An analog of Cercignani's conjecture for the Becker-Döring equation

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Cambridge, 12 May 2016

We present a recent work on entropy production inequalities for the Becker-Döring equation.

The Becker-Döring equations

$$\frac{\mathrm{d}}{\mathrm{d}t} c_i(t) = W_{i-1}(t) - W_i(t), \qquad i \geq 2,$$

$$\frac{\mathrm{d}}{\mathrm{d}t} c_1(t) = -W_1(t) - \sum_{k=1}^{\infty} W_k(t),$$

where

$$W_i := a_i c_i c_1 - b_{i+1} c_{i+1} \qquad i \geq 1.$$

$c_i \equiv$ density of clusters of size i

$W_i \equiv$ net rate of the reaction $\{i\} + \{1\} \rightleftharpoons \{i+1\}$

$\{a_i\}_{i\geq 1} \equiv$ coagulation coefficients

$\{b_i\}_{i\geq 2} \equiv$ fragmentation coefficients

Coagulation and fragmentation coefficients

We consider always the following coefficients, physically representative: we choose $0 \leq \alpha \leq 1$, $0 < \mu < 1$ and $z_s > 0$ and define

$$
\begin{aligned}
a_i &= i^\alpha && (\text{some } 0 \leq \alpha \leq 1, \text{ all } i \geq 1) \\
b_i &= a_{i-1} Q_{i-1} / Q_i && (i \geq 2) \\
Q_i &= e^{-(i-1)^\mu} z_s^{1-i} && (\text{some } 0 < \mu \leq 1)
\end{aligned}
$$

Q_i are the *detailed balance coefficients*.
z_s is the *critical monomer density*.

The entropy method

The use of Lyapunov functionals, sometimes called the "entropy method", has been key in the development of the theory for kinetic equations, and in particular the Boltzmann equation.

The idea is the following: if we have an evolution equation for f, with a Lyapunov functional H satisfying

$$\frac{\mathrm{d}}{\mathrm{d}t} H(f(t)) = -D(f(t)) \leq 0,$$

one may try to prove the following functional inequality:

$$\lambda H(f) \leq D(f)$$

for f in some family which is invariant by the flow of the equation. If we manage to do this, we get the differential inequality

$$\frac{\mathrm{d}}{\mathrm{d}t} H(f(t)) \leq -\lambda H(f(t)),$$

which often implies exponential convergence to equilibrium.

Previous results on speed of convergence to equilibrium

How fast do *subcritical* solutions converge to equilibrium? The first result on this was given by **Jabin & Niethammer (2003).** For the Becker-Döring system they showed that, assuming a bounded exponential moment and $\epsilon < c_1 < z_s - \epsilon$,

$$D \geq \frac{1}{C|\log H|^2} H,$$

which implies

$$H(t) \leq C e^{-t^{1/3}}.$$

This is slightly worse than an exponential convergence, and requires exponential moments.

Previous results: linearisation method

A natural approach in order to study the speed of convergence is to study the linearised equation around the equilibrium. This was done in a recent work, giving:

Theorem (C. & Lods, 2013)

Any subcritical solution with some exponential moment initially bounded converges exponentially fast to the unique equilibrium with its same mass: for some $\nu > 0$,

$$\sum_i e^{\nu i} \left| c_i(t) - c_i^{\mathrm{eq}} \right| \leq C e^{-\lambda t} \sum_i e^{\nu i} \left| c_i(0) - c_i^{\mathrm{eq}} \right|.$$

This improves the previous almost-exponential convergence (though it uses the Jabin & Niethammer result when the solution is far from equilibrium).

Cercignani's conjecture?

This still leaves open one question: is the inequality by Jabin & Niethammer optimal, or can we expect that

$$\lambda H \leq D$$

in some cases?

The corresponding question for the Boltzmann equation is known as Cercignani's conjecture (1983). If we have

$$\partial_t f = Q(f,f) \qquad \text{(homogeneous Boltzmann eq.)}$$

then

$$\frac{d}{dt} H(f|M) = -D(f)$$

and the question of whether (or under what conditions) we have

$$\lambda H(f|M) \leq D(f)$$

is *Cercignani's conjecture*. The inequality looks like

$$\lambda \int_{R^d} f \log \frac{f}{M}\, dv$$
$$\leq \iiint B(|v - v_*|) \Big(f(v) f(v_*) - f(v') f(v'_*) \Big) \log \frac{f(v) f(v_*)}{f(v') f(v'_*)}\, d\sigma\, dv\, dv_*$$

1. Counterexamples: **[Bobylev 84]** (Maxwell molecules), **[Wennberg 97]**, **[Bobylev & Cercigani 99]**
2. First positive results: **[Desvillettes 1989]**, **[Carlen & Carvalho 92, 94]**
3. In a series of papers **[Desvillettes 2000]**, **[Toscani and Villani 1999]**, **[Villani 2003]** the following answer was given:
    1. For some (unphysical) kernels it holds in complete generality: $B(|v - v_*|) = 1 + |v - v_*|^2$.
    2. For some others it does not (but one can then show slightly different inequalities by interpolation).

