The inverse droplet coagulation problem

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Coagulation of clusters and droplets

Many particles of one material dispersed in another.

Transport: diffusion, turbulence advection, ballistic...

Particles stick together on contact.

Applications: surface and colloid physics, atmospheric science, biology, cloud physics, astrophysics...
Mean field theory: Smoluchowski’s equation

Cluster size distribution, \( N_m(t) \), satisfies the kinetic equation:

**Smoluchowski equation**:

\[
\frac{\partial N_m(t)}{\partial t} = \frac{1}{2} \int_0^m dm_1 K(m_1, m - m_1) N_{m_1} N_{m-m_1} \]  

\[
- N_m \int_0^{M-m} dm_1 K(m, m_1) N_{m_1} + \frac{J}{m_0} \delta(m - m_0) 
\]

\[
- N_m \int_{M-m}^M dm_1 K(m, m_1) N_{m_1}
\]

Some additional features:

- Source of monomers, \( m_0 \), at rate \( J \).
- Removal of clusters larger than cut-off, \( M \).
Model kernels

At mean-field level all micro-physics is encoded into the kernel, $K(m_1, m_2)$. Kernel is often (approximately) homogeneous:

$$K(am_1, am_2) = a^\beta K(m_1, m_2)$$

$$K(m_1, m_2) \sim m_1^\mu m_2^\nu \quad m_1 \ll m_2.$$

A popular model kernel is the Van-Dongen kernel:

$$K(m_1, m_2) = \frac{1}{2} (m_1^\mu m_2^\nu + m_1^\nu m_2^\mu)$$

$K(m_1, m_2)$ for some physical models:

$$\left( \frac{m_1}{m_2} \right)^\nu + \left( \frac{m_2}{m_1} \right)^\nu + 2$$ Brownian coagulation, $\nu = \frac{1}{3}, \mu = -\frac{1}{3}$

$$\left( m_1^3 + m_2^3 \right)^2 \left| m_1^2 - m_2^2 \right|$$ Gravitational settling, $\nu = \frac{4}{3}, \mu = 0$

$$\left( m_1^3 + m_2^3 \right)^2 \sqrt{\frac{1}{m_1} + \frac{1}{m_2}}$$ Differential rotation, $\nu = \frac{2}{3}, \mu = \frac{1}{2}$
Self-similar solutions of Smoluchowski equation

For homogeneous kernels, cluster size distribution often self-similar. Without source: $s(t)$ is

$$N_m(t) \sim s(t)^{-2} F(z) \quad z = \frac{m}{s(t)}$$

the typical cluster size. The scaling function, $F(z)$, determining the shape of the cluster size distribution, satisfies:

$$-2F(z) + z \frac{dF(z)}{dz} = \frac{1}{2} \int_0^z dz_1 K(z_1, z - z_1) F(z_1) F(z - z_1)$$

$$- F(z) \int_0^\infty dz_1 K(z, z_1) F(z_1).$$
Stationary solutions of Smoluchowski eq. with source

Kernel is often homogeneous:

\[ K(am_1, am_2) = a^\beta K(m_1, m_2) \]
\[ K(m_1, m_2) \sim m_1^\mu m_2^\nu \quad m_1 \ll m_2. \]

Clearly \( \beta = \mu + \nu \). Model kernel:

\[ K(m_1, m_2) = \frac{1}{2} (m_1^\mu m_2^\nu + m_1^\nu m_2^\mu) \]

Stationary state for \( t \to \infty, m_0 \ll m \ll M \) (Hayakawa 1987):

\[ N_m = \sqrt{\frac{J (1 - (\nu - \mu)^2) \cos((\nu - \mu) \pi / 2)}{2\pi}} m^{-\frac{\beta + 3}{2}}. \] (1)

Describes a cascade of mass from source at \( m_0 \) to sink at \( M \).
Inverse problems

**Forward problem:** given kernel, $K(m_1, m_2)$, compute the size distribution, $N_m(t)$.

**Inverse problem:** given observations of the size distribution, $N_m(t)$, compute the kernel, $K(m_1, m_2)$ (Wright and Ramakrishna, 1992).

Inverse problem is *useful* because:

- Kernel may not be known.
- May help in building models and guiding micro-physics theory.
- Quantifies the sensitivity of the size distribution to variations in the kernel.

*but*

- Inverse problems are typically ill-posed.
The stationary inverse Smoluchowski problem

- The stationary size distribution satisfies:

\[-J \delta(m - 1) = S(N_m)[K(m_1, m_2)].\]

where \(S(N_m)\) is the integral operator defined by RHS of (1).

- **Linear** in \(K(z_1, z_2)\).

- If we measure \(N_m\), at \(M\) discrete masses, then this equation discretises to a set of \(M\) linear equations for the \(M^2\) values of the \(K(m_1, m_2)\).

\[b = Sk.\]

- This system is enormously under-determined \(\Rightarrow\) one can find many solutions but they are mostly determined by the noise in the measurements.
Dealing with ill-posedness

One strategy is to restrict the allowed $K(m_1, m_2)$ to a class of functions described by a much smaller set of parameters and find the “best fit” within this restricted class of functions.

Wright and Ramakrishna (1992)

Suggested the following representation of kernel:

$$K(m_1, m_2) = \sum_{i=1}^{N} \sum_{j=1}^{N} a_{i,j} \mathcal{L}_i(m_1) \mathcal{L}_j(m_2)$$

where $\mathcal{L}_i(x)$ are Laguerre polynomials.

