Augmented Lagrangian methods for gradient flows

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Plan

1. JKO scheme and PDEs
2. Augmented Lagrangian method
3. Porous medium equation
4. Interactions in the potential energy
5. Interactions in the internal energy

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JKO scheme ([Jordan, Kinderlehrer and Otto,1998])

- We define $(\rho_h^k)_{k\in\mathbb{N}}$ by induction such that $\rho_h^0 = \rho_0$ and for all $k \in \mathbb{N}$,

$$\rho_h^{k+1} \in \underset{\rho\in\mathcal{P}(\Omega)}{\operatorname{argmin}} W_2^2(\rho, \rho_h^k) + 2h\mathcal{F}(\rho), \tag{1}$$

and

$$\rho_h(t,\cdot) := \rho_h^k \qquad \text{if } t \in ((k-1)h, kh].$$

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- Under some asumptions on $\mathcal{F}$, $\rho_h \to \rho \in \mathcal{C}^{0,1/2}([0,T],\mathcal{P}(\Omega))$ and ρ is a weak solution, at least formally, of

$$\partial_t \rho + \text{div}(\rho\nabla\frac{\delta\mathcal{F}}{\delta\rho}) = 0, \qquad \rho_{|t=0} = \rho_0.$$

where $\frac{\delta\mathcal{F}}{\delta\rho}$ is the first variation of $\mathcal{F}$.

Examples

- If $\mathcal{F}(\rho) := \begin{cases} \int_\Omega \frac{1}{m-1}\rho^m & \text{if } \rho \ll \mathcal{L}, \\ +\infty & \text{otherwise,} \end{cases}$ for $m > 1$, then ρ solves

$$\partial_t \rho = \frac{m}{m-1} \operatorname{div}(\rho \nabla \rho^{m-1}) = \Delta \rho^m.$$

- If $\mathcal{V}(\rho) := \int_\Omega V(x)\, d\rho(x)$ then ρ solves

$$\partial_t \rho = \operatorname{div}(\rho \nabla V).$$

- If $\mathcal{W}(\rho) := \frac{1}{2} \int_{\Omega\times\Omega} W(x-y)\, d\rho(x) d\rho(y)$ then ρ solves

$$\partial_t \rho = \operatorname{div}(\rho \nabla W * \rho).$$

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Benamou-Brenier formulation

- The Benamou-Brenier formula,

$$W_2^2(\rho,\nu) = \inf_{\mu_t, m_t} \int_0^1 \int_\Omega \frac{|m_t|^2}{\mu_t}\, dxdt,$$

subject to constraints that $\mu \geqslant 0$, $m = 0$ when $\mu = 0$ and

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- As was observed in [Benamou,Brenier],

$$\Psi(\mu, m) = \begin{cases} \frac{|m|^2}{\mu} & \text{if } \mu \geqslant 0, \\ 0 & \text{if } \mu = 0, m = 0, \\ +\infty & \text{otherwise,} \end{cases}$$

is a convex, lsc, 1-homogenous function and can be rewrite as

$$\Psi(\mu, m) = \sup\left\{a\mu + b\cdot m \,:\, (a,b) \in K\right\},$$

where $K := \left\{(a,b) \in \mathbb{R}\times\mathbb{R}^n \,:\, a + \frac{1}{2}|b|^2 \leqslant 0\right\}$.

JKO scheme

- Let us consider one step of JKO where $\mathcal{F}$ is energy of the form

$$\mathcal{F}(\rho) = \int_\Omega F(\rho(x))\, dx + \int_\Omega V(x)\rho(x)\, dx.$$

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$$\mathcal{F}(\rho) = \int_\Omega F(\rho(x))\,dx + \int_\Omega V(x)\rho(x)\,dx.$$

- Using the Benamou-Brenier formula, one step of JKO scheme can be rewrite as a convex minimization problem:

$$\inf_{\mu_t, m_t} \int_0^1 \int_\Omega \Psi(\mu_t, m_t)\,dxdt + 2h\mathcal{F}(\mu_1),$$

subject to constraints that

$$\partial_t \mu + \mathrm{div}(m) = 0,\ \mu_{|t=0} = \rho_h^k.$$

dual problem

- Then the dual formulation

$$\inf_{\Phi(t,x)} \left\{ \int_\Omega \Phi(0,x)\rho_h^k + \mathcal{F}^*(-\Phi(1,.)) \,:\, (\partial_t \Phi, \nabla \Phi) \in K \right\},$$

where

$$\mathcal{F}^*(c) := \sup_{\mu \geqslant 0} \left\{ \int_\Omega ((c(x) - hV(x))\mu(x) - hF(\mu(x)))\, dx \right\}.$$

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- Another formulation is

$$\inf_{\phi,q} \left\{ F(\Phi) + G(q) \, : \, \Lambda\Phi = q \right\},$$

where $\Lambda\Phi = (\partial_t\Phi, \nabla\Phi, -\Phi(1,\cdot))$, $q = (a,b,c) \in \mathbb{R} \times \mathbb{R}^n \times \mathbb{R}$ and

$$F(\Phi) := \int_\Omega \Phi(0,\cdot)\rho_h^k, \; G(q) := \int_0^1 \chi_K(a,b)dxdt + h\mathcal{F}^*\left(\frac{c}{h}\right).$$

