (i, j), $i < j$, there is an exponential random variable $T_{i,j}$ with parameter

$$\lambda_{i,j} = N \binom{N}{2}^{-1} (1 + v_i^2 + v_j^2)^\gamma \ ,$$

where $0 \leq \gamma \leq 1$, and $\gamma = 1/2$ is the case of main interest, corresponding to “hard-sphere collisions”.

$T_{i,j}$ is the waiting time for particles i and j to collide, and the set of these random times is taken to be independent. The first collision occurs at time $T = \min_{i<j}\{T_{i,j}\}$, and then the process starts over after particles i, j collide.

Let $\mathcal{L}$ be the generator of this process, which is reversible, so that if the initial probability density for $\vec{v}$ is F, the density at time t is $e^{t\mathcal{L}}F$, where

$$\mathcal{L}F(\vec{v}) = N\binom{N}{2}^{-1}\sum_{i<j}(1+v_i^2+v_j^2)^{\gamma}(F^{i,j}-F) \ ,$$

$$F^{i,j}(\vec{v}) := \frac{1}{2\pi}\int_{-\pi}^{\pi}F(R_{i,j,\theta}\vec{v})\mathrm{d}\theta \ .$$

This form of the generator was discussed by Villani. Ideally, one would like to replace $(1 + v_i^2 + v_j^2)^\gamma$ with $(v_i^2 + v_j^2)^\gamma$, as in the work on the spectral gap by Carlen, C. and Loss. However, in the context of entropy production it is not clear how to do this, and we work with the form studied by Villani.

In terms of scaling, the rate $(v_i^2 + v_j^2)^{1/2}$ corresponds to the hard-sphere collisions.

Chaos

$$\frac{\partial}{\partial t} F = \mathcal{L} F$$

is the *Kac Master equation*. Its connection with the Boltzmann equation comes through Kac's notion of *chaos*. The coordinate functions on $\mathcal{S}_N$ are never independent, but for large N, they are almost pairwise independent.

This is because the unit Gaussian probability measure on $\mathbb{R}^N$ is strongly concentrated on $\mathcal{S}_N$, the sphere of radius $\sqrt{N}$.

In particular, as $e^{t\mathcal{L}}F$ tends to 1, its single particle marginals tend to

$$\frac{1}{\sqrt{2\pi}} e^{-v^2/2} \ .$$

Let μ be a probability measure on $\mathbb{R}$. A sequence $\{\mu^{(N)}\}$ of probability measures on $\mathcal{S}^N$ is μ chaotic in case

$$\int \chi(v_1, \dots, v_k) \mathrm{d}\mu^{(N)}(v_1, \dots, v_N) \to \int \chi(v_1, \dots, v_k) \mathrm{d}\mu(v_1) \cdots \mathrm{d}\mu(v_k)$$

That is, as $N \to \infty$, the k particle marginal looks more and more like a product, in the sense of weak convergence.

This is the "minimal" notion of chaos, as originally introduced to prove the following theorem:

Theorem 0.1 (Propagation of Chaos, Kac 1956). *Let* $\{F_0^{(N)}\sigma^{(N)}\}$ *be a* $f_0(v)\mathrm{d}v$*–chaotic sequence. Then* $\{e^{t\mathcal{L}}F_0^{(N)}\sigma^{(N)}\}$ *is a* $f(v,t)\mathrm{d}v$*–chaotic sequence and* $f(v,t)$ *is a solution of the initial value problem*

$$\frac{\partial}{\partial t}f = \frac{1}{\pi}\int_{-\pi}^{\pi}\mathrm{d}\theta\int_{\mathbb{R}}\mathrm{d}w R_\gamma(v,w)[f(v^*(\theta,t)f(w^*(\theta),t) - f(v,t)f(w,t)]$$

with $R_\gamma(v,w) = (1+v^2+w^2)^\gamma$*, and*

$$v^*(\theta) = \cos\theta v + \sin\theta w \quad \text{and} \quad w^*(\theta) = -\sin\theta v + \cos\theta w\ .$$

for the initial data $f(v,0) = f_0(v)$

This equation is called the Kac-Boltzmann equation.

If one wants to prove properties of the solution of the Kac-Boltzmann equation using an analysis of the N-particle model, it is useful to know that stronger notions of chaos, involving convergence to a product in a stronger topology, are valid. The Kac notion is the minimal one, just enough to prove his theorem relating the Kac Master Equations and the Kac Boltzmann equation.

