Self-similarity and eternal solutions for a model of min-driven clustering

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1. Prologue: Smoluchowski's coagulation equation with solvable kernels
2. "1D bubble bath model" of domain coarsening in the Allen-Cahn PDE
3. The Gallay-Mielke solution of a class of min-driven multiple clustering models
4. Domains of attraction, eternal solutions and Lévy-Khintchine representation
5. Dynamic scaling for a 1D uniform growth model (with J. Carr, preliminary)

• Smoluchowski's coagulation equations

$$\boxed{x} + \boxed{y} \Longrightarrow \boxed{x+y}$$

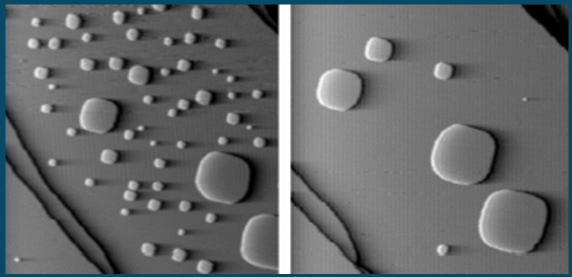
$$\boxed{x-y} + \boxed{y} \Longrightarrow \boxed{x}$$

Clusters of size x and y form $x+y$-clusters at rate $K(x,y)n(x,t)n(y,t)$,

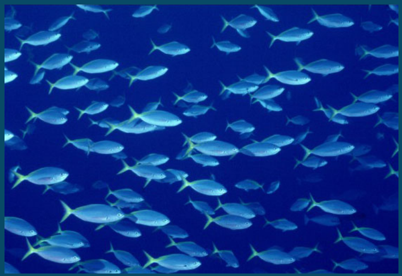
where $n(x,t)$ is the number density of size-x clusters:

$$\begin{aligned} \partial_t n(x,t) &= \frac{1}{2}\int_0^x K(x-y,y)n(x-y,t)n(y,t)\,dy \\ &\quad - \int_0^\infty K(x,y)n(x,t)n(y,t)\,dy \end{aligned}$$

Some scientific applications



- astrophysics: agglomeration of planetesimals, star clusters, galaxies
- aerosol physics: formation of clouds, smog, ink fog
- materials science: ripening of nanoscale structures & patterns
- probability: random graph theory, ancestral lines of descent
- Burgers' turbulence model: shock-wave clustering



Coagulation kernels arising in applications:

Particle coalescence due to: Brownian motion, shear flow, gravitational settling.
Effects of turbulence, inertia and large mean-free-path.
Condensation, polymerization, fractal aggregates.

$K(x,y)$
$(x^{1/3}+y^{1/3})(x^{-1/3}+y^{-1/3})$
$(x^{1/3}+y^{1/3})^2(x^{-1}+y^{-1})^{1/2}$
$(x^{1/3}+y^{1/3})^3$
$(x^{1/3}+y^{1/3})^{7/3}$
$(x^{1/3}+y^{1/3})^2\lvert x^{1/3}-y^{1/3}\rvert$
$(x^{1/3}+y^{1/3})^2\lvert x^{2/3}-y^{2/3}\rvert$
$(x-y)^2(x+y)^{-1}$
$(x+c)(y+c)$
$(x^{1/3}+y^{1/3})(xy)^{1/2}(x+y)^{-3/2}$

Often K is homogeneous: $K(ax,ay)=a^pK(x,y)$.

