Between Functional Inequalities and Cercignani's Conjecture

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24th of March, 2015

Boltzmann's Equation

- Boltzmann's Equation is an important equation in non-equilibrium Statistical Mechanics, describing the time evolution of the density function of a given ensemble (usually dilute gas).
- In its spatial homogeneous form, Boltzmann's Equation is given by

$$\begin{cases} \frac{\partial f}{\partial t}(t,v) = Q(f,f)(t,v) & t>0,\ v\in\mathbb{R}^d, \\ f(0,v) = f_0(v) & f_0\geq 0,\ f_0\in L^1\left(\mathbb{R}^d\right), \end{cases}$$

where $Q(f,f)(v)$ is given by the expression:

$$\int_{\mathbb{R}^d} dv_* \int_{\mathbb{S}^{d-1}} d\sigma B\left(v-v_*,\sigma\right)\left(f\left(v'\right)f\left(v_*'\right)-f\left(v\right)f\left(v_*\right)\right),$$

Boltzmann's Equation Cont.

and

$$v' = \frac{v+v_*}{2} + \frac{|v-v_*|}{2}\sigma,$$
$$v_*' = \frac{v+v_*}{2} - \frac{|v-v_*|}{2}\sigma.$$

The function $B(v-v_*,\sigma)$, called the Boltzmann Collision Kernel, is determined by the physics of the problem and relates to the physical cross section.

Kac's Model

- In 1956 Marc Kac introduced an $N-$particle linear model from which a caricature of the Boltzmann equation arose as a mean field limit.
- Kac's model consisted of N indistinguishable particles with one dimensional velocity that undergo random collision in the following manner: Suppose that a moment before the collision the velocity vector of the ensemble was $(v_1, \dots, v_N)$. When the collision occurs, we pick a pair of particles at random, say (v_i, v_j), with equal probability for any i, j, and collide them. After their collision the new velocity vector is given by $(v_1, \dots, v_i(\vartheta), \dots, v_j(\vartheta), \dots, v_N)$ where

$$\begin{pmatrix} v_i(\vartheta) \\ v_j(\vartheta) \end{pmatrix} = \begin{pmatrix} v_i \cos\vartheta + v_j \sin\vartheta \\ -v_i \sin\vartheta + v_j \cos\vartheta \end{pmatrix} = R_{i,j,\vartheta} \begin{pmatrix} v_i \\ v_j \end{pmatrix}$$

- Denoting by

$$Q(\psi)(\mathbf{v}) = \frac{1}{\begin{pmatrix} N \\ 2 \end{pmatrix}} \sum_{i<j} \frac{1}{2\pi} \int_0^{2\pi} \psi\left(R_{i,j,\vartheta}\mathbf{v}\right) d\vartheta,$$

  one finds that the evolution equation for the $N-$particles distribution function, F_N, is given by

$$\frac{\partial F_N}{\partial t}\left(v_1,\dots,v_N,t\right) = N(Q-I)F_N\left(v_1,\dots,v_N,t\right), \qquad (1)$$

  This equation is usually called Kac's Master equation.

- Kac's Master equation can be considered on $\mathbb{R}^N$, but a more realistic approach would be to restrict it to the manifold $\mathbb{S}^{N-1}(\sqrt{N})$ (which we will call 'Kac's sphere') where Q is a bounded, self adjoint operator satisfying $Q \leq I$ and

$$\mathrm{Ker}\left(I-Q\right) = \mathrm{span}\left\{1\right\}.$$

Connection to Boltzmann's Equation and Chaoticity.

- Integrating over all the velocities but v_1 in Kac's Master equation, and using symmetry one can see that

$$\partial_t \Pi_1(F_N)(v_1) = \frac{1}{\pi}\int_0^{2\pi}\int_{\mathbb{R}} \left(\Pi_2(F_N)(v_1(\vartheta), v_2(\vartheta)) - \Pi_2(F_N)(v_1, v_2)\right) d\vartheta dv_2$$

  where $\Pi_k(F_N)$ is the $k-$th marginal.
- The above equation looks very similar to a Boltzmann type equation if $\Pi_2(F_N) \approx \Pi_1(F_N) \otimes \Pi_1(F_N)$.