Existence of Chaotic initial data

Theorem 0.2 (Carlen, C., La Roux, Loss, Villani)**.** *Let f be a probability density on $\mathbb{R}$ satisfying, for some $p > 1$,*

$$\int_{\mathbb{R}} f(v) v^2 \mathrm{d}v = 1 \, , \; \int_{\mathbb{R}} f(v) v^4 \mathrm{d}v < \infty \, , f \in L^p(\mathbb{R})$$

and let $\mu(\mathrm{d}v) = f(v)\mathrm{d}v$, and let $[\mu^{\otimes N}]_{S^{N-1}(\sqrt{N})}$ be the normalized restriction of $f^{\otimes N}$ to the sphere. Then $\{[\mu^{\otimes N}]_{S^{N-1}(\sqrt{N})}\}$ is μ –chaotic

In this case, $[\mu^{\otimes N}]_{S^{N-1}(\sqrt{N})}$ will have a density F^N with respect to the uniform measure on the sphere:

$$[\mu^{\otimes N}]_{S^{N-1}(\sqrt{N})} = F^N \mathrm{d}\sigma \; .$$

Approach to Equilibrium

It is easy to see that under the Kac walk, the density tends to become uniform:

$$\lim_{t\to\infty} e^{t\mathcal{L}} F = 1 \ .$$

Kac proposed to measure this in terms of the *spectral gap* of $\mathcal{L}$ which is

$$\Delta_N := \inf\{\langle F, -\mathcal{L}F\rangle_{L^2(\mathcal{S}_N)} \ : \ \|F\|_2 = 1 \ , \langle F, 1\rangle_{L^2(\mathcal{S}_N)} = 0 \ \} \ .$$

$$\|e^{t\mathcal{L}} F - 1\|_2 = \|e^{t\mathcal{L}}(F-1)\|_2 \leq e^{-t\Delta_N}\|F-1\|_2 \ .$$

Kac conjectured that

$$\liminf_{N\to\infty} \Delta_N > 0 \ .$$

The Kac conjecture was proved by Janvresse with no estimate on the limiting gap. Carlen, C. and Loss gave the exact value:

$$\Delta_N = \frac{1}{2}\frac{N+2}{N-1} \ .$$

In subsequent work, this was extended to three dimensional collisions and hard sphere collisions, giving the exact gap for 3-dimensional Maxwellian molecules (Carlen, Geronimo and Loss) and bounds for hard sphere collisions (Carlen, C. and Loss).

We now discuss convergence in relative entropy for the Kac Master Equation and the Kac-Boltzmann equation, focusing on the relation between the two.

Entropy Production

Let f and g be two probability densities on a measure space $(X, \mathcal{F}, \mu)$. The *relative entropy of* $f\mathrm{d}\mu$ *with respect to* $g\mathrm{d}\mu$ is the quantity $H(f|g) = \int_X f[\ln f - \ln g]\mathrm{d}\mu$. Pinsker's inequality says that

$$H(f|g) \geq \frac{1}{2}\left(\int_X |f - g|\mathrm{d}\mu\right)^2 \quad (1)$$

Thus, while $H(f|g)$ is not itself a metric, it does control the L^1 distance between f and g.

The equilibrium solutions of the Kac-Boltzmann equation are the *centered Maxwellian densities* $M_T(v) = (2\pi T)^{-1/2} e^{-v^2/2T}$. The equilibrium to which the solution with initial data f_0 tends is the one with $T = \int_{\mathbb{R}} v^2 f_0(v) \mathrm{d}v$.

Consider a solution f with initial data f_0 for which $\int_{\mathbb{R}} v^2 f_0(v) \mathrm{d}v = 1$. Since the energy is conserved, Boltzmann's H theorem implies that $H(f(\cdot, t)|M_1)$ is monotone decreasing in t. Cercignani's conjecture for the Kac-Boltzmann equation was that for some constant $C_\gamma > 0$, all such solutions with initial data and with $H(f_0|M_1) < \infty$ satisfy

$$\frac{\mathrm{d}}{\mathrm{d}t} H(f(\cdot, t)|M_1) \leq -C_\gamma H(f(\cdot, t)|M_1) \ .$$

Pinsker's inequality would then yield

$$\|f(\cdot,t) - M_1\|_1 \leq [H(f_0|M_1)]^{1/2} e^{-C_\gamma t/2} \ .$$

Cercignani's conjecture is false for all $\gamma < 1$ – but it is true for $\gamma = 1$, as shown by Villani, who also showed how this result could be used to prove non-exponential bounds on the rate of relaxation for other values of γ and suitable constraints on the initial data. In this way he proved

$$\frac{\mathrm{d}}{\mathrm{d}t} H(f(\cdot,t)|M_1) \leq -C_{\gamma,\epsilon} \left(H(f(\cdot,t)|M_1)\right)^{1+\epsilon} \qquad (2)$$

for $\epsilon > 0$, $0 \leq \gamma < 1$, for suitable classes of initial data.

