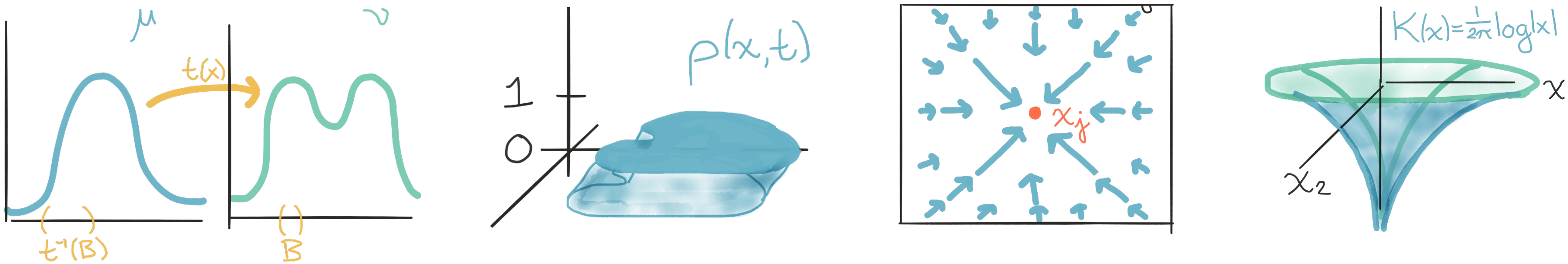

From slow diffusion to a hard height constraint: characterizing congested aggregation

Katy Craig
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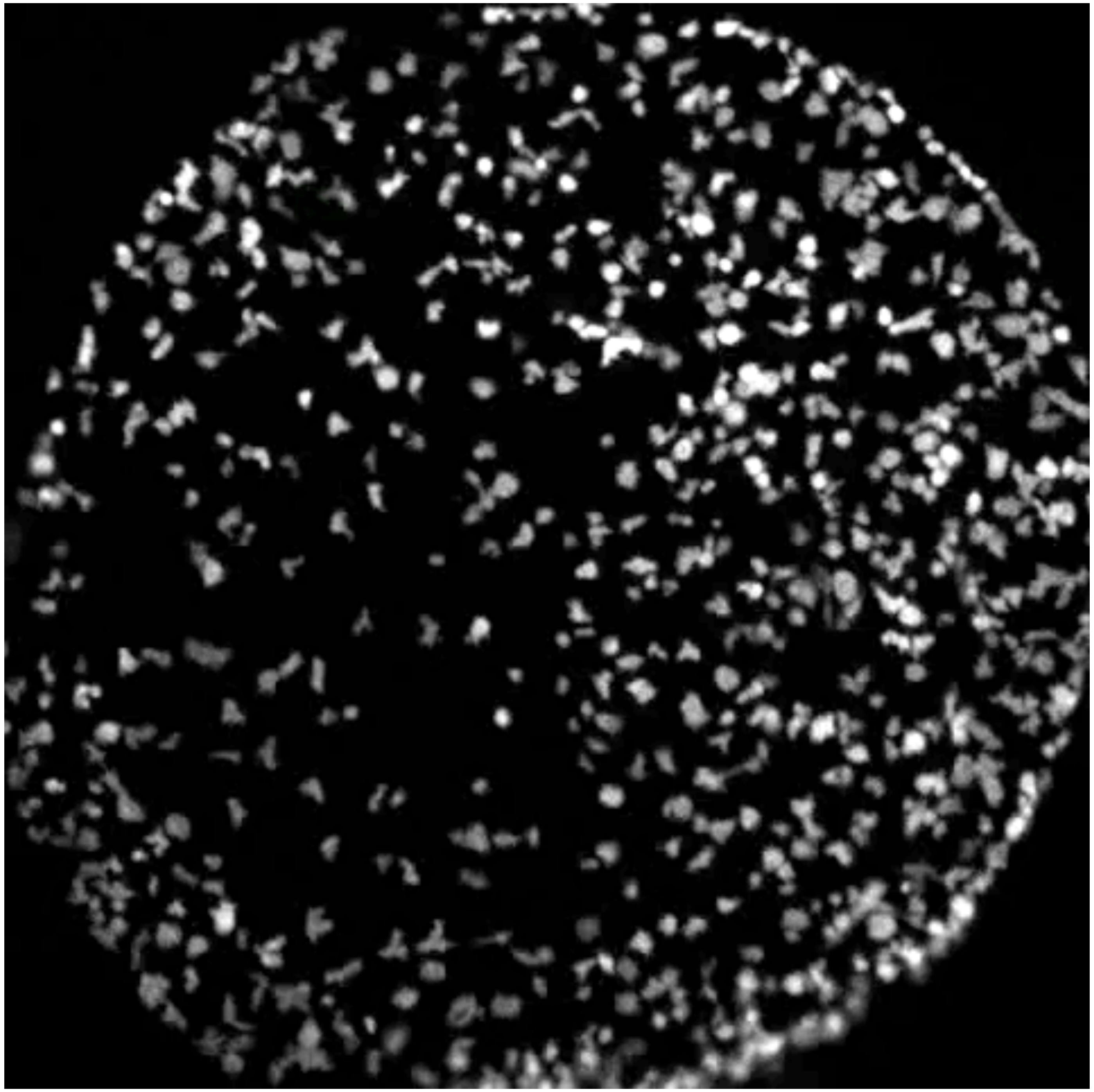
joint work with Inwon Kim (UCLA) and Yao Yao (Georgia Tech)