Definition

Let X be a Polish space. A family of symmetric probability measures on X^N, $\{\mu_N\}_{N\in\mathbb{N}}$, is called $\mu-$chaotic, where μ is a probability measure on X, if for any $k \in \mathbb{N}$

$$\lim_{N\to\infty} \Pi_k\left(\mu_N\right) = \mu^{\otimes k},$$

where $\Pi_k\left(\mu_N\right)$ is the $k-$th marginal of μ_N, and the limit is taken in the weak topology.

Connection to Boltzmann's Equation and Chaoticity Cont.

- Under the assumption of $f-$chaoticity on the family of density functions $\{F_N\}_{N\in\mathbb{N}}$ (i.e. assuming that the family $d\mu_N = F_N d\sigma^N$ is $d\mu = f(v)dv-$chaotic, where σ^N is the uniform probability measure on Kac's sphere), our marginal equation turns into the Boltzmann-Kac equation:

$$\partial_t f(v_1) = \frac{1}{\pi}\int_0^{2\pi}\int_{\mathbb{R}} \left(f(v_1(\vartheta))f(v_2(\vartheta)) - f(v_1)f(v_2)\right) d\vartheta dv_2.$$

- Kac showed that if the initial data is chaotic, then the solution to his Master equation is also chaotic for all $t>0$. Moreover, the limit function $f(t,v)$ satisfies the above caricature of the Boltzmann equation.

The Existence of Chaotic States.

- There is a simple formula to create chaotic states on Kac's sphere. Given a 'nice' enough distribution function, $f(v)$, on $\mathbb{R}$, one defines the following distribution function on Kac's sphere:

$$F_N\left(v_1,\dots,v_N\right)=\frac{\Pi_{i=1}^N f(v_i)}{\mathcal{Z}_N\left(f,\sqrt{N}\right)}, \tag{2}$$

  where $\mathcal{Z}_N\left(f,\sqrt{N}\right)=\int_{\mathbb{S}^{N-1}\left(\sqrt{N}\right)}\Pi_{i=1}^N f(v_i)d\sigma^N$. We call distributions of the form (2) *conditioned tensorisation of* f.

- Kac showed that under very restrictive integrability conditions on f, the above family is indeed $f-$chaotic. This was extended in 2010 by Carlen, Carvalho, Le Roux, Loss and Villani who managed to show the following:

Theorem

Let f be a distribution function on $\mathbb{R}$ such that $f\in L^p\left(\mathbb{R}\right)$ for some $p>1$, $\int_{\mathbb{R}}v^2f(v)dv=1$ and $\int_{\mathbb{R}}v^4f(v)dv<\infty$. Then the family of conditioned tensorisation of f is $f-$chaotic.

The Normalisation Function.

- The proof of Carlen et al's theorem relies *heavily* on an asymptotic approximation of the normalisation function

$$\mathcal{Z}_N\left(f,\sqrt{r}\right)=\int_{\mathbb{S}^{N-1}(r)}\Pi_{i=1}^N f(v_i)d\sigma_r^N,$$

where $d\sigma_r^N$ is the uniform probability measure on the sphere $\mathbb{S}^{N-1}(r)$, as it measures how well the tensoriastion of f is concentrated on the sphere of radius r.