Cases 'solvable' by Laplace transform: $K=2$, $x+y$, xy

General moment identity—weak form of coagulation equation

$$\partial_t \int_0^\infty a(x)n(x,t)\,dx = \frac{1}{2}\int_0^\infty \int_0^\infty \tilde{a}(x,y)K(x,y)n(x,t)n(y,t)\,dx\,dy$$

with

$$\tilde{a}(x,y) = a(x+y) - a(x) - a(y).$$

Choosing $\quad a(x) = 1 - e^{-sx} \quad$ yields $\quad \tilde{a}(x,y) = -(1-e^{-sx})(1-e^{-sy})$.

$$\text{Then} \quad \varphi(t,s) := \begin{cases} \int_0^\infty (1-e^{-sx})n(t,x)\,dx & \text{for } K = 2 \text{ or } x+y, \\ \int_0^\infty (1-e^{-sx})xn(t,x)\,dx & \text{for } K = xy \end{cases}$$

satisfies

$$\partial_t \varphi = -\varphi^2 \qquad \text{for } K = 2,$$

$$\partial_t \varphi - \varphi \partial_s \varphi = -\varphi \qquad \text{for } K = x+y,$$

$$\partial_t \varphi - \varphi \partial_s \varphi = 0 \qquad \text{for } K = xy.$$

Dynamic scaling analysis

See: G. Menon & R. L. Pego, CPAM 57 (2004) 1197-1232,
J. Nonl. Sci. 18 (2008) 143-190.

- What is a natural solution space for dynamics?
- What scaling solutions exist?
  (Fixed points of a renormalization group.)
- What are the domains of attraction?
  (Universality classes for scaling.)
- What other scaling limit points are possible?
  (Call the set of cluster points mod scaling the *scaling attractor*.)
- What is the "ultimate dynamics" on the scaling attractor?

(There is a *strong analogy* to classical limit theorems of probability)

Well-posed dynamics for solvable kernels

Smoluchowski's equation with

$$K = \begin{cases} 2 & (p=0) \\ x+y & (p=1) \\ xy & (p=2) \end{cases}$$

determines a dynamical system on the whole space of probability measures on $(0,\infty)$ determined by the p-th moment cumulative distribution function

$$F(x,t) = \int_0^x y^p\, n(y,t)\, dy \Big/ \int_0^\infty y^p\, n(y,t)\, dy,$$

under the topology of weak convergence — convergence in distribution.
(This topology is equivalent to pointwise convergence of the Laplace transform.)

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- Fournier & Laurencot 2006: general class of homogeneous kernels
- MP 2008: Dynamics extends to $\overline{\mathcal{P}} = \{$ probability measures on $\overline{E} = [0,\infty]\}$.

Coagulation with solvable kernels: $K(x,y) = 2, x+y, xy$

- There is a unique self-similar solution with finite $p+1$-st moment. ($p = 0, 1, 2$ resp. for $K = 2, x+y, xy$.) More generally, there are fat-tailed solutions with profiles related to important distributions in probability.

- Domains of attraction are classified by a necessary & sufficient criterion:

$$\int_0^x y^{p+1}\, n_0(y)\, dy \sim x^{2-\alpha} L(x) \quad \text{as } x \to \infty$$

  where $1 < \alpha \le 2$ and L is slowly varying.

- Points in the scaling attractor correspond 1-1 with eternal solutions and have a Lévy-Khintchine representation formulat in terms of measures G having $\int_0^\infty (1 \wedge x^{-1}) G(dx) < \infty$

- The Lévy-Khintchine representation *linearizes* coagulation dynamics on the scaling attractor. The corresponding measures evolve by a simple dilational scaling. Complicated dynamics with sensitive data dependence ensues!

Coagulation with solvable kernels: $K(x,y) = 2, x+y, xy$

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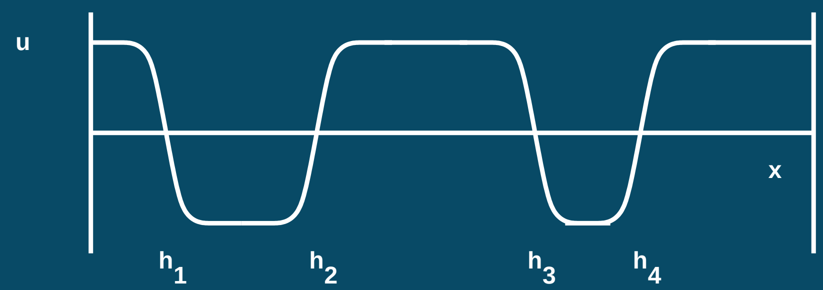
- The Lévy-Khintchine representation *linearizes* coagulation dynamics on the scaling attractor. The corresponding measures evolve by a simple dilational scaling. Complicated dynamics with sensitive data dependence ensues! $\sim$Doeblin's universal laws