Applied Math and Analysis Seminar
Duke University, 2/22/17

collective dynamics

biological chemotaxis (a colony of slime mold)



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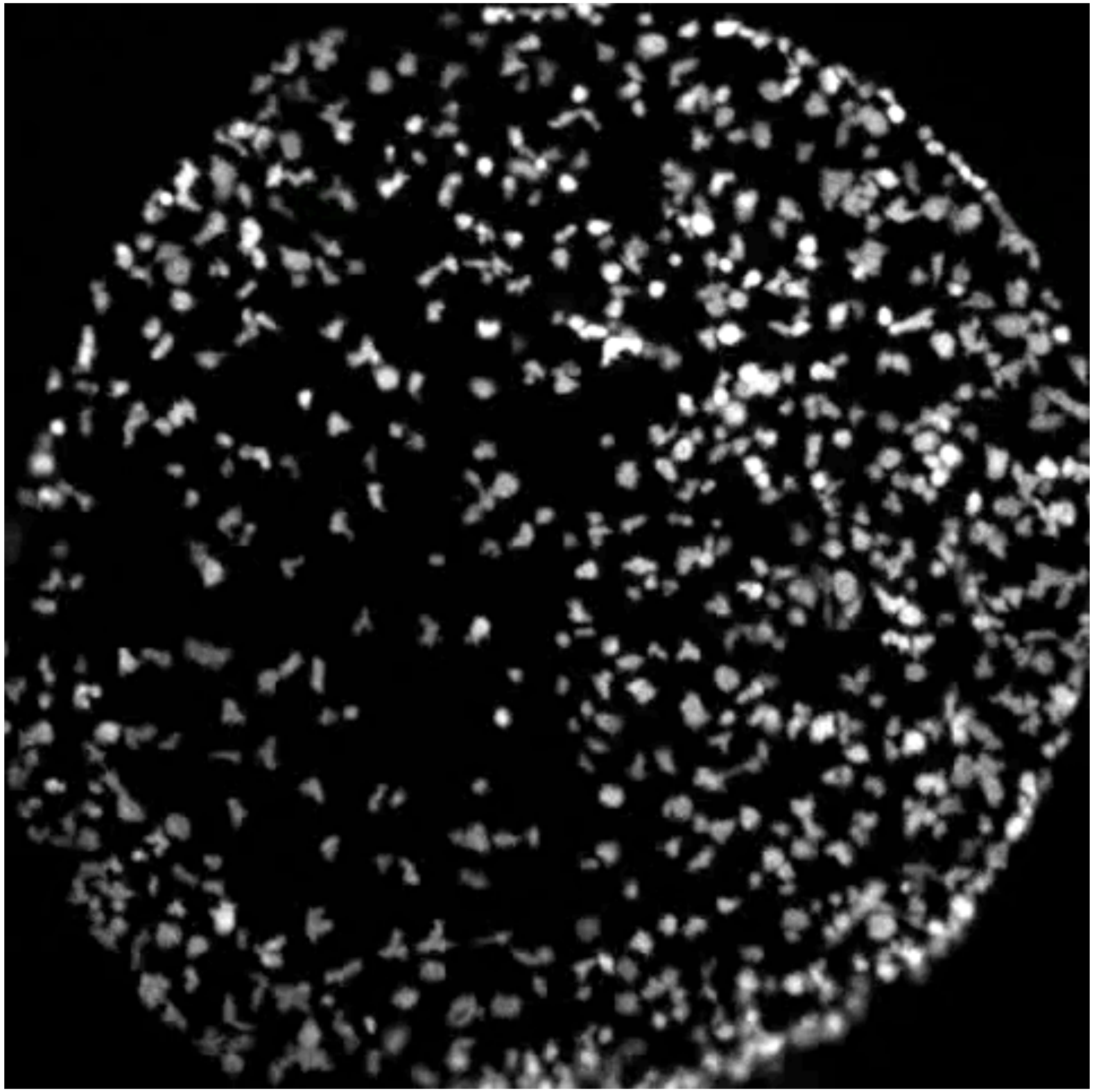

plan

- congested aggregation equation
- previous work and challenges
- well-posedness
  nonconvex Wasserstein gradient flow
- dynamics/long time behavior
  free boundary problem
- future work

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motivation

- ρ(x,t): $\mathbb{R}^d \times \mathbb{R} \rightarrow [0, +\infty)$ nonnegative density
- mass is conserved ⇒ $\int \rho(x)\, dx = 1$

aggregation equation with degenerate diffusion:

$$\boxed{\frac{d}{dt}\rho = \nabla \cdot ((\underbrace{\nabla K * \rho}_{\text{self attraction}})\rho) + \underbrace{\Delta \rho^m}_{\text{degenerate diffusion}}} \quad \text{for } K(x) : \mathbb{R}^d \to \mathbb{R} \text{ and } m \geq 1$$

interaction kernels:

- granular media: $K(x) = |x|^3$
- swarming: $K(x) = -e^{-|x|}$
- chemotaxis: $K(x) = \begin{cases} \frac{1}{2\pi} \log |x| & \text{if } d = 2, \\ C_d |x|^{2-d} & \text{otherwise.} \end{cases}$

degenerate diffusion:

- $\Delta \rho^m = \nabla \cdot (\underbrace{m\rho^{m-1}}_{D} \nabla \rho)$

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interaction kernels:

K = Δ^{-1}

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degenerate diffusion:

