When do interacting organisms gravitate to the vertices of a regular simplex?

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Slides at ‘Talk 3’ at www.math.toronto.edu/mccann

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Animals forming patterns: flocking, milling, swarming
and schooling
Led scientists to make models...

e.g. (very incomplete)
Lennard-Jones (1924) 6-12 potential for molecular interactions
Parr (1927)
Breder (1954) attractive-repulsive power law interaction for fish separation
Keller-Segal (1971) purely attractive, 1st order (2d cell chemotaxis)

Mogilner and Edelstein-Keshet (1999) 1d attractive-repulsive + diffusion
Levine, Rappel and Cohen (2000) 2nd order, preferred speed
Topaz, Bertozzi and Lewis (2006)
Cucker and Smale (2007) 2nd order, matched speeds

... analyze and simulate
e.g. (just as incomplete) Albi, Balague, Bertozzi, Burchard, Carrillo, Choksi, Craig, Fetecau, Figalli, Frank, Huang, Kolokolnikov, Laurent, Lieb, Lopes, Pavlovski, Pattachini, Raoul, Sun, Topaloglu, Uminsky, von Brecht,
Attractive-repulsive pair potentials on $x \in \mathbb{R}^n$:

$$V_{a,b}(x) := V_a(x) - V_b(x)$$

$$V_a(x) := \frac{1}{a} |x|^a \quad \text{exponents } a > b$$

- minimized at separation $|x| = 1$
First-order, interacting $J$ particle dynamics

ODE description: $x_k(t) \in \mathbb{R}^n$ for $i \in \{1, \ldots, J\}$:

$$\frac{dx_k}{dt} = \frac{1}{J-1} \sum_{i \neq k} \nabla V_{a,b}(x_i - x_k)$$

PDE description:

the probability measure $\mu(t) := \frac{1}{J} \sum_{i=1}^{J} \delta_{x_i}(t)$ on $\mathbb{R}^n$ satisfies
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$$= \quad$$
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$$= \frac{1}{2} \nabla \cdot [\mu \nabla (\delta E \delta \mu)],$$

which dissipates the energy

$$E(\mu) = E_{a,b}(\mu) := \int_{\mathbb{R}^n} \int_{\mathbb{R}^n} V_{a,b}(x - y) d\mu(x) d\mu(y)$$
The aggregation / self-assembly equation

\[
\frac{d\mu}{dt} = \nabla \cdot [\mu \nabla (V_{a,b} \ast \mu)] = \frac{1}{2} \nabla \cdot [\mu \nabla (\frac{\delta E}{\delta \mu})],
\]

defines a flow on \( P(\mathbb{R}^n) \), where

\[
P(K) := \{ \mu \geq 0 \text{ on } \mathbb{R}^n \mid \mu[K] = 1 = \mu[\mathbb{R}^n] \}
\]
denotes the space of Borel probability measures on \( K \subset \mathbb{R}^n \).
The continuumum $J \to \infty$ limiting dynamics

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defines a flow on $\mathcal{P}(\mathbb{R}^n)$, where

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denotes the space of Borel probability measures on $K \subset \mathbb{R}^n$.

Minimizers of $E_{a,b}(\mu)$ on $\mathcal{P}(\mathbb{R}^n)$ represent attracting fixed points of the flow (as do local minimizers in a suitable topology).
Figure 1: Steady states of (1) with $F(r) = \min (ar + b, 1 - r)$, using $N = 1000$ particles and with $a, b$ as indicated. A snapshot at $t = 10,000$ is shown. Integration was performed using forward Euler method with stepsize 0.5.
Fig. 9. $N = 1000$ particles, $a = 5, |u_0| = 0.5$. The Figure shows the evolution of a mill ring for increasing values of $b$, i.e., decreasing repulsion. The evolution of the second and third rows is computed starting from the stable pattern of the previous line.

Figure 9 we show the evolution of a mill ring solution with $b$ taken equal to 0.5, 1.25, and 3.5, respectively. The parameter choices are marked as (*) in Figure 7. The plot is generated using the main
Parameter space

[Hand-drawn graph with axes labeled 0 to 4 and 0 to b, with annotations such as 'mildly aggressive', 'social/physical', and 'O. Luyba 18']
Some related results

M. '94, '05 introduced $d_\infty$-local minimization to find stable rotating stars

Balague, Carrillo, Laurent, Raoul '13: showed $d_\infty$-local minimizers $\mu$ of $E_{a,b}$ on $\mathcal{P}(\mathbb{R}^n)$ have support with Hausdorff dimension at least $2 - b$. 

Sun, Uminsky, Bertozzi '12: for $b = 2$ showed spherical shell linearly stable iff $a < 4$ while vertices of regular simplex are linearly stable iff $a > 4$.

Inquired about nonlocal stability and global attraction.

• moreover, in the mildly repulsive regime $b \geq 2$

Carrillo, Figalli, Patachini '17: showed if $b > 2$ then $d_\infty$-local minimizers are supported only at isolated points (and indeed only finitely many such points in the case of global energy minimizers).

