STOCHASTIC COALESCENCE

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First 3 talks based on survey article *Deterministic and Stochastic Models for Coalescence (Aggregation, Coagulation); A Review of the Mean-Field Theory for Probabilists*. **Bernoulli** 5 (1999) 3–48.

Final talk describes subsequent work of Bertoin, Chassaing et al.

Lots of open problems remain!

Survey paper and these slides available at
`www.stat.berkeley.edu/`

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We study models of physical matter in clusters; as time passes, the clusters meet and merge into larger and larger clusters. Such models have been studied in a variety of scientific disciplines.

- Two disciplines: formation of planets; aerosols
- Stochastic fragmentation (easier analog)
- The basic math models: stochastic and deterministic
- Using physics to derive rate kernels

3 Stages

1. Formation of billions of planetisimals (size $<$ 1 km)

(duration $\gg$ 200 million years)

2. Formation of 30–50 smaller planets : Luna $<$ size $<$ Mars

($\approx$ 1 million years)

3. Formation of current 4 planets $+$ ......

($\approx$ 200 million years)

Our later math theory will indicate why stage 2 happened fast.

Aerosol: solid or liquid particles suspended in gas.

- water droplets in clouds
- volcanic dust
- plant spores (seeds, pollen)
- smoke particles from fires
- smog, dust from industry

Behavior of such particles depends on their size. Dominant effect:
radius $< 10^{-5}$ cm: Brownian motion
radius $> 10^{-4}$ cm: gravitational settling.

We'll see later what math says about the Brownian case.

Start with a more familiar related topic
Fragmentation as a Branching process.

Initially, one cluster of mass 1. The clusters undergo binary splitting in continuous time, according to a fragmentation kernel $F(x;y)$.

A mass-x cluster splits at rate $F(x;y)\ dy$ into a "left" cluster of mass y and a "right" cluster of mass $x-y$.

In this stochastic model, we can consider the mean size spectrum

$$m(x,t)dx =$$

$E(\#$ particles of size $\in [x, x+dx]$ at time $t)$.

And $m(x,t)$ satisfies the equations

$$\begin{aligned}\frac{d}{dt}m(x,t) &= -m(x,t)\int_0^x F(x;y)dy \\ &+ 2\int_x^1 m(y,t)F(y;x)dy.\end{aligned}$$

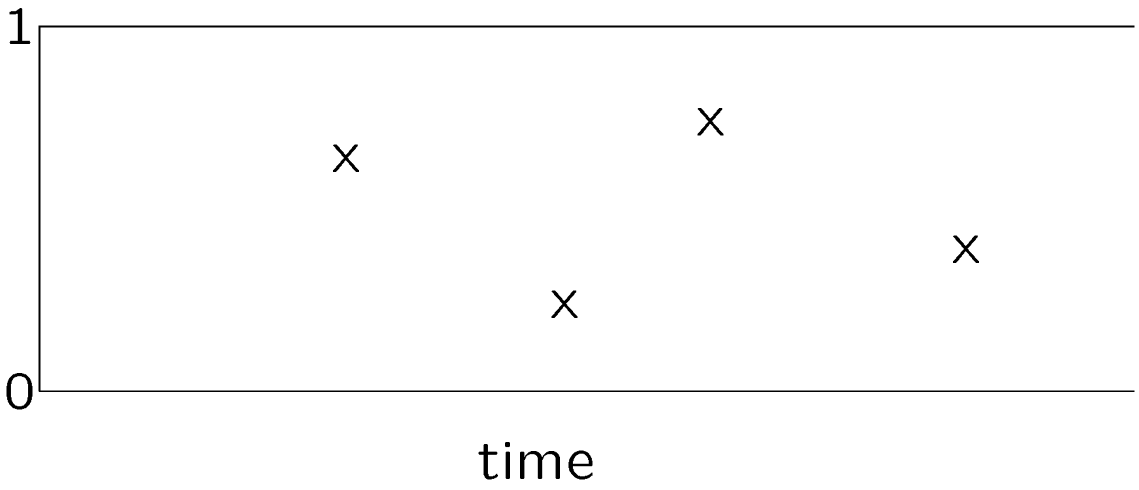
Simplest example of stochastic fragmentation

Take $F(x;y) = 1$. So a mass-x cluster splits at rate x, and the daughter clusters have $U(0,x)$ sizes. For this example there is an explicit construction.