Relaxation problem and augmented Lagrangian method

- Then when we relax the problem, the JKO scheme is equivalent to find a saddle-point of the Lagrangian

$$L(\Phi, q, \sigma) := F(\Phi) + G(q) + \sigma \cdot (\Lambda\Phi - q),$$

where $\sigma := (\mu, m, \mu_1)$, $q := (a, b, c) \in \mathbb{R} \times \mathbb{R}^n \times \mathbb{R}$,
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$\Lambda\Phi := (\partial_t \Phi, \nabla\Phi, -\Phi(1, \cdot))$,

- Now for $r > 0$, we consider the augmented Lagrangian function

$$L_r(\Phi, q, \sigma) := F(\Phi) + G(q) + \sigma \cdot (\Lambda\Phi - q) + \frac{r}{2}|\Lambda\Phi - q|^2.$$

We note that being a saddle-point of L is equivalent to being a saddle-point of L_r.

Augmented Lagrangian algorithm ALG2 splitting scheme (1)

This algorithm consists, starting from (Φ^0, q^0, σ^0), to generate inductively a sequence as follows:

- **Step 1:** minimization w.r.t Φ:

$$\Phi^{n+1} := argmin\left\{F(\Phi) + \sigma^n \cdot \Lambda\Phi + \frac{r}{2}|\Lambda\Phi - q^n|^2\right\},$$

- **Step 2:** minimization w.r.t q:

$$q^{n+1} := argmin\left\{G(q) - \sigma^n \cdot q + \frac{r}{2}|\Lambda\Phi^{n+1} - q|^2\right\},$$

- **Step 3:** update the multiplier by the gradient ascent formula

$$\sigma^{n+1} = \sigma^n + r(\Lambda\Phi^{n+1} - q^{n+1}).$$

Augmented Lagrangian algorithm ALG2 splitting scheme (2)

- Step 1 corresponds to solve an elliptic problem

$$-\Delta_{t,x}\Phi^{n+1} = \mathrm{div}_{t,x}((\mu^n, m^n) - r(a^n, b^n)), \text{ in } (0,1)\times\Omega,$$

with the boundary conditions

$$\begin{aligned} r\partial_t\Phi^{n+1}(0,\cdot) &= \rho_h^k - \mu^n(0,\cdot) + ra^n(0,\cdot), \\ r(\partial_t\Phi^{n+1}(1,\cdot) + \Phi^{n+1}(1,\cdot)) &= \mu_1^n - \mu^n(1,\cdot) + r(a^n(1,\cdot) - c^n(\cdot)), \\ (r\nabla\Phi^{n+1} + m^n - rb^n)\cdot\nu &= 0, \text{ on } \partial\Omega. \end{aligned}$$

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- Step 2 splits into two convex pointwise problems

$$(a^{n+1}(t,x), b^{n+1}(t,x)) = P_K\left(D_{t,x}\phi^{n+1}(t,x) + \frac{1}{r}(\mu^n(t,x), m^n(t,x))\right),$$

and

$$c^{n+1}(x) = argmin_{c\in\mathbb{R}}\left\{\frac{r}{2}|\Phi^{n+1}(1,x) - \frac{1}{r}\mu^n(1,x) + c|^2 + h\mathcal{F}^*\left(\frac{c}{h}\right)\right\}.$$

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Porous media equation

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Porous media equation

- We want to solve, for $m > 1$,

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- In this case

$$\mathcal{F}^*(c) = \frac{1}{rh^{\frac{1}{m-1}}} \left(\frac{m}{m-1} \right)^{\frac{m-1}{m}} \int_\Omega \left((c(x) - hV(x))_+ \right)^{\frac{m-1}{m}} \, dx.$$

Then

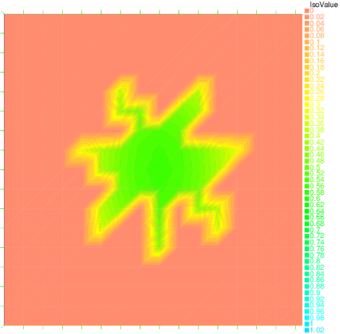
$$c^{n+1}(x) = \begin{cases} \frac{1}{r}\mu^n(1,x) - \Phi^{n+1}(1,x) & \text{if } \overline{c} \leqslant hV(x), \\ \text{the root in } (hV(x), +\infty) \text{ of } (2) & \text{otherwise,} \end{cases}$$

where (2) is the equation

$$c - \overline{c} + \frac{1}{rh^{\frac{1}{m-1}}} \left(\frac{m-1}{m} \right)^{\frac{1}{m-1}} (c - hV(x))^{\frac{1}{m-1}} = 0 \qquad (2)$$

Simulation

$$m = 3, \qquad V(x) = \frac{|x|^2}{2}.$$



The algorithm converges to the Barenblatt profile

$$\rho_\infty = \frac{m-1}{2m}(1-|x|^2)_+^{1/(m-1)}.$$

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System with nonlocal interactions

- We consider I species solving, for all $i \in \{1, \dots, I\}$,

$$\begin{cases} \partial_t \rho_i = \alpha_i \Delta \rho_i + \mathrm{div}(\rho_i \nabla V_i[\boldsymbol{\rho}]) \\ \rho_{i|t=0} = \rho_{i,0}, \end{cases}$$

  with no-flux boundary condition, and where $\boldsymbol{\rho} := (\rho_1, \dots, \rho_I)$.