Theorem (Carlen et. al. 2010)

Let f be a distribution function on $\mathbb{R}$ such that $f\in L^p(\mathbb{R})$ for some $p>1$, $\int_{\mathbb{R}} v^2 f(v)dv=1$ and $\int_{\mathbb{R}} v^4 f(v)dv<\infty$. Then

$$\mathcal{Z}_N(f,\sqrt{r})=\frac{2}{\sqrt{N}\Sigma\left|\mathbb{S}^{N-1}\right|r^{\frac{N-2}{2}}}\left(\frac{e^{-\frac{(r-N)^2}{2N\Sigma^2}}}{\sqrt{2\pi}}+\lambda_N(r)\right),$$

where $\Sigma^2=\int_{\mathbb{R}} v^4 f(v)dv-1$ *and* $\sup_r\left|\lambda_N(r)\right|\underset{N\to\infty}{\longrightarrow}0.$

Equilibrium and Rate of Convergence

- The operator Q in Kac's Master Equation is easily seen to be self adjoint, between 0 and I, and with a one dimensional eigenspace to the eigenvalue $\lambda = 1$, spanned by the constant function $F \equiv 1$.
- The structure of Kac's equation, along with the above, proves that for a fixed N, the solution to the evolution equation must converge to the stationary solution $F \equiv 1$ as the time goes to infinity.
- The rate of convergence is of great interest, especially if it is independent of the number of particles. In that case, we hope it might help show convergence to the equilibrium state of the associated Boltzmann equation.

The Spectral Gap

- A natural way to measure the rate of convergence is the spectral gap, defined as

$$\Delta_N = \inf \left\{ \langle \varphi_N, N(I-Q)\varphi_N \rangle \mid \varphi_N \perp 1 \quad \langle \varphi_N, \varphi_N \rangle = 1 \right\}.$$

- In his 1956 paper Kac conjectured that $\liminf_{N\to\infty} \Delta_N > 0$.
- The conjecture remained open until 2000, when Janvresse showed it to be true. Later on that year Carlen, Carvalho and Loss managed to compute the spectral gap explicitly and showed that

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

The Spectral Gap Problem

- Kac's conjecture might fool us to think that since the spectral gap can be bounded below independently of N we can get exponential convergence to equilibrium since

$$\left\|F_N(t)-1\right\|_{L^2\left(\mathbb{S}^{N-1}(\sqrt{N})\right)} \leq e^{-\liminf_{N\to\infty}\Delta_N t}\left\|F_N(0)-1\right\|_{L^2\left(\mathbb{S}^{N-1}(\sqrt{N})\right)}.$$

  Such is not the case.

- The main problem lies with the initial data. Heuristically speaking, many chaotic families (particularly those which are common examples) satisfy $F_N \approx f^{\otimes N}$ in some sense. This leads us to a very high L^2 norm that will depend on N very strongly.

- Indeed, one can easily find examples of chaotic families F_N satisfying

$$\left\|F_N\right\|_{L^2} \geq C^N,$$

  where $C > 1$ (conditioned tensorisation are the appropriate candidates).

The Entropy Solution

- Since the linear theory is not helpful as we hoped it to be, we'd like to find another quantity (probably non linear) that would help us measure the distance from equilibrium.
- Two important quantities that appear frequently in Statistical Mechanics are the entropy and relative entropy. The relative entropy of two measures $\mu \ll \nu$ is defined to be

$$H(\mu|\nu) = \int h \log h d\nu$$

  where $h = \frac{d\mu}{d\nu}$.
- We can thus define

$$H_N(F_N) = H(F_N d\sigma^N | d\sigma^N) = \int_{\mathbb{S}^{N-1}(\sqrt{N})} F_N \log F_N d\sigma^N,$$

  where $d\sigma^N$ is the uniform measure on $\mathbb{S}^{N-1}(\sqrt{N})$.

The Entropy Solution Cont.

- A crucial difference between the entropy method and the linear one lies in the extensivity of the entropy. Namely, for certain types of chaotic families we have that

$$H_N(F_N) \approx NH(f|\gamma)$$

  where γ is the standard Gaussian.
- The known Kullback-Pinsker inequality

$$\|\mu - \nu\|_{TV}^2 \leq 2H(\mu|\nu)$$

  gives us a way to use the relative entropy to measure distances between measures.