For future reference, we express this as a functional inequality. Define

$$D_\gamma(f(\cdot,t)) := -\frac{\mathrm{d}}{\mathrm{d}t} H(f(\cdot,t)|M_1)$$

where $f(v,t)$ is the solution of the Kac-Boltzmann equation with $f(v,0) = f(v)$. Then we may restate (2) as

$$D_\gamma(f(\cdot,t)) \geq C_{\gamma,\epsilon} \left(H(f(\cdot,t)|M_1)\right)^{1+\epsilon} \ . \tag{3}$$

The main question that we address here is the following:

To what extent can one do something similar for the Kac Master equation?

To investigate this question, let F be a probability density with respect to $\mathrm{d}\sigma_N$. The relative entropy of F with respect to the uniform density 1 is simply $\int_{\mathbb{S}^{N-1}(\sqrt{N})} F \ln F \mathrm{d}\sigma_N$. To simplify our notation, we define

$$H_N(F) = \int_{\mathbb{S}^{N-1}(\sqrt{N})} F \ln F \mathrm{d}\sigma_N \ . \tag{4}$$

We are thus led to investigate the *relative entropy dissipation* under the dynamics generated by $\mathcal{L}_{N,\gamma}$. This dissipation, sometimes called *the entropy production* is the non-negative quantity $D_{N,\gamma}(F)$ that is given by

$$D_{N,\gamma}(e^{t\mathcal{L}_{N,\gamma}}F) = -\frac{\mathrm{d}}{\mathrm{d}t}H_N(e^{t\mathcal{L}_{N,\gamma}}F) \ .$$

With $\psi(x,y) = (x-y)\log\left(\frac{x}{y}\right)$,

$$D_{N,\gamma}(F_N) = \frac{1}{4\pi}\frac{N}{\binom{N}{2}}\times$$

$$\sum_{i<j}\int_{\mathbb{S}^{N-1}(\sqrt{N})}\int_0^{2\pi}\left(1+(v_i^2+v_j^2)\right)^\gamma \psi\left(F_N, F_N\circ R_{i,j,\theta}\right) d\sigma^N d\theta \ .$$

Inequalities relating $H_N(F)$ and $D_{N,\gamma}(F)$ are useful for quantifying the aforementioned rate of convergence. As we only connect the Kac Walk with the Kac-Boltzmann equation in the limit $N \to \infty$, we are ultimately only interested in inequalities that are *uniform in* N.

In particular, one might hope to find $C_\gamma > 0$, independent of N, such that

$$D_{N,\gamma}(F) \geq C_\gamma H_N(F).$$

This is known as *Cercignani's Conjecture for the Kac Walk*.

A significant breakthrough in its study was done in 2003 by Villani who introduced the family of operators $\{\mathcal{L}_{N,\gamma}\}_{\gamma\in[0,1]}$ and showed that

$$D_{N,\gamma}(F) \geq C_\gamma \frac{H_N(F)}{N^{1-\gamma}}. \qquad (5)$$

Again for $\gamma = 1$, we have the conjectured bound, but only for $\gamma = 1$. For $\gamma < 1$, this gives a decay rate of order $e^{-CN^{\gamma-1}t}$ which is meaningless in the limit $N \to \infty$.

Einav proved that this bound is essentially sharp, as Villani had conjectured.

For the Kac Walk, the intuition that chaotic data with a one particle marginal f behaves like $f^{\otimes N}$ is true in some cases, and one can show (see [CCRLV] for precise statements)

$$\frac{H_N(F_N)}{N} \approx H(f|M), \qquad \frac{D_{N,\gamma}(F_N)}{N} \approx D_\gamma(f).$$

This suggests that we seek inequalities of the form

$$\frac{D_{N,\gamma}(F_N)}{N} \geq C_{\gamma,\epsilon} \left(\frac{H_N(F_N)}{N} \right)^{1+\epsilon} .$$

Can we estimate $D_{N,\gamma}(F_N)$ in terms of $D_{N,1}(F_N)$ and propagated regularity of F_N to obtain such a result?

In this way, Villani used the $\gamma = 1$ bounds to control entropy production in the Boltzmann equation for physical models. It is not so easy for the Kac Master equation because the two particle marginal of F_N is not *exactly* a product even for large N, as it is for Boltzmann.

We present two results in this direction. One requires only a form of chaos known to be propagated. However, in this inequality, the constant depends weakly on N, so it cannot be used to prove results for the Kac-Boltzmann equation.

The second inequality has a constant that is independent of N, but involves a new notion of chaos that we do not know to be propagated. Despite this, we show that this inequality may be used to bound the rate of relaxation to equilibrium for solutions of the Kac-Boltzmann equation.