- $\Delta \rho^m = \nabla \cdot (\underbrace{m\rho^{m-1}}_{D} \nabla \rho)$

motivation

Inspired by the aggregation equation with degenerate diffusion, we consider the congested aggregation equation.

$$\frac{d}{dt}\rho = \nabla \cdot ((\nabla K * \rho)\rho) + \Delta \rho^m$$

“ $$\begin{cases} \frac{d}{dt}\rho = \nabla \cdot (\nabla(K * \rho)\rho) \text{ if } \rho < 1 \\ \rho \leq 1 \text{ always} \end{cases}$$ ”

- Both models have self-attraction from $\nabla K * \rho$.
- The role of repulsion is played by hard height constraint instead of degenerate diffusion.
- Heuristically, hard height constraint is singular limit of degenerate diffusion:

Idea: $\Delta \rho^m = \nabla \cdot (\underbrace{m\rho^{m-1}}_{D} \nabla \rho)$, so as m→+∞, $D \to \begin{cases} +\infty & \text{if } \rho > 1 \\ 0 & \text{if } \rho < 1 \end{cases}$

questions

Congested aggregation eqn: “$\begin{cases} \frac{d}{dt}\rho = \nabla \cdot (\nabla (K * \rho)\rho) \text{ if } \rho < 1 \\ \rho \leq 1 \text{ always} \end{cases}$”

- In what sense?
- Well-posed? Stable?
- Dynamics?
- Long time behavior?

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previous work

Congested drift equation: “$\begin{cases} \frac{d}{dt}\rho = \nabla \cdot ((\nabla V)\rho) \text{ if } \rho < 1 \\ \rho \leq 1 \text{ always} \end{cases}$”

[Maury, Roudneff-Chupin, Santambrogio 2010]

- introduced as a model of crowd motion in an evacuation scenario, where $V(x)$ = distance to exit.
- showed well-posedness as a W_2 gradient flow for $V(x)$ convex.

[Alexander, Kim, Yao 2014] showed

$$\frac{d}{dt}\rho = \nabla \cdot ((\nabla V)\rho) + \Delta \rho^m \xrightarrow{m \to +\infty} \begin{cases} \frac{d}{dt}\rho = \nabla \cdot ((\nabla V)\rho) \text{ if } \rho < 1 \\ \rho \leq 1 \text{ always} \end{cases}$$

and used this to characterize dynamics in terms of free boundary problem

previous work

V convex

Congested drift equation: “ $\begin{cases} \frac{d}{dt}\rho = \nabla \cdot ((\nabla V)\rho) \text{ if } \rho < 1 \\ \rho \leq 1 \text{ always} \end{cases}$ ”

- In what sense? Wasserstein gradient flow
- Well-posed? Stable? Yes

[MRS 2010]

- Dynamics? Hele-Shaw type free boundary problem
- Long time behavior? exponential conv. to ! equilibrium

[AKY 2014]

Challenges:

- $K * \rho$ not convex ⇒ W_2 gradient flow theory comparatively undeveloped
- $K * \rho$ nonlocal ⇒ no comparison principle

questions

K= Δ^{-1}

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combination of Wasserstein gradient flow with viscosity solution theory

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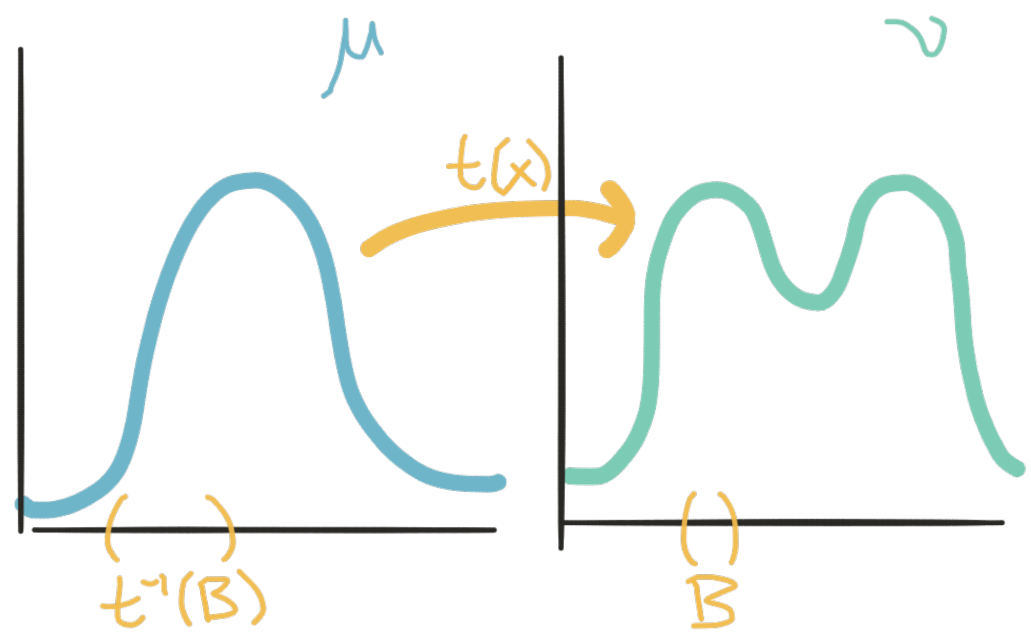
Wasserstein metric

- Given two probability measures μ and ν on $\mathbb{R}^d$, $\mathbf{t} : \mathbb{R}^d \to \mathbb{R}^d$ *transports* μ *onto* ν if $\nu(B) = \mu(\mathbf{t}^{-1}(B))$. Write this as $t\#\mu = \nu$.