Poisson(1) space-time point process

For large t, there will be about t clusters with approximately exponential (t) distribution;

$$m(x,t) \approx t \times te^{-tx}.$$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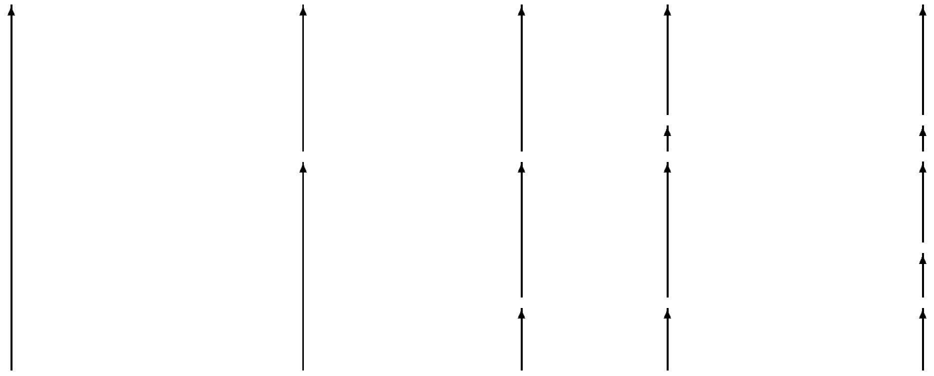
0
time



Think of stochastic fragmentation as a branching process with types, in which

individual = cluster; type = mass.

The theory of stable type structure for supercritical branching processes (Jagers - Nerman 1984) has an analogy for fragmentation, in the case where the kernel is homogeneous with scaling exponent α:

$$F(cx; cy) = c^{\alpha} F(x; y).$$

If $\alpha > -1$ then (Brennan - Durrett 1987)

$$m(x,t) \sim b t^{2/(1+\alpha)} \psi(x t^{1/(1+\alpha)}).$$

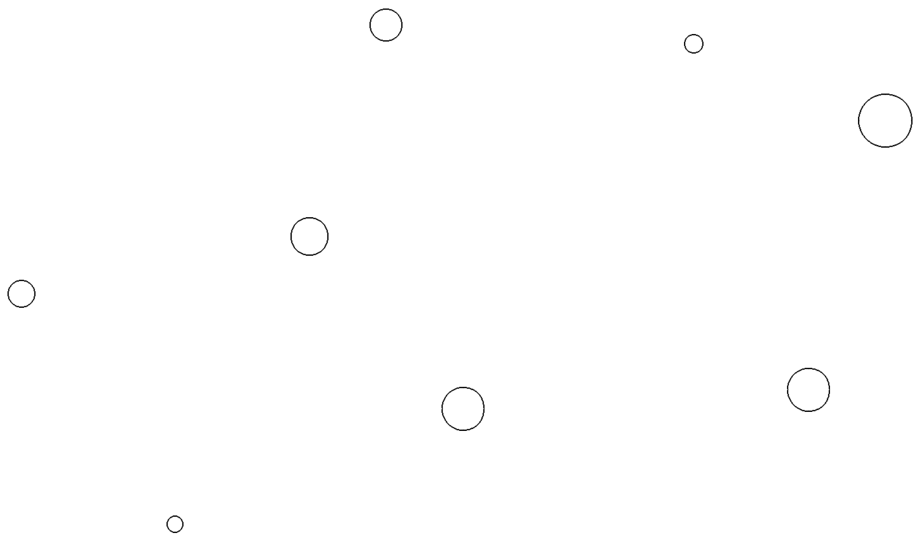
That is, there is some limit distribution $\psi(\cdot)$ of relative masses of clusters as $t \to \infty$.

Math point.

Stochastic fragmentation theory is easier than stochastic coalescence because it is a linear theory; there are exact equations for $m(x,t)$ which are just the continuous-time analog of convolution of the kernel F. By contrast, stochastic coalescence is a quadratic theory and there are no exact equations for the analogous $n(x,t)$.

Mental picture

Clusters of different masses x move in space. When two clusters (masses x and y) come close, they may merge into a single cluster, mass $x + y$.



Mass x may be discrete ($x = 1, 2, 3, \ldots$) or continuous ($0 < x < \infty$). Time t is always continuous.

Models involve a rate kernel $K(x, y)$ which specifies the propensity for mass-x and mass-y clusters to merge. The physics of the specific physical phenomenon being modeled are used to derive the rate kernel $K(x, y)$, by considering two clusters only. We then make a many-cluster model by assuming each pair of clusters behaves independently, ignoring the geometry of cluster positions. Loosely, we use mean-field models.

Most kernels have a scaling exponent γ:

$$K(cx, cy) = c^{\gamma} K(x, y).$$

Note that by scaling time we can remove constant factors; if $K(x, y) = \alpha(x + y)$ we just say $K(x, y) = x + y$.

Some examples of $K(x,y)$.

Physical Brownian motion:

$$(x^{1/3}+y^{1/3})(x^{-1/3}+y^{-1/3})$$

Shear (linear velocity profile):

$$(x^{1/3}+y^{1/3})^3$$

Gravitational settling:

$$(x^{1/3}+y^{1/3})^2|x^{1/3}-y^{1/3}|$$

Polymerization: branched polymers:

$$(x+c)(y+c)$$

Polymerization: linear polymers:

$$c$$

Planetisimals (stage 2):

$$\max(x^{4/3},y^{4/3}).$$

We'll derive some of these soon.