- Inverse problem becomes a linear least squares problem for the $N^2$ coefficients $a_{i,j}$.
- One can hope to use cross-validation techniques to find optimal $N$.
- Not too good for kernels with fractional exponents.
An alternative parameterisation

Inverse problem is very sensitive to the form of the kernel for very large and very small masses. Can we find a parameterisation which is better at capturing this?

Any *homogeneous* kernel with asymptotic exponents $\mu$ and $\nu$ can be represented as:

$$K(m_1, m_2) = \frac{1}{2} \left( m_1^\mu m_2^\nu + m_1^\nu m_2^\mu \right) f \left( \frac{m_1}{m_2} \right)$$

where the “shape function" is by definition

$$f \left( \frac{m_1}{m_2} \right) = \frac{K(m_1, m_2)}{\frac{1}{2} \left( m_1^\mu m_2^\nu + m_1^\nu m_2^\mu \right)}.$$ 

It is a function of the single variable $\frac{m_1}{m_2}$, because it is homogeneous of degree zero and has the symmetry $f(x) = f(1/x)$. 

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Computational strategy

Step 1:
- Assume \( f(x) = 1 \) and find the "best" values of \( \mu \) and \( \nu \).
- This is a two-dimensional (nonlinear) minimization problem. We used the Nelder-Mead algorithm.

Step 2:
- After estimating \( \mu \) and \( \nu \), try to improve our estimate of kernel by fitting the one-dimensional function \( f(x) \).
- Representation of \( f(x) \) which enforces required symmetry?
  \[
  f(x) = g(\log(x))
  \]

where

  \[
  g(y) = \sum_{n=1}^{N} a_n \cos \left( \frac{n \pi y}{\log M} \right).
  \]

- This is a linear least squares problem for the \( a_n \).
Results: model kernel (stationary)

Test of step 1 for Van-Dongen kernel:

\[ K(m_1, m_2) = \frac{1}{2} \left( m_1^{\frac{1}{4}} m_2^{-\frac{1}{2}} + m_1^{-\frac{1}{2}} m_2^{\frac{1}{4}} \right) \]

Stationary \( N_m \) for \( \nu = 1/4, \mu = -1/2, M = 250 \) compared to exact solution for \( M = \infty \).

Slices through the reconstructed kernel. Exponents obtained are effectively exact.
Results: Stationary Brownian coagulation $\mu = -\nu = \frac{1}{3}$

Full test for Brownian coagulation of spherical droplets:

$$K(m_1, m_2) = \left( \frac{m_1}{m_2} \right)^{\frac{1}{3}} + \left( \frac{m_2}{m_1} \right)^{\frac{1}{3}} + 2$$

Stationary $N_m$ for Brownian coagulation, $M = 250$

compared to exact solution for $M = \infty$.

Slices through the reconstructed kernel compared to exact values. $\nu_{est} \approx 0.486$, $\mu_{est} \approx -0.484$. 
Results: shear-like kernel (stationary) $\nu = 1, \mu = -\frac{1}{4}$

Full test for a toy model variation on the shear kernel:

$$K(m_1, m_2) = \left( \sqrt{m_1} + \sqrt{m_2} \right)^2 \sqrt{\frac{1}{\sqrt{m_1}} + \frac{1}{\sqrt{m_2}}}$$

Stationary $N_m$ for a toy model with $\nu = 1, \mu = -\frac{1}{4}$.

Slices through the reconstructed kernel compared to exact values. $\nu_{\text{est}} \approx 0.97, \mu_{\text{est}} \approx 0.24$. 

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What about the nonstationary case?

Method applies to the nonstationary case in the scaling limit:

\[ N_m(t) \sim s(t)^{-2} F(z) \quad z = \frac{m}{s(t)} \]

The scaling function, \( F(z) \) satisfies:

\[
-2F(z) + z \frac{dF(z)}{dz} = \frac{1}{2} \int_0^z dz_1 K(z_1, z - z_1) F(z_1) F(z - z_1)
- F(z) \int_0^\infty dz_1 K(z, z_1) F(z_1).
\]

which is similar to stationary Smoluchowski equation.

\[ s(t) = \sum_{i=1}^M m^2 N_m(t) / \sum_{i=1}^M m N_m(t) \]

is typical size used to collapse data.

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Results: Sum kernel (nonstationary) $\nu = \frac{1}{4}, \mu = 0$

Nonstationary test case for a toy model variation on the sum kernel:

$$K(m_1, m_2) = m_1^{\frac{1}{4}} + m_2^{\frac{1}{4}}$$

Nonstationary $N_m$ and data collapse for a toy model with $\nu = \frac{1}{4}, \mu = 0$.

Slices through the reconstructed kernel compared to exact values. $\nu_{\text{est}} \approx 0.29, \mu_{\text{est}} \approx -0.03$. 

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Concluding remarks

Summary

- Despite clear difficulties, some features of the collision kernel can be reconstructed from measurements of the size distribution.
- We have presented an approach to the stationary inverse problem which works reasonably well for homogeneous kernels and can be extended to time-dependent problems in the scaling limit.

Issues and future work

- Need better ways of selecting the optimal number of Fourier coefficients to represent the shape function.
- Sensitivity to noise in the data should be explored.
- What can be done for non-homogeneous kernels?