- The *Wasserstein distance* between μ and ν ∈ $P_2(\mathbb{R}^{\mathbf{d}})$ is

$$W_2(\mu,\nu) := \inf\left\{ \underbrace{\left(\int |t(x)-x|^2 d\mu(x)\right)^{1/2}}_{\text{effort to rearrange } \mu \text{ to look like } \nu \text{, using } t(x)} : \underbrace{t\#\mu = \nu}_{t \text{ sends } \mu \text{ to } \nu} \right\}$$

geodesics

Not just a metric space… a geodesic metric space: there is a constant speed geodesic $\sigma : [0,1] \to \mathcal{P}_2(\mathbb{R}^d)$ connecting any μ and ν.

$$\sigma(0) = \mu, \;\; \sigma(1) = \nu, \;\; W_2(\sigma(t), \sigma(s)) = |t-s| W_2(\mu, \nu)$$

Monge Kantorovich

μ Wasserstein geodesic $\sigma(t)$ ν

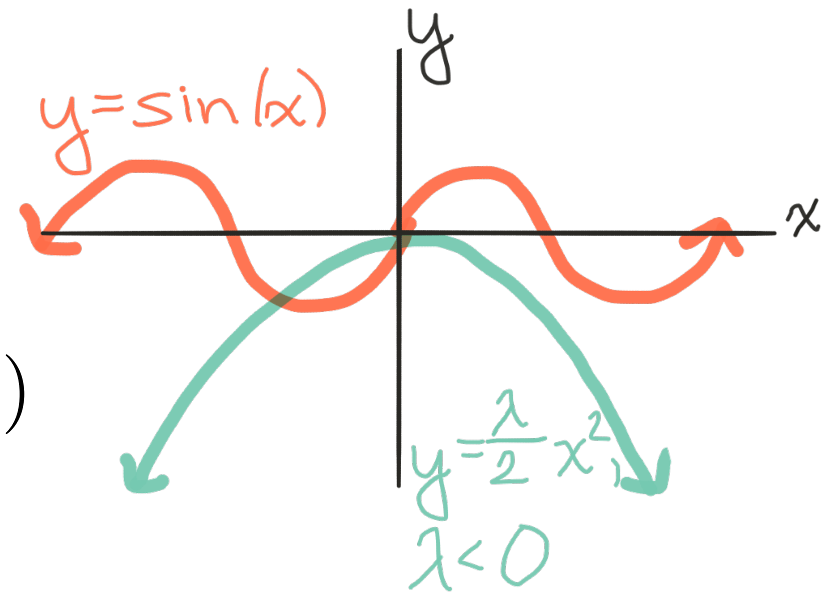
μ linear interpolation $(1-t)\mu + t\nu$ ν

[Payré, Papadakis, Oudet 2013]

convexity

Since the Wasserstein metric has geodesics, it has a notion of convexity.

Recall: in **Euclidean space**, E: $\mathbb{R}^d \to \mathbb{R}$ is…



convex

$D^2E \geq 0 \Longleftrightarrow E((1-t)x+ty) \leq (1-t)E(x)+tE(y)$

λ-convex

$D^2E \geq \lambda I_{d\times d} \Longleftrightarrow E((1-t)x+ty) \leq (1-t)E(x)+tE(y) - t(1-t)\frac{\lambda}{2}|x-y|^2$

Likewise, in the **Wasserstein metric**, E: $P_2(\mathbb{R}^d) \to \mathbb{R}$ is λ-convex if

$$E(\sigma(t)) \leq (1-t)E(\mu)+tE(\nu) - t(1-t)\frac{\lambda}{2}W_2^2(\mu,\nu)$$

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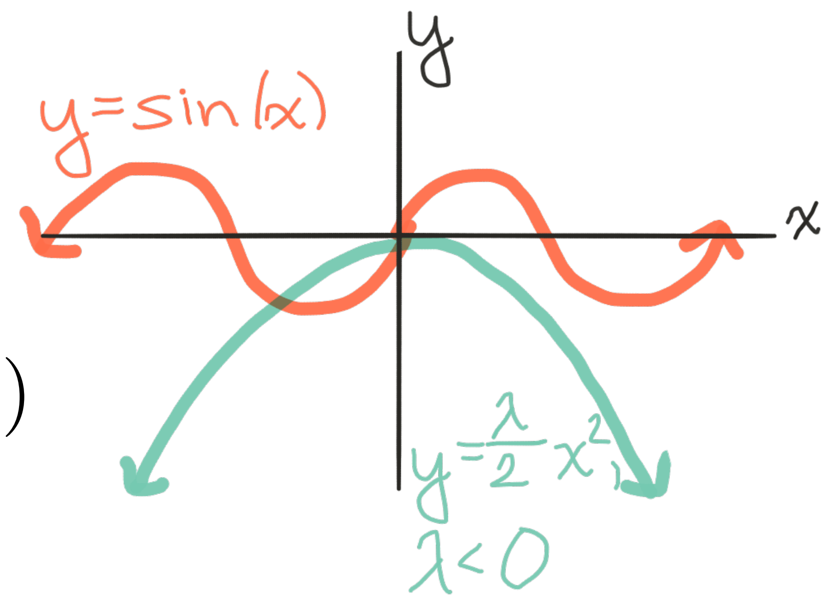