An analog for the Becker-Döring equation

In the Becker-Döring case we are able to show the following analog of this result:

Theorem (C., Einav & Lods (2015))

1. *When $a_i = i$ there exists $\lambda > 0$ such that*

$$\lambda H(c) \leq D(c)$$

in general, when $\epsilon < c_1 < z_s - \epsilon$ (no assumption on moments).

2. *When $a_i = i^\alpha$, by interpolation one finds*

$$\tilde{\lambda} H(c)^{\frac{\beta-\alpha}{\beta-1}} \leq (M_\beta)^{\frac{1-\alpha}{\beta-1}} D(c)$$

for all c with a bounded moment M_β of order $\beta > 1$.

The entropy method for the Becker-Döring equation

For the Becker-Döring system we may use

$$H(c|Q_i z^i) = \sum_{i=1}^{\infty} \left(c_i \log \frac{c_i}{Q_i z^i} - c_i + Q_i z^i \right)$$
$$= \sum_{i=1}^{\infty} \mathcal{Q}_i \Psi \left(\frac{c_i}{\mathcal{Q}_i} \right)$$

$$D = \sum_{i=1}^{\infty} (a_i c_1 c_i - b_{i+1} c_{i+1}) \left(\log(a_i c_1 c_i) - \log(b_{i+1} c_{i+1}) \right)$$
$$= \sum_{i=1}^{\infty} a_i \mathcal{Q}_1 \mathcal{Q}_i \left(\frac{c_1 c_i}{\mathcal{Q}_1 \mathcal{Q}_i} - \frac{c_{i+1}}{\mathcal{Q}_{i+1}} \right) \left(\log \frac{c_1 c_i}{\mathcal{Q}_1 \mathcal{Q}_i} - \log \frac{c_{i+1}}{\mathcal{Q}_{i+1}} \right)$$

and we have $\frac{d}{dt} H = -D$.

Let us look more closely at the inequality: is it true that...?

$$\lambda \sum_{i=1}^{\infty} \mathcal{Q}_i \left(\frac{c_i}{\mathcal{Q}_i} \log \frac{c_i}{\mathcal{Q}_i} - \frac{c_i}{\mathcal{Q}_i} + 1 \right)$$
$$\leq \sum_{i=1}^{\infty} a_i \mathcal{Q}_1 \mathcal{Q}_i \left(\frac{c_1 c_i}{\mathcal{Q}_1 \mathcal{Q}_i} - \frac{c_{i+1}}{\mathcal{Q}_{i+1}} \right) \left(\log \frac{c_1 c_i}{\mathcal{Q}_1 \mathcal{Q}_i} - \log \frac{c_{i+1}}{\mathcal{Q}_{i+1}} \right),$$

for all c_i with

$$\sum_{i=1}^{\infty} i \mathcal{Q}_i c_i = \rho,$$

where

$$\mathcal{Q}_i := Q_i z^i.$$

In other words,

$$\lambda \sum_{i=1}^{\infty} \sum_{i=1}^{\infty} \mathcal{Q}_i \Psi(u_i) \le \sum_{i=1}^{\infty} a_i \mathcal{Q}_1 \mathcal{Q}_i (u_1 u_i - u_{i+1}) \log \frac{u_1 u_i}{u_{i+1}}$$

with

$$u_i = \frac{c_i}{\mathcal{Q}_i}.$$

This looks a bit like "modified logarithmic Sobolev" inequalities for a discrete Markov process:

$$\lambda \sum_{i=1}^{\infty} \sum_{i=1}^{\infty} \mu_i \Psi(u_i) \le \sum_{i=1}^{\infty} \mu_i (u_i - u_{i+1}) \log \frac{u_i}{u_{i+1}}.$$

This was already noted by Jabin & Niethammer.

