Extending the JKO scheme beyond gradient flows

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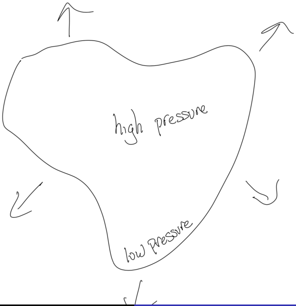
Tumor growth models

$$\begin{cases} \partial_t \rho - \nabla \cdot (\rho \nabla p) = \rho G(p), \\ p = e'(\rho) \end{cases} \tag{1}$$

- Models the growth of a tumor (or cell population) where the main limitation to growth is a competition for space.
- $p = e'(\rho)$ is the system pressure where e is a convex and increasing function.
- G is a decreasing function determining the growth rate.



Hele Shaw limit (Perthame, Quirós, Vázquez 2014)

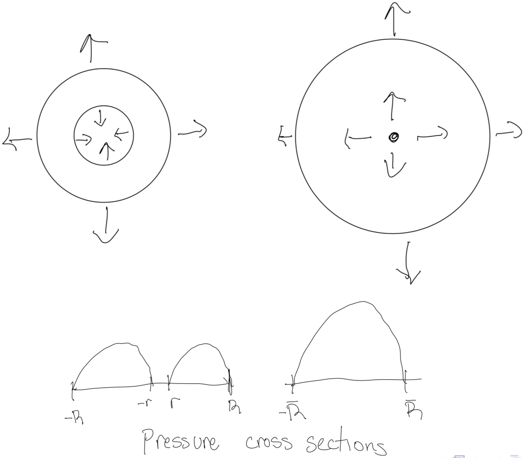
- A common choice for the pressure is $p = \rho^\gamma$ for some $\gamma > 0$.
- Sending $\gamma \to \infty$, the pressure becomes a Lagrange multiplier for the incompressibility constraint $\rho \leq 1$.

$$\begin{cases} \partial_t \rho - \nabla \cdot (\rho \nabla p) = \rho G(p), \\ p(1-\rho) = 0 \end{cases} \tag{2}$$

- This is a free boundary problem with a sharp interface between the occupied/empty regions i.e. $\rho \in \{0, 1\}$.

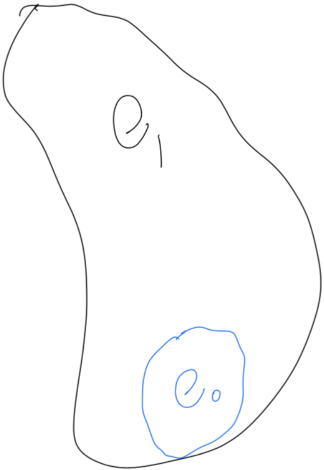
Challenges/Features

- The tumor may undergo topological changes as it grows.
- Pressure regularity can badly degenerate at topological changes.



Challenges/Features

- The equation satisfies a comparison principle.
- Not entirely obvious since smaller mass has a lower pressure and hence faster growth rate.



Goal

Can we design a numerical method to simulate this model that satisfies the following properties?

- Unconditionally stable.
- Preserves the comparison principle.
- Converges to the continuum PDE as the approximation vanishes.

Very tempting to use a JKO (like) scheme!

Recent previous works

$$\begin{cases} \partial_t \rho - \nabla \cdot (\rho \nabla p) = \rho G(p), \\ p = e'(\rho) \end{cases}$$

- View the equation as a gradient flow with respect to unnormalized/unbalanced optimal transport (Chizat, Di Marino 2018).
- Use a splitting scheme to separately handle the right and left hand sides of the equation (Gallouet, Laborde, Monsaingeon 2019).

Is it really not a gradient flow?

- Integrating the equation against the pressure gives the energy "dissipation" inequality:

$$\int_{\Omega} e(\rho(t,x))\,dx + \int_0^t \int_{\Omega} \rho(s,x)|\nabla p(s,x)|^2\,dx\,ds$$

$$\leq \int_{\Omega} e(\rho(0,x))\,dx + \int_0^t \int_{\Omega} p(s,x)\rho(s,x)G(p(s,x))\,dx\,ds$$

- The space-time integral on the second line should not show up in a $W2$ gradient flow.
- Energy is not necessarily being dissipated! We have to pay for adding mass to the system.