convex

endpoints

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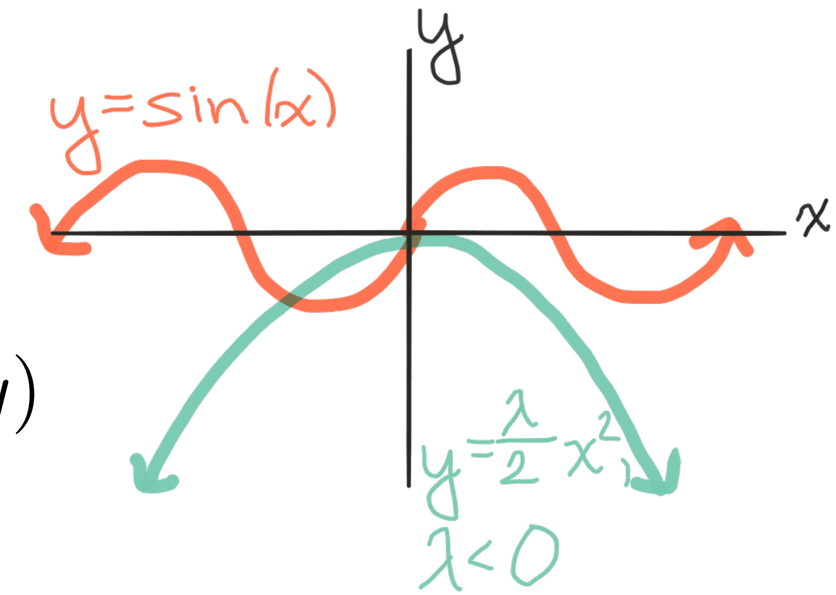

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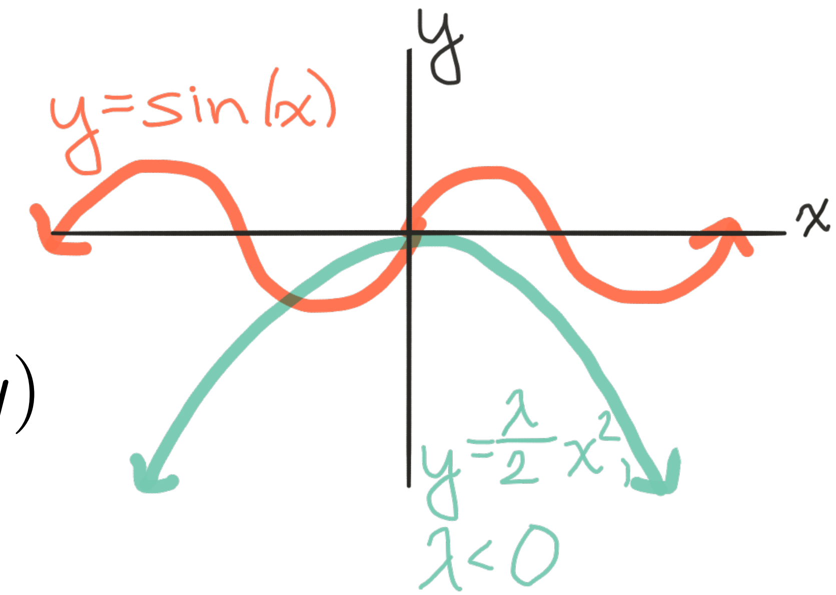

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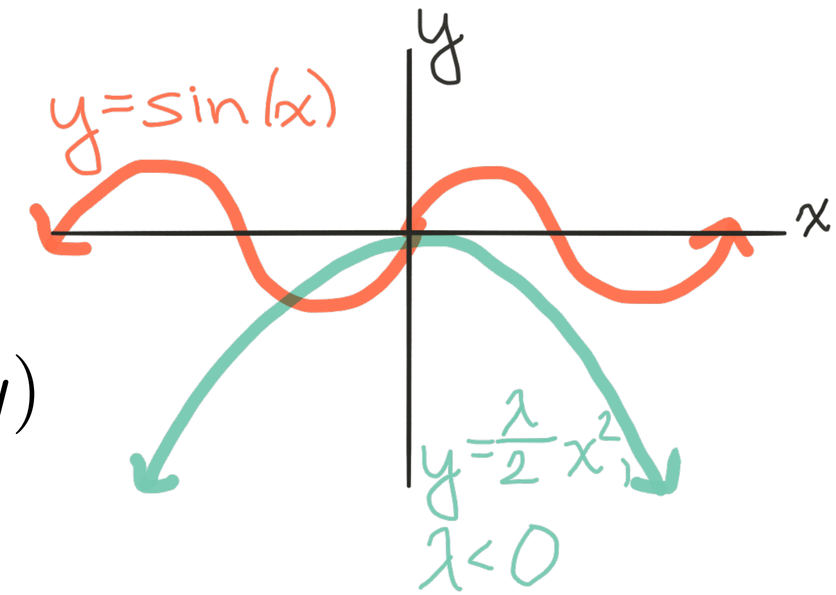

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gradient flow

How does this relate to PDE? Wasserstein gradient flow.