• Domain coarsening for the 1D Allen-Cahn PDE

• L^2 gradient flow for $\quad E(u) = \int \frac{1}{2}u_x^2 + \frac{1}{8}(u^2-1)^2\,dx$

$$u_t = u_{xx} + \frac{1}{2}(u - u^3)$$



• (J. Neu, Fusco-Hale, Carr-P '89,'92) $\exists$ 'metastable' invariant manifold:

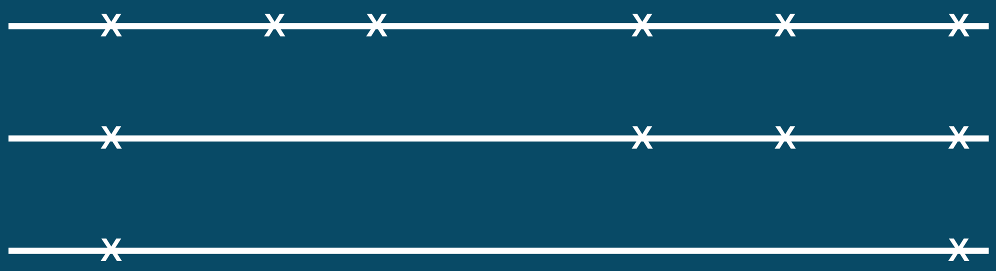
$$h \mapsto u^h(x), \qquad h = (h_1, \dots, h_N), \qquad S = \min\{h_j - h_{j-1}\} \gg 1$$

Domain wall dynamics:

$$\frac{d}{dt}h_j(t) = \Big(V'\,(h_{j+1} - h_j) - V'\,(h_j - h_{j-1})\Big)\Big(\frac{3}{2} + O(e^{-S/2})\Big),$$

$$V'(\ell) = 8e^{-\ell} + O(e^{-3\ell/2}). \qquad \text{Roughly} \quad \dot{S}(t) \approx 24e^{-S}.$$