Definition 0.3. *Let* $F_N \in P(\mathbb{S}^{N-1}(\sqrt{N}))$ *be symmetric. We say that* F_N *is log-scalable if there exists* $C > 0$*, independent of* N*, such that*

$$\sup_{v \in \mathbb{S}^{N-1}(\sqrt{N})} |\log F_N(v)| \leq CN. \qquad (6)$$

Theorem 0.4. *Let* $F_N \in P(\mathbb{S}^{N-1}(\sqrt{N}))$ *be symmetric and log-scalable with associated constant* $C_F > 0$*. Assume there exists* $k > 1$ *such that* $M_{2k} = \sup_N M_{2k}(\Pi_1(F_N)) < \infty$*. Then,*

$$\frac{D_{N,\gamma}(F_N)}{N} \geq \mathcal{C}_{k,\gamma,N} \left(\frac{H_N(F_N)}{N} \right)^{1+\frac{1-\gamma}{k-1}}, \qquad (7)$$

with $\mathcal{C}_{k,\gamma,N}$ *is a multiple of* $N^{\epsilon(k)}$, $\lim_{k\to\infty} \epsilon(k) = 0$.

A strong chaotic condition

Definition 0.5. *A symmetric family of probability densities* $\{F_N\}_{N\in\mathbb{N}} \in P(\mathbb{S}^{N-1}(\sqrt{N}))$ *has the log-power property of order* $\beta > 0$*, if there exists* $C > 0$*, independent of* N*, such that*

$$\frac{1}{2\pi}\int_0^{2\pi}\int_{\mathbb{S}^{N-1}(\sqrt{N})}\psi_\beta(F_N, F_N\circ R_{1,2,\theta})d\sigma^N d\theta \leq C^{1+\beta}$$

where $\psi_\beta(x,y) = |x-y|\left|\log\frac{x}{y}\right|^{1+\beta}$*.*

The condition that $\{F_N\}_{N\in\mathbb{N}}$ have the log-power property of order $\beta > 0$ is a quantitative chaoticity condition because it can be easily verified when $\{F_N\}_{N\in\mathbb{N}}$ is a family of *normalized tensor product states*, as constructed in [CCRLV] from a suitable probability density f on $\mathbb{R}$.

Theorem 0.6. *Let* $F_N \in P(\mathbb{S}^{N-1}(\sqrt{N}))$ *have the log-power property of order* β *with associated constant* $C_F > 0$*. If there exists* $k > 1 + \frac{1}{\beta}$ *such that* $M_{2k} = \sup_N M_{2k}(\Pi_1(F_N)) < \infty$*. Then*

$$\frac{D_{N,\gamma}(F_N)}{N} \geq \mathcal{C}_\epsilon \left(\frac{H_N(F_N)}{N} \right)^{1+\epsilon}$$

where $\epsilon = 1 + \dfrac{(1-\gamma)(1+\beta)}{k\beta - (1+\beta)}$ *and* $\mathcal{C}_\epsilon$ *is explicitly computable.*

If we knew that our new strong notion of chaos was propagated by the Kac Master Equation, the previous theorem would tell us that the relative entropy per particle decays to zero at a uniform exponential rate.

We do not know this, but the conditions on f that are required for the normalized products to yield a log power chaotic family are easily shown to be propagated by the Kac-Boltzmann equation, and this crucial fact allows us to side-step the interesting question as to whether the log-power property of order β might be propagated by the Kac Master Equation.

This yields:

Theorem 0.7. *Let* $f \in P(\mathbb{R})$ *be such that* $M_2(f) = 1$. *Assume in addition that there exists* $\beta > 0$ *and* $k > 1 + 1/\beta$ *such that*

$$M_{\max\{2k, k(1+\beta), 4\}}(f) < \infty,$$

that $I(f) = \displaystyle\int_{\mathbb{R}} \frac{(f'(x))^2}{f(x)} dx < \infty$ *and that*

$$f(v) \geq Ce^{-|v|^2} \qquad \forall v \in \mathbb{R}.$$

Then, there exists an explicit constant, $\mathcal{C}$, *depending only on the parameters of the problem such that*

$$D_\gamma(f) \geq \mathcal{C} H(f|M)^{1+\epsilon} \quad \text{where} \quad \epsilon = \frac{(1-\gamma)(1+\beta)}{k\beta - (1+\beta)}$$

The last result is the Kac-Boltzmann equation analog of Vilani's result for the Boltzmann equation. The interest in the result is not that it provides new information about this equation, but that the best currently known estimates on the entropic rate of convergence can be obtained as corollaries of an analysis of the Kac Master Equation, thus vindicating Kac's purpose in introducing the model.

We have also seen that in order to prove uniform in N entropic convergence results for the Kac Master equation, one does not necessarily need better entropy inequalities *per se*: Better propagation of chaos results would suffice. This will be the subject of further research.