- In general, given a complete metric space (X,d), a curve x(t): $\mathbb{R} \to$ X is the gradient flow of an energy E: X $\to$ $\mathbb{R}$ if

$$\boxed{\frac{d}{dt}x(t) = -\nabla_X E(x(t))}$$

- "x(t) evolves in the direction of steepest descent of E"

Examples:

metric	energy functional	gradient flow
$(L^2(\mathbb{R}^d), \|\cdot\|_{L^2})$	$E(f) = \frac{1}{2}\int \|\nabla f\|^2$	$\frac{d}{dt}f = \Delta f$
$(\mathcal{P}_2(\mathbb{R}^d), W_2)$	$E(\rho) = \int \rho \log \rho$	$\frac{d}{dt}\rho = \Delta \rho$
	$E(\rho) = \frac{1}{m-1}\int \rho^m$	$\frac{d}{dt}\rho = \Delta \rho^m$

gradient flow

$\rho(t): \mathbb{R} \to P_2(\mathbb{R}^d)$ is the *Wasserstein gradient flow* of energy $E: P_2(\mathbb{R}^d) \to \mathbb{R}$ if

$$\frac{d}{dt}\rho(t) = -\nabla_{W_2} E(\rho(t))$$

Relationship between Wasserstein gradient flow and PDE:

- If E sufficiently regular, gradient flow $\Longleftrightarrow$ PDE
- More generally, gradient flow $\not\Longleftrightarrow$ PDE

For *λ-convex* energies, gradient flow theory is well-developed.

Theorem (Ambrosio, Gigli, Savaré 2005): If E is λ-convex, lower semicontinuous, and bounded below, solutions of its W_2 gradient flow

- exist
- are unique
- contract ($\lambda>0$)/expand ($\lambda\leq 0$) exponentially:

$$W_2(\rho_1(t), \rho_2(t)) \leq e^{-\lambda t} W_2(\rho_1(0), \rho_2(0))$$

gradient flow

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$$W_2(\rho_1(t), \rho_2(t)) \leq e^{-\lambda t} W_2(\rho_1(0), \rho_2(0))$$

This ensured well-posedness of the congested drift equation for V(x) convex.

gradient flow and aggregation

The congested aggregation equation is (formally) a Wasserstein gradient flow of the height constrained interaction energy:

$$\begin{cases} \frac{d}{dt}\rho = \nabla \cdot (\nabla(K * \rho)\rho) \text{ if } \rho < 1 \\ \rho \leq 1 \text{ always} \end{cases}$$

$$E_\infty(\rho) = \begin{cases} \frac{1}{2}\iint K(x-y)\rho(x)\rho(y)dxdy & \text{if } \|\rho\|_\infty \leq 1 \\ +\infty & \text{otherwise} \end{cases}$$

Fact: If K: $\mathbb{R}^d \to \mathbb{R}$ is λ-convex, then E_∞ is λ-convex.

Problem: $K(x) = \begin{cases} \frac{1}{2\pi}\log|x| & \text{if } d = 2 \\ C_d|x|^{2-d} & \text{otherwise} \end{cases}$ is not λ-convex.

E_∞ falls outside the scope of the existing theory.

ω-convexity

Solution: Even though we don't have

$$E_\infty(\sigma(t)) \leq (1-t)E_\infty(\mu) + tE_\infty(\nu) - \frac{\lambda}{2}t(1-t)W_2^2(\mu,\nu)$$

λ-convexity

E_∞ does satisfy a similar inequality for a different modulus of convexity

$$E_\infty(\sigma(t)) \leq (1-t)E_\infty(\mu) + tE_\infty(\nu) - \frac{\lambda}{2}\left[(1-t)\omega\left(t^2 W_2^2(\mu,\nu)\right) + t\omega\left((1-t)^2 W_2^2(\mu,\nu)\right)\right]$$

ω-convexity

where ω(x) = x |log(x)|.

Remark: The above two inequalities coincide for ω(x) = x: ω-convexity is a generalization of λ-convexity.

aside: ω-convexity & Euler equations

In fact, when $\omega(x) = x\,|\log(x)|$, ω-convexity is related to well-posedness of bounded solutions of the the Euler equations.

- λ-convexity in W_2 is analogous to D^2E being bounded from below in Euclidean space, or that ∇E is one-sided Lipschitz.

- Likewise, ω-convexity in W_2 is analogous to D^2E being BMO in Euclidean space, or that ∇E is log-Lipschitz.

- Log-Lipschitz regularity of the velocity field was precisely what allowed [Yudovich 1963] to prove uniqueness of bounded solutions of the two dimensional Euler equations.

ω-convexity: well-posedness

For merely ω-convex energies, the gradient flow is well-posed.

Theorem (C. 2016): If E is ω-convex for ω(x) = x |log(x)|, lower semicontinuous, and bounded below, solutions of its W_2 gradient flow

- exist
- are unique
- contract (λ>0)/expand (λ≤0) double exponentially:

$$W_2(\rho_1(t), \rho_2(t)) \leq W_2(\rho_1(0), \rho_2(0))^{e^{2\lambda t}}$$

In fact, well-posedness holds for all ω(x) that satisfy Osgood's condition.

Corollary (C. 2016): Since E_∞ is ω-convex for ω(x) = x |log(x)| and λ<0, the congested aggregation equation is well-posed as a Wasserstein gradient flow and expands at most double exponentially.

questions

$K = \Delta^{-1}$

Congested aggregation eqn: "$\begin{cases} \frac{d}{dt}\rho = \nabla \cdot (\nabla(K * \rho)\rho) \text{ if } \rho < 1 \\ \rho \leq 1 \text{ always} \end{cases}$"

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(nonconvex) Wasserstein gradient flow

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combination of Wasserstein gradient flow with viscosity solution theory

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motivation for free boundary problem

How does congested aggregation equation relate to free boundary problem?