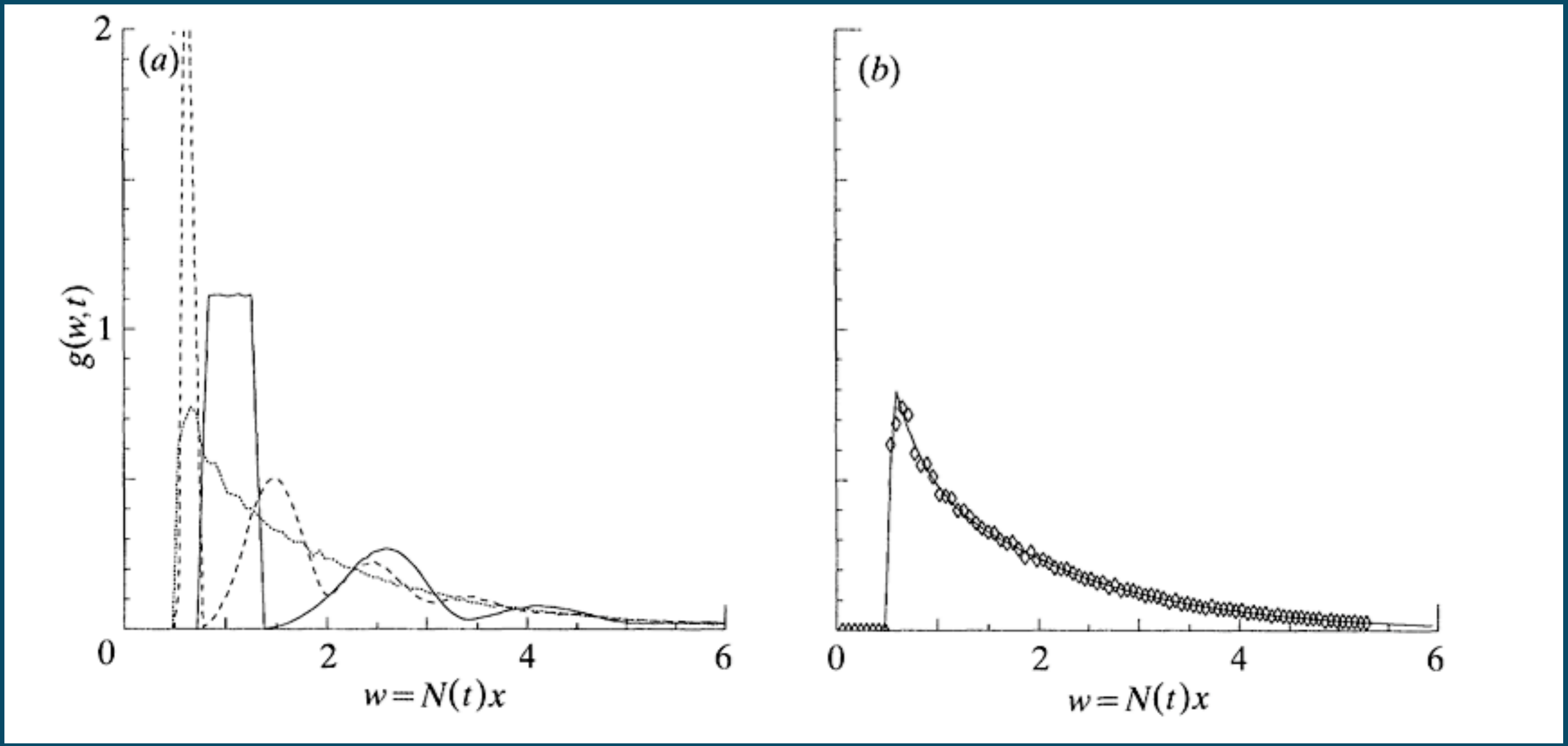
“1D bubble bath” cartoon of coarsening dynamics:



(i) The *smallest* domain collapses, combining with its two neighbors.

(ii) Repeat

Simulations show that the *domain size distribution* approaches self-similar form, with a variety of initial domain size distributions (e.g., Poisson, uniform on [1,3]).



Scaled size distributions: 45%, 25%, 5% of 10^5 domains remain

Initial distribution: Uniform on [1,3] (Carr-P 1992)

Solid curve $n_*(x)$ satisfies:
$$\int_0^\infty e^{-qx} n_*(x)\, dx = \tanh\left(\frac{1}{2}\int_q^\infty \frac{e^{-z}}{z}\, dz\right).$$

Rate equation: min-driven coagulation model

$n(t,x)$: number density at time t for domains of size x.

$S = S(t)$: min (minimum size). $N(t) = \int_S^\infty n(t,x)\,dx$: total number.

$$\partial_t n(t,x) = n(t,S)\dot{S}\left(\int_0^x \frac{n(x-y-S)}{N}\frac{n(y)}{N}\,dy - 2\int_0^\infty \frac{n(x)}{N}\frac{n(y)}{N}\,dy.\right)$$

event rate gain loss

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This model is invariant under arbitrary reparametrization of time.

T. Gallay & A. Mielke 2003 found a remarkable solution procedure through Fourier transform: Choosing $S(t) = t$,

$$w(t,\cdot) = \mathcal{F}^{-1} \circ \tanh^{-1} \circ \mathcal{F} n(t.\cdot) \quad \Rightarrow \quad w(t,x) = H(x-t)w(t_0,x), \quad t \geq t_0.$$

Analysis of min-driven clustering

Results of Gallay & Mielke (2003) using $S(t) = t$

- Well-posedness in L^1: $\int_1^\infty n(0,x)\,dx < \infty$.
- Existence of self-similar solutions, including ones with fat tails: $n^{(\theta)}(x) \sim c_\theta x^{-1-\theta}$, $0 < \theta < 1$.
- Sufficient conditions for approach to self-similar form
- Rates of approach to self-similar form from decay of initial data