Kang, Kim, Lim, Seo '19+: catalog $d_\infty$-local and global minimizers in $n = 1$ dimension.
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Theorem (Minimizing strong attraction with mild repulsion)

1. If $a >> b > 2$ then $E(\mu)$ is uniquely minimized on $\mathcal{P}(\mathbb{R}^n)$ (up to rotations and translations) by equidistributing the mass of $\mu$ over the vertices of a regular simplex:

$$\mu = \frac{1}{n+1} \sum_{i=0}^{n} \delta_{x_i}$$

where $|x_i - x_k| = 1$ for all $0 \leq i < k \leq n$. 
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Theorem (Many local minima throughout the mildly repulsive regime)

2. If $a > b > 2$ and $0 < m_0 \leq \cdots \leq m_n$ with $1 = \sum_{i=0}^{n} m_i$ then

\[ \mu = \sum_{i=0}^{n} m_i \delta_{x_i} \]  
where $|x_i - x_k| = 1$ as above

is a $d_\infty$-local minimizer of $E(\mu)$ (minimizing strictly up to rigid motions).
Given $p > 1$ and $K \subset \mathbb{R}^n$ compact,

$$d_p(\mu, \nu) := \left( \inf_{\gamma \in \Gamma(\mu, \nu)} \int_{\mathbb{R}^n \times \mathbb{R}^n} |x - y|^p \, d\gamma(x, y) \right)^{1/p}$$

metrizes the weak topology on $\mathcal{P}(K)$, where

$$\Gamma(\mu, \nu) := \left\{ \gamma \in \mathcal{P}(\mathbb{R}^{2n}) \mid \mu[U] = \gamma[U \times \mathbb{R}^n], \quad \gamma[\mathbb{R}^n \times U] = \nu[U] \quad \forall U \subset \mathbb{R}^n \right\}$$

denotes the set of joint measures with given marginals.
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$$d_{\infty}(\mu, \nu) := \lim_{p \to \infty} d_p(\mu, \nu)$$

metrizes a much finer topology.

Tongseok Lim & Robert McCann (UToronto) Isodiametry, variance and pattern formation 6 July 2020 15 / 20
What distinguishes $b = 2$? (and for that matter $a = 2$)?

Introducing the mean

$$\bar{x}(\mu) := \int_{\mathbb{R}^n} xd\mu(x),$$

the quadratic contribution

$$\frac{1}{2} \int_{\mathbb{R}^n} \int_{\mathbb{R}^n} |x - y|^2 d\mu(x)d\mu(y) = -|\bar{x}(\mu)|^2 + \int_{\mathbb{R}^n} |x|^2 d\mu(x) =: \text{Var}(\mu)$$
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to the energy of $\mu$ becomes linear on the centered measures

$$
\mathcal{P}_0(\mathbb{R}^n) := \{\mu \in \mathcal{P}(\mathbb{R}^n) \mid d_2(\mu, \delta_0) < \infty, \quad \bar{x}(\mu) = 0\}
$$
Thus

\[- \min_{\mu \in P_0(\mathbb{R}^n)} E_{\infty,2}(\mu) = \max_{\text{diam spt } \mu \leq 1} \text{Var}(\mu)\]

- although the diameter constraint is non-convex (unless \( n = 1 \)), the variance maximizers can be found by solving an infinite-dimensional linear program for each compact set \( K \subset \mathbb{R}^n \) of unit diameter. As described in a companion work, they turn out to be precisely the measures from THM 1.
Variance maximization under diameter constraint

Thus

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• by comparison, the same measures minimize $E_{\infty,b}(\mu)$ for all $b > 2$.

• $\Gamma$-convergence: since $E_{a,b} \Gamma \rightarrow E_{\infty,b}$ on $(\mathcal{P}_0(\mathbb{R}^n), d_2)$, subsequences of minimizers $\mu_{a,b}$ converge weakly to minimizers $\mu_{\infty,b}$ of the limiting problem.
First and second variations

- this convergence can be strengthened using the Euler-Lagrange equation

\[ V_{a,b} \ast \mu_{a,b}(x) \geq 2E_{a,b}(\mu_{a,b}) \quad \text{with equality holding } \mu_{a,b}-\text{a.e.} \]
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• for large $a$, the mass of $\mu_{a,b}$ is thus localized to a union of small balls around the vertices of a regular simplex; a 2nd variation calculation (exploiting the uniform radial convexity of $V_{a,b}$ at its minimum and its lack of uniform concavity at the origin) then shows the energy is reduced by concentrating all of the mass in each ball at a single point.

The regular simplex is the only shape which succeeds in placing all $n + 1$ points at unit distance from each other, hence is energetically optimal.

The same 2nd variation calculation establishes THM 2; the $d_\infty$-closeness to a measure supported on a regular simplex replaces the $\Gamma$-convergence argument to provide the required localization in this case.
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Thank you