“
$$\begin{cases} \frac{d}{dt}\rho = \nabla \cdot (\nabla(K * \rho)\rho) \text{ if } \rho < 1 \\ \rho \leq 1 \text{ always} \end{cases}$$
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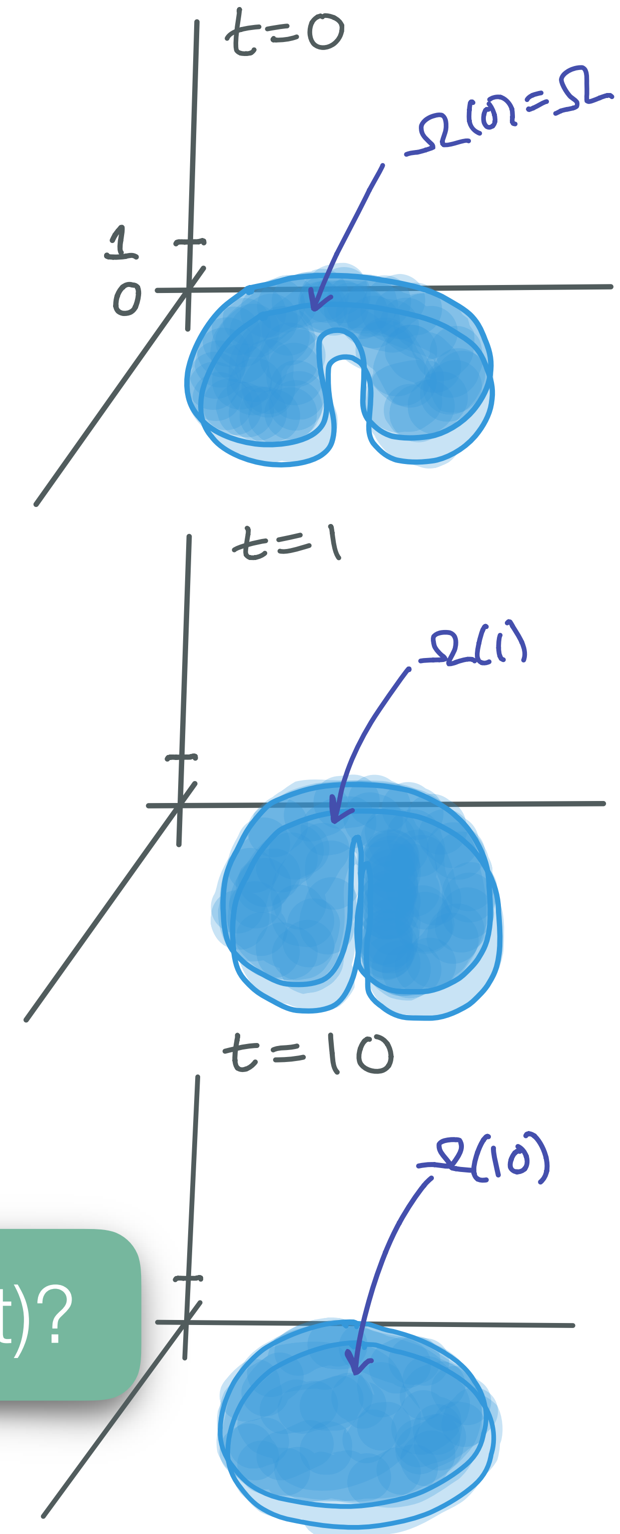

- Consider patch solutions. For a domain Ω, suppose that ρ(x,t) is a solution with initial data
$$\rho(x,0) = \begin{cases} 1 & \text{if } x \in \Omega, \\ 0 & \text{otherwise.} \end{cases}$$
- Since $K = \Delta^{-1}$, $\nabla K * \rho$ causes self-attraction. Thus, we expect ρ(x,t) to remain a characteristic function.
- Let Ω(t)={ρ=1} be *congested region*, so $\rho(x,t)=1_{\Omega(t)}(x)$.

What free boundary problem describes evolution of Ω(t)?

formal derivation

- Here is a **formal** derivation of the related free boundary problem.
- Suppose ρ(x,t) solves "$\begin{cases} \frac{d}{dt}\rho = \nabla \cdot (\nabla(K * \rho)\rho) \text{ if } \rho < 1 \\ \rho \leq 1 \text{ always} \end{cases}$"
- Since mass is conserved, we expect ρ(x,t) satisfies a continuity equation

$$\frac{d}{dt}\rho = \nabla \cdot \big(\underbrace{(\nabla K * \rho + \nabla \mathbf{p})}_{v}\,\rho\big)$$

where **∇p(x,t)** is the pressure arising from the height constraint.

Height constraint is active on the congested region {**p**>0} = Ω(t).

Height constraint is inactive outside the congested region {**p**=0}= $\Omega(t)^c$.

formal derivation

Given $$\frac{d}{dt}\rho = \nabla \cdot \Big(\underbrace{(\nabla K * \rho + \nabla \mathbf{p})}_{v}\,\rho\Big)$$ what happens on congested region?

- Because of hard height constraint, on the congested region Ω(t)={ρ=1}, the velocity field is incompressible, **∇**·v=0.