New results (MNP Trans. Amer. Math. Soc 2009): Choose time so $N(t) = 1/t$

- Well-posedness for arbitrary size distributions (finite measures with positive *min*)
- *Necessary & sufficient* conditions for approach to self-similar form
- Characterize all *eternal* solutions by a Lévy-Khintchine formula

Model with multiple collisions

The smallest remaining cluster, with size $S(t)$, combines with k other clusters at random with probability p_k.

Generating function: $Q(z) = \sum p_k z^k$, $\qquad \sum p_k = 1$, $Q'(1) = \sum k p_k < \infty$.

Moment identity (weak form) for the CDF $\quad F_t(x) = \int_0^x n(y,t)\,dy/N(t)$:

$$\frac{d}{dt}\int_0^\infty a(x)F_t(dx) = \sum_{k=1}^\infty p_k \int_{\mathbb{R}_+^k} \left[a\left(S(t) + \sum_{i=1}^k y_i\right) - a(S(t))\right] \prod_{i=1}^k F_t(dy_i)\,\frac{N}{Q'(1)}.$$

$a(x) = e^{-qx}$ gives the Laplace transform: $\bar{F}_t(q) = \int_0^\infty e^{-qx}F_t(dx)$ satisfies

$$\partial_t \bar{F}_t(q) = \frac{Q(\bar{F}_t(q)) - 1}{Q'(1)}\,\frac{e^{-qS(t)}}{t}.$$

Solution formula

$$\Phi(\bar{F}_t(q)) = \int_t^\infty \frac{e^{-qS(s)}}{s} ds, \qquad \Phi(p) = \int_0^p \frac{Q'(1)}{1 - Q(z)}\, dz.$$

À la Gallay-Mielke, the solution is determined as follows:

i) Initial data F_{t_0} determine the Laplace transform $\bar{F}_{t_0}(q)$.

ii) This determines the min history $S(s)$, $s \geq t_0$.

iii) The truncation $S(s)$, $s \geq t$ determines $\bar{F}_t(q)$.

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Remark: The solution formula is degenerate. We can write $(w = 1 - \bar{F})$

$$\exp(-\Phi(1-w)) = w\kappa(w) \quad \text{where } \kappa(w) \text{ is slowly varying as } w \to 0:$$

$$-\log \kappa(w) = \Phi(1-w) + \log w = \int_0^{1-w} \left(\frac{Q'(1)}{1-Q(s)} - \frac{1}{1-s} \right) ds$$

The limit as $w \to 0$ is finite if and only if $\sum p_k(k \log k) < \infty$

Domains of attraction for dynamic scaling

Theorem (Necessary & sufficient conditions for approach to self similar form)

Let F_{t_0} be an arbitrary probability measure on $(0, \infty)$ with positive min, and let F_t $(t \geq t_0)$ be the corresponding measure solution.

(i) Suppose there is a probability measure F_* with positive min S_*, and a positive $\lambda(t) \to \infty$ as $t \to \infty$ such that

$$F_t(\lambda(t)x) \to F_*(x) \quad \text{for a.e. } x > 0.$$

Then there exists $\theta \in (0, 1]$ and slowly varying L, $\tilde{L}$ such that as $x, t \to \infty$,

$$\int_0^x yF_{t_0}(dy) \sim x^{1-\theta}L(x) \qquad \text{and} \qquad \lambda(t)S_* \sim S(t) \sim t^{1/\theta}\tilde{L}(t).$$

(ii) Conversely, the condition on F_{t_0} is sufficient to ensure $S(t)$ is as described and

$$F_t(S(t)x) \to F^\theta(x), \qquad \text{where} \quad \bar{F}^\theta(q) = \Phi^{-1}(\theta\, \mathrm{Ei}(q))$$

Rigidity of scaling limits — regular variation

We say L is *slowly varying* at ∞ if $\quad \forall c > 0\ \dfrac{L(cx)}{L(x)} \to 1 \ \ (x \to \infty).$

Examples: $\log x$, $\log\log x$ are slowly varying at ∞, but $1 + \epsilon \sin x$ is not.