The Entropy Production

- We'd like to follow a similar route to the one we had in the linear case and define an appropriate 'spectral gap' for the entropy.
- a simple calculation shows that if F_N solves the Master equation then

$$\frac{\partial H_N(F_N)}{\partial t} = \langle N(Q-I)F_N, \log F_N\rangle_{L^2\left(\mathbb{S}^{N-1}(\sqrt{N})\right)}.$$

- The above leads us to define the *Entropy-Entropy Production* ratio as

$$\Gamma_N = \inf_{\psi_N} \frac{\langle N(I-Q)\psi_N, \log\psi_N\rangle_{L^2\left(\mathbb{S}^{N-1}(\sqrt{N})\right)}}{H_N(\psi_N)} = \inf_{\psi_N} \frac{D_N(\psi_N)}{H_N(\psi_N)},$$

where ψ_N are symmetric probability densities of the N-particles.
- For substantial decay we'd like to find $C>0$ such that $\Gamma_N > C$ for all N.

Villani's Conjecture

- In 2003 Villani managed to show that

$$\Gamma_N \geq \frac{2}{N-1}$$

- Villani conjectured that

$$\Gamma_N = O\left(\frac{1}{N}\right)$$

Theorem (E. - 2011)

For any $0 < \eta < 1$ there exists a constant $C_\eta > 0$, depending only on η, such that

$$\Gamma_N \leq \frac{C_\eta}{N^\eta}$$

- On $\mathbb{R}^N$, the relative entropy with respect to the Gaussian measure enjoys a subadditivity property. Given a density function $F_N \in P\left(\mathbb{R}^N\right)$, then for any $1 \leq i \leq N$ we define the first marginal in the $i-$th variable of F_N as

$$\Pi_1^{(i)}\left(F_N\right)\left(v_i\right) = \int_{\mathbb{R}^{N-1}} F_N\left(v_1, \dots, v_N\right) dv_1 \dots dv_{i-1} dv_{i+1} \dots dv_N .$$

Alternatively, $\Pi_1^{(i)}\left(F_N\right)\left(v_i\right)$ can be defined as the unique probability density in $P\left(\mathbb{R}\right)$ that satisfies

$$\int_{\mathbb{R}} \phi(v_i) \Pi_1^{(i)}\left(F_N\right)\left(v_i\right) dv_i = \int_{\mathbb{R}^N} \phi(v_i) F_N\left(v_1, \dots, v_N\right) dv_1 \dots dv_N .$$

Theorem

Let $F_N \in P\left(\mathbb{R}^N\right)$ have a finite second moment. Then

$$\sum_{i=1}^{N} H\left(\Pi_1^{(i)}\left(F_N\right) | \gamma\right) \leq H\left(F_N | \gamma_N\right), \tag{3}$$

where $\gamma_k\left(v_1, \dots, v_k\right) = \frac{e^{-\frac{\sum_{i=1}^k v_i^2}{2}}}{\left(2\pi\right)^{\frac{k}{2}}}$ and $\gamma = \gamma_1$.

Marginals on the Spherical

- Much like the Euclidean space, we'd like to develop a notion of marginal on the appropriate sphere. Taking a leaf from the alternative definition of the first marginal in the $i-$th variable we define the first marginal *on the sphere* in the $i-$th variable of the density function $F_N \in P\left(\mathbb{S}^{N-1}\left(\sqrt{N}\right), d\sigma_N\right)$, $F_i^{(N)}$, as the unique density function such that

$$\int_{\mathbb{S}^{N-1}(\sqrt{N})} \phi(v_i) F_i^{(N)}(v_i)\, d\sigma_N = \int_{\mathbb{S}^{N-1}(\sqrt{N})} \phi(v_i) F_N(v_1, \dots, v_N)\, d\sigma_N.$$

- It is easy to show that

$$F_i^{(N)}(v_i) = \int_{\mathbb{S}^{N-2}\left(\sqrt{N-v_i^2}\right)} F_N d\sigma^{N-1}_{\sqrt{N-v_i^2}},$$

where $d\sigma_r^k$ is the uniform probability measure on $\mathbb{S}^{k-1}(r)$.