Modified JKO scheme (J., Kim, Tong 2021)

Given a time step $\tau > 0$ we iterate

$$\rho^{n+1} = \operatorname*{argmin}_{\rho} \min_{\alpha} \int_{\Omega} e(\rho) + \tau \int_{\Omega} \rho^n f(\alpha) + \frac{1}{2\tau} W_2^2(\rho, \rho^n(1 + \tau\alpha)) \tag{3}$$

- No issue that ρ^{n+1} and ρ^n have different mass since we are matching ρ^{n+1} to $\rho^n(1 + \tau\alpha^{n+1})$.
- f is a convex term (linked to G) encouraging mass change (can be taken to be spatially dependent).

Duality and c-transforms

- All of our analysis and numerics will be based on the dual rather than the primal problem.
- We will constantly use the following notation/results:

c-transform:

$$p^c(y) := \inf_x p(x) + \frac{|y-x|^2}{2\tau}.$$

conjugate c-transform:

$$q^{\bar{c}}(x) = \sup_y q(y) - \frac{|y-x|^2}{2\tau}.$$

Induced transport maps:

$$T_p(y) := \operatorname*{argmin}_x p(x) + \frac{|y-x|^2}{2\tau}, \quad \bar{T}_q(x) := \operatorname*{argmax}_y q(y) - \frac{|y-x|^2}{2\tau}.$$

c-transform variation:

$$\lim_{t\to 0^+} \frac{(p+tu)^c(y) - p^c(y)}{\tau} = u(T_p(y)).$$

Minimax formulation

Using Kantorovich duality

$$\frac{1}{2\tau} W_2^2(\rho, \rho^n(1+\tau\alpha)) = \int_\Omega p^c \rho^n (1+\tau\alpha) - p\rho$$

We transform the original primal problem

$$\min_{\alpha,\rho} \int_\Omega e(\rho) + \tau\rho^n f(\alpha) + \frac{1}{2\tau} W_2^2(\rho, \rho^n(1+\tau\alpha))$$

into the minimax problem

$$\min_{\rho,\alpha} \sup_p \int_\Omega p^c \rho^n (1+\tau\alpha) + e(\rho) - p\rho + \tau\rho^n f(\alpha)$$

Fixing p and minimizing over ρ we get

$$\min_{\alpha} \sup_p \int_\Omega p^c \rho^n (1+\tau\alpha) - e^*(p) + \tau\rho^n f(\alpha)$$

Determining the growth rate

If we fix p and minimize over α in the minimax problem

$$\min_{\alpha} \sup_{p} \int_{\Omega} p^c \rho^n (1 + \tau\alpha) - e^*(p) + \tau \rho^n f(\alpha)$$

the optimality condition for α requires

$$f'(\alpha) + p^c = 0 \quad \implies \quad \alpha = f^{*\prime}(-p^c).$$

- Choosing f such that $f^{*\prime}(-a) = G(a)$ allows us to obtain the desired growth rate.
- As long as G is decreasing there exists a convex function f with this property.

The dual problem

Plugging in the optimal choice for α, we obtain the maximization problem

$$\sup_p \int_\Omega \rho^n(p^c + \tau \bar{G}(p^c)) - e^*(p) \tag{4}$$

where $\bar{G}$ is an antiderivative of G.