How can we take advantage of this? Rewrite the inequality as:

$$\lambda \sum_{i=1}^{\infty} \sum_{i=1}^{\infty} \mathcal{Q}_i \Psi\left(u_i\right) \leq \sum_{i=1}^{\infty} a_i \tilde{\mathcal{Q}}_1 \tilde{\mathcal{Q}}_i \left(\tilde{u}_i - \tilde{u}_{i+1}\right) \log \frac{\tilde{u}_i}{\tilde{u}_{i+1}}.$$

where

$$\tilde{\mathcal{Q}}_i := \mathcal{Q}_i (c_1/z)^i = Q_i c_1^i, \qquad \tilde{u}_i := \frac{c_i}{\tilde{\mathcal{Q}}_i}.$$

Now recall a property of the relative entropy $H(c|Q_i r^i)$: *it is lowest when $Q_i r^i$ is the equilibrium with the same mass as c.* Hence it is enough to show

$$\lambda \sum_{i=1}^{\infty} \sum_{i=1}^{\infty} \tilde{\mathcal{Q}}_i \Psi\left(\tilde{u}_i\right) \leq \sum_{i=1}^{\infty} a_i \tilde{\mathcal{Q}}_1 \tilde{\mathcal{Q}}_i \left(\tilde{u}_i - \tilde{u}_{i+1}\right) \log \frac{\tilde{u}_i}{\tilde{u}_{i+1}}.$$

This kind of inequality is sometimes called "modified logarithmic Sobolev" inequality in probability literature (**Bobkov & Tetali, 2004**) or "Φ-entropy inequalities" (**Gentil & Imbert 2008**). I would call it an **entropy-entropy production inequality** in agreement with kinetic literature.

Not much is known about them in general. It has been proved that it holds for Poisson measure $\mu_i = Cz^i/i!$ (**Ledoux 98**):

$$\lambda \sum_{i=1}^{\infty} \sum_{i=1}^{\infty} \mu_i \Psi(u_i) \leq \sum_{i=1}^{\infty} \mu_i (u_i - u_{i+1}) \log \frac{u_i}{u_{i+1}}$$

for all u_i with

$$\sum_{i=1}^{\infty} \mu_i u_i = 1.$$

Logarithmic Sobolev inequalities

Instead of

$$\lambda \sum_{i=1}^{\infty} \sum_{i=1}^{\infty} \mu_i \Psi(u_i) \leq \sum_{i=1}^{\infty} \mu_i (u_i - u_{i+1}) \log \frac{u_i}{u_{i+1}}$$

one may use that

$$(u_i - u_{i+1}) \log \frac{u_i}{u_{i+1}} \geq 4(\sqrt{u_i} - \sqrt{u_{i+1}})^2$$

and instead try to prove that

$$\lambda \sum_{i=1}^{\infty} \sum_{i=1}^{\infty} \mu_i \Psi(u_i) \leq 4 \sum_{i=1}^{\infty} \mu_i \left(\sqrt{u_i} - \sqrt{u_{i+1}}\right)^2.$$

The latter is a **logarithmic Sobolev inequality.**

The latter inequalities are better understood:

1. **Bobkov & Götze (1999)** gave general conditions for a continuous logarithmic Sobolev inequality to hold on $(0, +\infty)$, without any weights (so this only covers the case $a_i = 1$, i.e., $\alpha = 0$).
2. **Barthe & Roberto (2003)** generalised this to general weights. Essentially,

$$\lambda \sum_{i=1}^{\infty} \sum_{i=1}^{\infty} \mu_i \Psi(u_i) \leq \sum_{i=1}^{\infty} \nu_i \left(\sqrt{u_i} - \sqrt{u_{i+1}}\right)^2 .$$

holds for all $\{u_i\}$ with $\sum_{i=1}^{\infty} \mu_i u_i = 1$ if and only if

$$\sup_{k \geq 1} \left\{ \left(\sum_{i=k+1}^{\infty} \mu_i \right) \left(-\log \sum_{i=k+1}^{\infty} \mu_i \right) \left(\sum_{i=1}^{k} \frac{1}{\nu_i} \right) \right\} < \infty.$$

One can test the above condition with

$$\mu_i = \text{const} \cdot \tilde{\mathcal{Q}}_i, \qquad \nu_i = \text{const} \cdot i\tilde{\mathcal{Q}}_i \qquad \text{(normalised)}$$

and show that we have

$$\lambda \sum_{i=1}^{\infty} \sum_{i=1}^{\infty} \tilde{\mathcal{Q}}_i \Psi(u_i) \leq \sum_{i=1}^{\infty} {\color{red} i} \tilde{\mathcal{Q}}_i \left(\sqrt{u_i} - \sqrt{u_{i+1}} \right)^2 .$$

holds for all $\{u_i\}$ with $\sum_{i=1}^{\infty} \mu_i u_i = 1$, when $\tilde{\mathcal{Q}}_i$ is exponentially decreasing.