Lemma (in Feller's book) Suppose that f is monotone and that there exist $\lambda_j \to \infty$ and $a_j/a_{j+1} \to 1$ such that

$$h(x) = \lim_{j\to\infty} a_j f(\lambda_j x) \ \text{ exists } \forall x > 0.$$

Then necessarily $\quad h(x) = cx^p \quad$ for some c, $p \in \mathbb{R}$, and furthermore, f is regularly varying at ∞, meaning

$$f(x) \sim x^p L(x) \quad \text{where } L \text{ is slowly varying.}$$

Sketch of the argument

1. Regular variation of the min history is necessary (and sufficient):

The hypotheses imply $\bar{F}_t(q/\lambda)) \to \bar{F}_*(q)$ $(q > 0)$. From the solution formula,

$$\int_1^\infty \exp\left(\frac{-qS(ts)}{\lambda(t)}\right)\frac{ds}{s} \to \int_1^\infty \exp(-qS_*(s))\frac{ds}{s},$$

whence we infer

$$\frac{S(ts)}{\lambda(t)} \to S_*(s) \quad \text{at each point of continuity of } S_*.$$

By a rigidity argument one deduces

$$S_*(s) = cs^{1/\theta} \text{ and } S(t) \sim t^{1/\theta}L_1(t) \text{ is regularly varying.}$$

2. Tauberian arguments:

The right inverse $S^\dagger(\tau) \sim \tau^\theta L_2(\tau)$ is regularly varying. Write

$$\int_{t_0}^{\infty} e^{-qS(s)} \frac{ds}{s} = \int_{\tau_0}^{\infty} e^{-q\tau} A(d\tau) = \bar{A}(q), \quad \text{where } e^{A(\tau)} := S^\dagger(\tau).$$

By the handy exponential Tauberian theorem of de Haan,

$$e^{A(1/q)} e^{-\bar{A}(q)} \to e^{\gamma\theta} \quad (q \to 0), \quad \gamma = 0.577\ldots$$

Hence $\quad e^{-\bar{A}(q)} = w\,\kappa(w) \sim q^\theta L_3(1/q) \quad$ with $w = 1 - \bar{F}_{t_0}(q)$.

Standard inversion and Tauberian arguments yield $\displaystyle\int_0^x y F_{t_0}(dy) \sim x^\theta L_4(x)$.

Eternal solutions

Since $N(t) = 1/t$, 'eternal solutions' are those defined for all $t \in (0, \infty)$.

To F_t we associate the "g-measure"

$$G_t(dx) = \frac{x\, F_t(dx)}{t\kappa^{\#}(t)}$$

$(\kappa^{\#} = \ldots)$ and its 'Laplace exponent'

$$\eta_t(q) = \int_0^\infty \frac{1 - \exp(-qx)}{x} G_t(dx) \quad = \frac{1 - \bar{F}_t(q)}{t\kappa^{\#}(t)}$$

Eternal solutions are characterized in the limit $t \downarrow T_{\min} = 0$ as follows

Lévy-Khintchine parametrization

Measures arising as backward-time limits:

Definition: G is a g-measure if $(1 \wedge y^{-1})G(dy)$ is a finite measure on $[0, \infty]$.

Define $$x(G) := \int_{[0,\infty]} (x^{-1} \wedge y^{-1}) G(dy) = x^{-1} \int_{[0,x]} G(dy) + \int_{(x,\infty]} y^{-1} G(dy).$$

We say $G_n \to G$ if $x(G_n) \to x(G)$ for all x non-atomic for G.

We say G is divergent if $x(G) \to \infty$ as $x \to 0$.

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Theorem (a) Each eternal solution F has an associated divergent g-measure G_* such that $G_t \to G_*$ as $t \to 0$.