In the case $e(\rho) = \frac{1}{\gamma+1}\rho^{\gamma+1}$ we get the dual problem

$$\sup_p \int_\Omega \rho^n(p^c + \tau \bar{G}(p^c)) - \frac{\gamma}{\gamma+1}\max(p^{1+\frac{1}{\gamma}}, 0)$$

The dual problem

- For any function p we have $p^{c\bar{c}} \leq p$ and $p^c = p^{c\bar{c}c}$.
- e^* is always an increasing function therefore

$$\sup_p \int_\Omega \rho^n(p^c + \tau \bar{G}(p^c)) - e^*(p)$$

$$\leq \sup_p \int_\Omega \rho^n(p^{c\bar{c}c} + \tau \bar{G}(p^{c\bar{c}c})) - e^*(p^{c\bar{c}})$$

- Any maximizer $\bar{p}$ of the dual problem must be a c-concave function i.e. $\bar{p}^{c\bar{c}} = \bar{p}$.
- If we let $q = p^c$ then we can write the dual problem in the following equivalent way

$$\sup_q \int_\Omega \rho^n(q + \tau \bar{G}(q)) - e^*(q^{\bar{c}})$$

Optimality for the dual problem

p_{n+1} is a solution to the dual problem if

$$T_{p_{n+1}\,\#}\Big(\rho^n(1+\tau G(p^c_{n+1})\big) = e^{*\prime}(p_{n+1})$$

If we choose

$$\bar\rho = T_{p_{n+1}\,\#}\Big(\rho^n(1+\tau G(p^c_{n+1})\big), \quad \bar\alpha = G(-p^c_{n+1})$$

then

$$J(p_{n+1}) = F(\bar\rho, \bar\alpha)$$

where F and J denote the values of the primal and dual problems respectively.

Relations and the approximate equation

Combining our work the primal and dual variables satisfy the equations

$$\begin{cases} T_{p_{n+1}\#}\Big(\rho^n(1+\tau G(p_{n+1}^c)) = \rho^{n+1}, \\ \rho^{n+1} = e^{*\prime}(p_{n+1}) \iff p_{n+1} = e'(\rho^{n+1}) \end{cases}$$

Rewriting

$$T_{p_{n+1}}^{-1}\rho^{n+1} = \rho^n(1+\tau G(p_{n+1}^c))$$

we see that given a smooth test function φ

$$\int_\Omega \frac{\rho^{n+1}-\rho^n}{\tau}\varphi = \int_\Omega \rho^{n+1}\frac{\varphi - \varphi\circ T_{p_{n+1}}^{-1}}{\tau} + \varphi\rho^n G(p_{n+1}^c)$$

Relations and the approximate equation

Since

$$T_{p_{n+1}}^{-1} = x + \tau \nabla p_{n+1},$$

We have

$$\int_\Omega \rho^{n+1} \frac{\varphi - \varphi \circ T_{p_{n+1}}^{-1}}{\tau} = \int_\Omega -\rho^{n+1} \nabla \varphi \cdot \nabla p_{n+1}$$

$$+ O\big(\tau \|D^2 \varphi\|_{L^\infty(\Omega)} \|\nabla p\|_{L^2(\Omega)}^2\big)$$

As long as we can control $\|\nabla p_{n+1}\|_{L^2(\Omega)}^2$ and prove the weak convergence of the nonlinear terms $e'(\rho^{n+1})$, $\rho^{n+1}\nabla p_{n+1}$ and $G(p_{n+1}^c)$ then the scheme converges to a weak solution of the tumor growth model.

Comparison principle

Theorem (J., Kim, Tong 2021)

Given two densities ρ_0, ρ_1 let

$$\bar{\rho}_i = \operatorname*{argmin}_{\rho} \int_\Omega e(\rho) + \tau \rho_i f(\alpha) + \frac{1}{2\tau} W_2^2(\rho, \rho_i(1+\tau\alpha)).$$

If $\rho_0 \leq \rho_1$ a.e., then $\bar{\rho}_0 \leq \bar{\rho}_1$ a.e.

To prove this we work with the dual problem. If we let

$$\bar{p}_i = \operatorname*{argmax}_{p} \int_\Omega \rho_i(p^c + \tau \bar{G}(p^c)) - e^*(p)$$

then it will be enough to show that $\bar{p}_0 \leq \bar{p}_1$ a.e.