The two stochastic models

1. The Marcus-Lushnikov process. Start with N separate atoms. As time increases, atoms merge into clusters according to the rule:
each pair of clusters (sizes x and y, say) merge at rate $K(x,y)/N$.

2. The general stochastic coalescent. Scale total mass to be 1, and allow countably many clusters. State-space is infinite-dimensional simplex

$$\Delta := \{(x_i) : x_i > 0, \sum_i x_i = 1\}$$

for continuous cluster-masses x_i. Evolution rule is:
each pair of clusters (masses x and y, say) merge at rate $K(x,y)$.

Remarks on the models

(a) In subsequent lectures we suppose a formula for $K(x,y)$ is given; our goal is math analysis of the processes.

(b) If the kernel has a scaling exponent then the Marcus-Lushnikov process is a special case of the stochastic coalescent, by scaling mass and time.

(c) The Marcus-Lushnikov process is more elementary, in that for fixed N it clearly exists as a finite-space continuous-time Markov chain. But having different state-space for different N is inelegant; the general stochastic coalescent has a fixed state space Δ. On the other hand, it's not rigorously obvious whether our verbal description really specifies a unique "well-behaved" Markov process on Δ.

(d) The $t \to \infty$ asymptotics are trivial; all the mass goes into one cluster. In the context of the Marcus-Lushnikov process, we study $N \to \infty$ limit behavior at intermediate times; for instance

how long does it take (as a function of N) for large clusters to appear?

(e) In the Marcus-Lushnikov process, write $\mathbf{ML}_N(x,t)$ for number of size-x clusters at time t. Consider expectations

$$m(x,t) = E\left(\mathbf{ML}_N(x,t)\right).$$

In contrast to the fragmentation setting, we cannot write an equation for $\frac{d}{dt}m(x,t)$ in terms of the $m(\cdot,t)$, because it involves the covariances $E\left(\mathbf{ML}_N(x,t)\mathbf{ML}_N(y,t)\right)$.

(f) Literature also treats coalescence combined with fragmentation, removal, imigration, etc.

In the Marcus-Lushnikov process, write $\mathbf{ML}_N(x,t)$ for number of size-x clusters at time t. It seems intuitively clear that as $N \to \infty$ there should be a weak law of large numbers

$$N^{-1}\mathbf{ML}_N(x,t) \ \overset{p}{\to}\ n(x,t)$$

with a deterministic limit satisfying a certain set of differential equations, the **Smoluchowski coagulation equation**

$$\begin{aligned}\frac{d}{dt}n(x,t) &= \frac{1}{2}\sum_{y=1}^{x-1} K(y,x-y)n(y,t)n(x-y,t)\\ &- n(x,t)\sum_{y=1}^{\infty} K(x,y)n(y,t),\ x=1,2,\ldots\end{aligned}$$

[analogous integro-differential equation for continuous x]

These equations are the subject of extensive scientific literature. Drake (1972) gave a 175-page survey with 250 citations.

Physics interpretation of $K(x, y)$

In infinite-volume system, take

$$n(x,t) = \text{ave number of size-}x\text{ clusters per unit volume at time } t.$$

Define K by

ave number of merges of size-x and size-y clusters per unit volume per unit time $= K(x,y)n(x,t)n(y,t)$.

Single tagged particle interpretation: a tagged size-x particle merges with particles of some size y at rate $K(x,y)n(y,t)$.

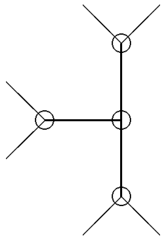
Two tagged particles interpretation: for two tagged particles of sizes x and y, started "in general position", then their chance of merging in a short time $\propto K(x,y)$.

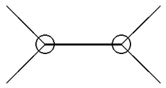
Examples: deriving $K(x,y)$ from physics

Linear polymers. Mass x = number of monomers. When ends come close, a new bond forms.

If motion of polymers does not depend on size then $K(x,y)$ = constant.

Branched polymers: trivalent case.





mass x mass y

$x + 2$ potential bonds $y + 2$ potential bonds

$$K(x, y) = (x + 2)(y + 2).$$

Such crude models of polymerization go back to Flory (1941). Modern theory involves 3-dimensional geometry, e.g. self-avoiding walks.

von Smoluchowski (1916) considers physical Brownian motion (diffusion under thermal noise) in R^3, where for spherical clusters of radius r

$$\text{variance rate } \equiv \sigma^2(r) \propto 1/r.$$

Mathematically, distance between centers is just another Brownian motion with variance rate $\sigma^2(r_1)+\sigma^2(r_2)$. Clusters meet when this distance hits sphere of radius r_1+r_2 centered at origin. But in R^3

$$P(\text{ hit sphere of radius r}) \propto r$$

and so the meeting rate is

$$\propto (\sigma^2(r_1)+\sigma^2(r_2))(r_1+r_2).$$

This gives

$$K(x,y) = (x^{-1/3}+y^{-1/3})(x^{1/3}+y^{1/3})$$

in terms of mass x.