- Since K= Δ^{-1}, $\nabla \cdot v = \Delta K * \rho + \Delta \mathbf{p} = \rho + \Delta \mathbf{p}$, so incompressibility means

$$-\Delta \mathbf{p} = \rho \text{ on } \Omega(t) = \{\rho = 1\}$$

- Using that the height constraint is active on the congested region, Ω(t)={**p**>0}, we obtain the following equation for the pressure:

$$\boxed{-\Delta \mathbf{p} = 1 \text{ on } \{\mathbf{p} > 0\}}$$

formal derivation

Given $\boxed{\frac{d}{dt}\rho = \nabla\cdot(\underbrace{(\nabla K * \rho + \nabla \mathbf{p})}_{v}\rho)}$ what about bdy of congested region?

outward normal velocity of ∂Ω(t)

- By conservation of mass,

$$0 = \frac{d}{dt}\int_{\Omega(t)} \rho = \int_{\Omega(t)} \frac{d}{dt}\rho + \int_{\partial\Omega(t)} V\rho$$

- Using that ρ(x,t) solves the above continuity equation, this equals

$$= \int_{\Omega(t)} \nabla\cdot((\nabla K * \rho + \nabla \mathbf{p})\rho) + \int_{\partial\Omega(t)} V\rho = \int_{\partial\Omega(t)} (\partial_\nu K * \rho + \partial_\nu \mathbf{p} + V)\rho$$

- Using that $\rho(x,t)=1_{\Omega(t)}(x)$, for $\Omega(t)=\{\mathbf{p}>0\}$, we again obtain an equation for **p**,

$$\boxed{\partial_\nu K * 1_{\{\mathbf{p}>0\}} + \partial_\nu \mathbf{p} + V = 0 \text{ on } \partial\{\mathbf{p}>0\}}$$

free boundary problem

Combining the observations that…

- on the congested region,

$$-\Delta \mathbf{p} = 1 \text{ on } \{\mathbf{p} > 0\}$$

- and on the boundary of the congested region,

outward normal velocity of $\partial\Omega(t)$

$$\partial_\nu K * 1_{\{\mathbf{p}>0\}} + \partial_\nu \mathbf{p} + V = 0 \text{ on } \partial\{\mathbf{p} > 0\}$$

Theorem (C., Kim, Yao 2016):

- Suppose ρ(x,t) solves congested aggregation eqn with ρ(x,0) = $1_{\Omega(0)}$(x).
- Then ρ(x,t)=$1_{\Omega(t)}$(x), for Ω(t) = {**p(x,t)**>0}, where **p** a viscosity solution of

$$\begin{cases} -\Delta \mathbf{p} = 1 & \text{on } \quad \{\mathbf{p} > 0\} \\ \quad V = -\partial_\nu K * 1_{\{\mathbf{p}>0\}} - \partial_\nu \mathbf{p} & \text{on } \partial\{\mathbf{p} > 0\}. \end{cases}$$

long time behavior

Using the characterization of the dynamics of patch solutions provided by the free boundary problem, we are able to study their long time behavior:

Theorem (C., Kim, Yao 2016):

- Suppose ρ(x,t) solves congested aggregation eqn with $\rho(x,0) = 1_{\Omega(0)}(x)$.
- Then, in two dimensions,

$$\rho(x,t) \xrightarrow{L^p} 1_B(x) \text{ for all } 1 \leq p < +\infty$$

and

$$|E_\infty(\rho(\cdot,t)) - E_\infty(1_B)| \leq C_{\Omega(0)} t^{-1/6}$$

- In any dimension, the Riesz Rearrangement Inequality guarantees that the unique minimizer of E_∞ is $1_B(x)$.

- The difficult part is showing that mass of ρ(x,t) doesn't escape to +∞. To accomplish this, we use an inequality due to Talenti, which holds in d=2.

plan

- congested aggregation equation
- previous work and challenges
- well-posedness
  nonconvex Wasserstein gradient flow
- dynamics/long time behavior
  free boundary problem
- future work

future work:

Does Keller-Segel converge to congested aggregation?

$$\frac{d}{dt}\rho = \nabla \cdot ((\nabla K * \rho)\rho) + \Delta \rho^m \quad \xrightarrow{m \to +\infty} \quad \begin{cases} \frac{d}{dt}\rho = \nabla \cdot (\nabla(K * \rho)\rho) \text{ if } \rho < 1 \\ \rho \leq 1 \text{ always} \end{cases}$$

- For V(x) convex, [Alexander, Kim, Yao 2014] showed

$$\frac{d}{dt}\rho = \nabla \cdot ((\nabla V)\rho) + \Delta \rho^m \quad \xrightarrow{m \to +\infty} \quad \begin{cases} \frac{d}{dt}\rho = \nabla \cdot ((\nabla V)\rho) \text{ if } \rho < 1 \\ \rho \leq 1 \text{ always} \end{cases}$$

- Connecting Keller-Segel and the congested aggregation eqn would…
  - ✦ Lead to new numerical methods for congested aggregation.
  - ✦ Lead to greater insight in long-time behavior of supercritical (m>2-2/d) Keller-Segel.

future work:

What about non-patch solutions?

- Relates to recent work on $m \to +\infty$ limit in PME-type models for tumor growth by [Kim and Pozar 2015] and [Mellet, Perthame, Quiros 2015]

What about non-Newtonian kernels $K(x)$?

- While well-posedness theory extends to a range of interaction kernels, free boundary problem strongly uses Newtonian structure.

future work:

Other characterizations of dynamics?

- Can we show $\boxed{\frac{d}{dt}\rho = \nabla \cdot ((\underbrace{\nabla K * \rho + \nabla \mathbf{p})}_{v}\, \rho)}$ in a weak sense?
- For the congested drift equation [Maury, Roudneff-Chupin, Santambrogio 2010] showed that the analogous continuity equation holds, where v is obtained by projecting ∇V onto a space of admissible velocities.

Further examples of ω-convex energies?

More applications with a height constraint?

Thank you!