Key lemma

Recall that

$$T_p(y) = \operatorname*{argmin}_x p(x) + \frac{|y-x|^2}{2\tau}$$

Lemma (J., Kim, Tong 2021)

Let p_0, p_1 be c-concave functions and let $U = \{x \in \Omega : p_0(x) > p_1(x)\}$. If $T_{p_0}(y) \in U$, then $T_{p_1}(y) \in U$ and $p_1^c(y) \leq p_0^c(y)$.

Remark: This doesn't use any property of the quadratic cost beyond existence of optimal maps.

Comparison principle

Let χ be the characteristic function of $U = \{x \in \Omega : \bar{p}_0(x) > \bar{p}_1(x)\}$. Optimality of the $\bar{p}_i$ implies that

$$\int_\Omega \chi e^{*\prime}(\bar{p}_i) = \int_\Omega \rho_i \big(1 + \tau G(\bar{p}_i^c)\big)\chi \circ T_{\bar{p}_i}$$

Therefore we have the chain of inequalities

$$\int_\Omega \chi e^{*\prime}(\bar{p}_0) \geq \int_\Omega \chi e^{*\prime}(\bar{p}_1) = \int_\Omega \rho_1 \big(1 + \tau G(\bar{p}_1^c)\big)\chi \circ T_{\bar{p}_1}$$

$$\geq \int_\Omega \rho_1 \big(1+\tau G(\bar{p}_0^c)\big)\chi\circ T_{\bar{p}_0} \geq \int_\Omega \rho_0 \big(1+\tau G(\bar{p}_0^c)\big)\chi\circ T_{\bar{p}_0} = \int_\Omega \chi e^{*\prime}(\bar{p}_0)$$

Numerics (Back-and-Forth Method J. Léger 2020, J. Léger, Lee 2021)

- Evolve the scheme by solving the dual problem using BFM.
- BFM performs alternating H^1 gradient ascent on the two equivalent dual problems:

$$J_n(p) = \int_\Omega \rho^n(p^c + \tau \bar{G}(p^c)) - e^*(p), \quad I_n(q) = \int_\Omega \rho^n(q + \tau \bar{G}(q)) - e^*(q^{\bar{c}})$$

- Once we have recovered the optimal pressure p_{n+1} we can recover the optimal density ρ^{n+1} through either of the relations

$$\rho^{n+1} = e^{*\prime}(p_{n+1}), \quad \rho^{n+1} = T_{p_{n+1}\#}\Big(\rho^n(1 + \tau G(p^c_{n+1}))\Big).$$

BFM

Given an initial pressure p^0 and step size σ we iterate

$$p^{k+1/2} = p^k + \sigma \nabla_{H_1} J_n(p^k),$$

$$q^{k+1/2} = (p^{k+1/2})^c,$$

$$q^{k+1} = q^{k+1/2} + \sigma \nabla_{H_1} I_n(q^{k+1/2}),$$

$$p^{k+1} = (q^{k+1})^{\bar{c}}.$$

- H^1 gradient is equivalent to preconditioning the standard L^2 gradient by $(I - \Delta)^{-1}$

$$\nabla_{H_1} J_n(p) = (I - \Delta)^{-1}\Big(T_{p\#}\rho^n\big(1 + \tau G(p^c)\big) - e^{*\prime}(p)\Big)$$

$$\nabla_{H_1} I_n(q) = (I - \Delta)^{-1}\Big(\rho^n\big(1 + \tau G(q)\big) - \bar{T}_{q\#}e^{*\prime}(q^{\bar{c}})\Big)$$

BFM

- H^1 is the weakest inner product where I and J have a hope of being L-smooth for some $L < \infty$ (c-transform is not stable in weaker norms).
- Functions like $\max(p, 0)$ that are not L^2 smooth are H^1 smooth as long as $\partial\{p > 0\}$ is nondegenerate (trace inequality!)
- Alternating between I and J is beneficial because their Hessians are almost inverses of one another.
- On a grid with N points the $c/\bar{c}$-transforms as well as the induced maps T_p and $\bar{T}_q$ can be computed in $O(N)$ time.

Simulations