(b) Given any divergent g-measure G_* there corresponds a unique eternal F with $G_t \to G_*$ as $t \to 0$.

Thank you!

What $\kappa^{\#}(t)$ is

- If $Q(z) = z^2$ then $\kappa^{\#} = 2$. (back)
- If $\sum p_k k \log k < \infty$ then $\kappa^{\#} = \exp\left(\int_0^1 \frac{Q'(1)}{1-Q(s)} - \frac{1}{1-s}\,ds\right)$.
- In general $\kappa^{\#}(\tau)$ is *slowly varying*, found as $w = 1 - \bar{F} \to 0$ by an inversion:

$$-\log \kappa(w) = \Phi(1-w) + \log w = \int_0^{1-w} \left(\frac{Q'(1)}{1-Q(s)} - \frac{1}{1-s}\right) ds$$

$$\tau = w\kappa(w) = \exp(-\Phi(1-w))$$

$$w \sim \tau \kappa^{\#}(\tau)$$

• The scaling attractor for $K = x + y$

The scaling attractor $\mathcal{A}$ is the set of all probability distributions F_* on $[0, \infty]$ that arise as cluster points

$$F_*(x) = \lim_{n\to\infty} F_n(b_n x, t_n), \quad b_n, t_n \to \infty$$

Points in $\mathcal{A}$ correspond 1-1 with (extended) eternal solutions:

$$F(x,t) = \lim_{n\to\infty} F_n(b_n x, t + t_n) \quad \text{is defined for } -\infty < t < \infty.$$

The set of F_t for eternal solutions is the *maximal invariant set* for the dynamics of the system (meaning both positively and negatively invariant).

These are the analog of *infinitely divisible laws* in probability theory.

Lévy-Khintchine parametrization of eternal solutions

(Bertoin 2002, Menon-P 2008)

To any solution F associate $G_t(dx) = e^t x^2 n(e^t dx, t) = xF(e^t dx, t)$.

Theorem (a) Each eternal solution F has an associated divergent g-measure G_* such that $G_t \to G_*$ as $t \to -\infty$.

(b) Given any divergent g-measure G_* there corresponds a unique eternal F with $G_t \to G_*$ as $t \to -\infty$.

• Linearization of ultimate dynamics

The nonlinear "time τ map" acts by *linear scaling* through a bicontinuous map

$$\mathcal{A} \quad \leftrightarrow \quad \text{extended eternal } F \quad \leftrightarrow \quad g\text{-meas } G_*.$$

Theorem Let $F(x,t)$ be eternal with associated divergent g-measure G_*. Then

$$\tilde{F}(x,t) = F(bx, t+\tau)$$

has associated divergent g-measure $\tilde{G}_*$ given by the pure scaling relation

$$\tilde{G}_*(dx) = b^{-1}e^{2\tau}G_*(be^{-\tau}dx).$$

Proof:

$$\tilde{G}_t(dx) = b^{-1}e^{2\tau}G_{t+\tau}(be^{-\tau}dx).$$

Take $t \to -\infty$.

Signatures of chaos for heavy-tailed dynamics

For solutions with $K = x + y$ and total mass 1, long-time scaling behavior is sensitive to the mass distribution of the largest clusters:

- All domains of attraction are dense.
- There is an uncountable dense set of scaling-periodic solutions.
- There are dense trajectories on the scaling attractor — *Doeblin solutions*.
- Asymptotic shadowing: If the tails of F_0 and $\tilde{F}_0$ agree (more generally, if $\varphi_0(s)/\tilde{\varphi}_0(s) \sim 1$ as $s \to 0$), then
  - ⋆ The scaling ω-limit sets $\omega(F) = \omega(\tilde{F})$
  - ⋆ For any size rescaling $b(t)$, in $\overline{\mathcal{P}}$ (a metric space) we have

$$\operatorname{dist}(F(b(t)\cdot, t), \tilde{F}(b(t)\cdot, t)) \to 0 \quad \text{as } t \to \infty.$$