- Given $F_N \in P\left(\mathbb{S}^{N-1}\left(\sqrt{N}\right), d\sigma_N\right)$ we denote by

$$H_N\left(F_N\right) = H\left(F_N d\sigma_N | d\sigma_N\right),$$

the appropriate entropy on the sphere.

- In 2004 Carlen, Lieb and Loss managed to show that in general (3) *does not hold* on the sphere. They have shown that

Theorem (Carlen, Lieb, Loss (2004))

Given $F_N \in P\left(\mathbb{S}^{N-1}\left(\sqrt{N}\right), d\sigma_N\right)$ *then*

$$\sum_{i=1}^{N} H_N\left(F_i^{(N)}\right) \leq 2H_N\left(F_N\right). \tag{4}$$

Moreover, the constant 2 *is sharp.*

Connection to Cercignani's Conjecture

- Surprisingly enough, in 2007 Carlen has shown that using the above inequality one can find an alternative, inductive, proof to the lower bound for Γ_N (Villanis original proof involved a clever semigroup argument on the sphere using the heat semigroup). Moreover, the fact that we had the factor 2 in the theorem was a vital part of why we get such a strong N dependency. Had the 2 been $1+\epsilon_N$, where ϵ_N goes to zero appropriately, a uniform lower bound would have been found.

Main Theorem

Theorem (E. (2014))

Let $F_N \in P\left(\mathbb{S}^{N-1}\left(\sqrt{N}\right), d\sigma_N\right)$ *be such that:*

(i) $\mathcal{A}_k = \sup_N \frac{\sum_{i=1}^N M_k\left(\Pi_1^{(i)}(F_N)\right)}{N} < \infty$ *for some* $k > 2$ *where*

$$M_k\left(\Pi_1^{(i)}\left(F_N\right)\right) = \int_{\mathbb{R}} |v|^k\, \Pi_1^{(i)}\left(F_N\right)(v) dv = \int_{\mathbb{S}^{N-1}\left(\sqrt{N}\right)} |v_i|^k F_N d\sigma_N.$$

(ii) $\inf_N \frac{H_N(F_N)}{N} \geq C_H > 0.$

and either

(iii) (Non-intrinsic condition) $\mathcal{A}_I = \sup_N \frac{\sum_{i=1}^N I\left(\Pi_1^{(i)}(F_N)\right)}{N} < \infty$, *or*

(iii') (Intrinsic conditions) $\sup_N \frac{I_N(F_N)}{N} \leq C_I < \infty$ *and there exists* $2 < q < k$ *such that*

$$\mathcal{A}_q^P = \sup_N \frac{\sum_{i=1}^N P_q^{(i)}\left(F_N\right)}{N} < \infty$$

where $P_q^{(i)}\left(F_N\right) = \int_{\mathbb{R}} \frac{\Pi_1^{(i)}(F_N)(v)}{\left(1-\frac{v^2}{N}\right)^{\frac{q}{q-2}}} dv = \int_{\mathbb{S}^{N-1}\left(\sqrt{N}\right)} \frac{F_N}{\left(1-\frac{v_i^2}{N}\right)^{\frac{q}{q-2}}} d\sigma_N$

Main Theorem Cont

Then there exists ϵ_N depending on $\mathcal{A}_k$, C_H and $\mathcal{A}_l$ or C_l and $\mathcal{A}_q^P$ that goes to zero like a negative power of N, depending on k and possibly q, such that

$$\sum_{i=1}^{N} H_N\left(F_i^{(N)}\right) \leq (1+\epsilon_N)\, H_N(F_N)\,. \tag{5}$$

- Unfortunately, the induction doesn't work as well so far, but the theorem does identifies a few key ingredients that we feel play an important role in the validation of the conjecture.

Thank You!