How can one use this for the Becker-Döring equation? We recall the inequality we would like to prove:

$$\lambda H(c|\mathcal{Q}) = \lambda \sum_{i=1}^{\infty} \mathcal{Q}_i \Psi\left(u_i\right) \leq \sum_{i=1}^{\infty} a_i \tilde{\mathcal{Q}}_1 \tilde{\mathcal{Q}}_i \left(\tilde{u}_i - \tilde{u}_{i+1}\right) \log \frac{\tilde{u}_i}{\tilde{u}_{i+1}}.$$

for all $\{c_i\}$ with $\sum_{i=1}^{\infty} i c_i = \rho$, with

$$\tilde{\mathcal{Q}}_i := Q_i c_1^i, \qquad \tilde{u}_i := \frac{c_i}{\tilde{\mathcal{Q}}_i}$$

Instead, we look at

$$\lambda H(c|\tilde{\mathcal{Q}}) = \lambda \sum_{i=1}^{\infty} \tilde{\mathcal{Q}}_i \Psi\left(\tilde{u}_i\right) \leq \sum_{i=1}^{\infty} a_i \tilde{\mathcal{Q}}_1 \tilde{\mathcal{Q}}_i \left(\sqrt{\tilde{u}_i} - \sqrt{\tilde{u}_{i+1}}\right)^2$$

which is enough.

We may use the discrete log-Sobolev inequality to get

$$\sum_{i=1}^{\infty} i\tilde{\mathcal{Q}}_i \left(\sqrt{\tilde{u}_i} - \sqrt{\tilde{u}_{i+1}}\right)^2 \gtrsim H(c|\tilde{\mathcal{Q}}) - \left(\sum_{i=1}^{\infty} \tilde{Q}_i\right) \psi \left(\frac{\sum_{i=1}^{\infty} c_i}{\sum_{i=1}^{\infty} \tilde{\mathcal{Q}}_i}\right)$$

We then need to show that

$$\psi\left(\frac{\sum c_i}{\sum \tilde{\mathcal{Q}}_i}\right) \lesssim \left(\frac{\sum c_i}{\sum \tilde{\mathcal{Q}}_i} - 1\right)^2 \lesssim \sum_{i=1}^{\infty} i\tilde{\mathcal{Q}}_i \left(\sqrt{\tilde{u}_i} - \sqrt{\tilde{u}_{i+1}}\right)^2,$$

which is a consequence of the Csiszár-Kullback-Pinsker inequality.

This shows the inequality.

Interpolation for $a_i = i^\alpha$

For $\gamma \geq 0$ call

$$D_\gamma(c) := \sum_{i=1}^{\infty} i^\gamma \mathcal{Q}_1 \mathcal{Q}_i \left(\sqrt{\frac{c_1 c_i}{\mathcal{Q}_i}} - \sqrt{\frac{c_{i+1}}{\mathcal{Q}_{i+1}}} \right)^2 .$$

By interpolation, choosing $\theta = (\beta - 1)/(\beta - \alpha)$ we have

$$H(c|\mathcal{Q}) \lesssim D_1(c) \leq D_\alpha(c)^\theta D_\beta(c)^{1-\theta} \lesssim D(c)^\theta \left(\sum_{i=1}^{\infty} i^\beta c_i \right)^{1-\theta} .$$

This gives

$$H(c) \leq C(1+t)^{-\frac{\beta-1}{1-\gamma}} .$$

Compare also to **[Murray & Pego 2015]**

One can also “interpolate with exponential moments” and obtain a family of inequalities which includes the Jabin-Niethammer one: if we assume that an exponential moment is bounded,

$$D(c) \geq \frac{\lambda H(c)}{|\log H(c)|^{1-\gamma}} \qquad \text{for } H \text{ small.}$$

This gives a rate of convergence

$$H(c) \leq C \exp\left(-\lambda t^{\frac{1}{2-\gamma}}\right).$$

Optimality

Surprisingly, we do not lose anything by considering the log-Sobolev inequality instead of the modified log-Sobolev: if $a_i = i^\gamma$ with $\gamma < 1$ (and under reasonable conditions on the Q_i) consider the sequence

$$c_i^{(\epsilon)} := Ae^{-ri} + B_\epsilon e^{-\epsilon i},$$

with B_ϵ chosen so that the total mass is fixed. *Then this sequence gives a counterexample to Cercignani's inequality for the B-D equations.*

Thanks!