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  with no-flux boundary condition, and where $\boldsymbol{\rho} := (\rho_1, \ldots, \rho_I)$.
- The proof of existence is based on a semi-implicit JKO scheme (defined by [DiFrancesco and Fagioli]): we construct by induction $(\rho_{i,h}^k)$ such that

$$\rho_{i,h}^{k+1} \in \mathrm{argmin}\, W_2^2(\rho, \rho_{i,h}^k) + 2h \left(\alpha_i \int_\Omega \rho \log \rho + \int_\Omega V_i[\boldsymbol{\rho}_h^k] \rho \right).$$

Proximal

- We note $Prox_{\mathcal{F}}(\overline{c})$ the solution of

$$\inf_{c\in\mathbb{R}} \left\{ \frac{r}{2}|c-\overline{c}|^2 + \mathcal{F}(c) \right\}.$$

Moreover, $Prox_{\mathcal{F}^*}(\overline{c}) = \overline{c} - Prox_{\mathcal{F}}(\overline{c})$.

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  Moreover, $Prox_{\mathcal{F}^*}(\overline{c}) = \overline{c} - Prox_{\mathcal{F}}(\overline{c})$.
- Then $c_i^{n+1}(x) = \overline{c}_i - \tilde{c}_i$, where

$$\overline{c}_i = \frac{1}{r} \mu_i^n(1, x) - \Phi_i^{n+1}(1, x),$$

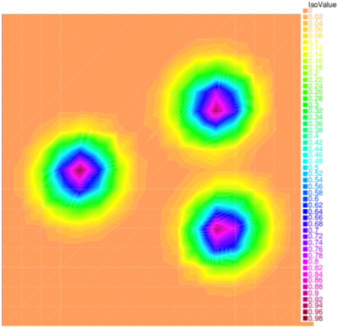
  and $\tilde{c}_i$ is the root of

$$\tilde{c}_i - \overline{c}_i + h V_i[\boldsymbol{\rho}_h^k] + h \log(\tilde{c}_i) = 0.$$

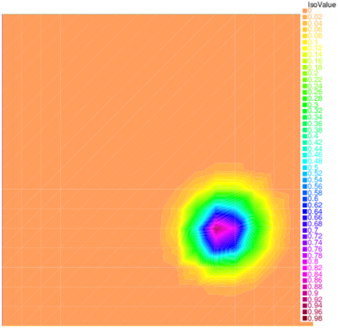
Simulations for 3 species

$$V_1[\rho_1, \rho_2, \rho_3] = |x|^2 * \rho_2 - |x|^2 * \rho_3, \; V_2[\rho_1, \rho_2, \rho_3] = |x|^2 * \rho_3 - |x|^2 * \rho_1,$$

and $V_3[\rho_1, \rho_2, \rho_3] = |x|^2 * \rho_1 - |x|^2 * \rho_2$.



$\rho_1 + \rho_2 + \rho_3$



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Crowd motion

- We consider two species solving

$$\begin{cases} \partial_t \rho_1 - \Delta \rho_1 - \mathrm{div}(\rho_1(\nabla V_1 + \nabla p)) = 0 \\ \partial_t \rho_2 - \Delta \rho_2 - \mathrm{div}(\rho_2(\nabla V_2 + \nabla p)) = 0 \\ p \geqslant 0,\ \rho_1 + \rho_2 \leqslant 1,\ p(1 - \rho_1 - \rho_2) = 0, \\ \rho_{1|t=0} = \rho_{1,0}, \qquad \rho_{2|t=0} = \rho_{2,0} \end{cases}$$

with no-flux boundary conditions (see for one density [Mészá ros,Santambrogio] and [Maury, Roudneff-Chupin, Santambrogio] without diffusion).

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- Gradient flow structure with

$$\mathcal{F}(\rho_1, \rho_2) := \sum_{i=1}^{2} \int_\Omega (\rho_i \log \rho_i + V_i \rho_i) + \chi_{[0,1]}(\rho_1 + \rho_2).$$

Proximal

Using, the formualtion $Prox_{\mathcal{F}^*}(\overline{c}) = \overline{c} - Prox_{\mathcal{F}}(\overline{c})$ we compute

$$\tilde{c}_i := \operatorname{argmin} \frac{1}{2}|c - \overline{c}_i|^2 + c(hV_i + h\log(c)).$$

- If $\tilde{c}_1 + \tilde{c}_2 \leqslant 1$, then

$$c_i^{n+1}(x) = \overline{c}_i - \tilde{c}_i,$$

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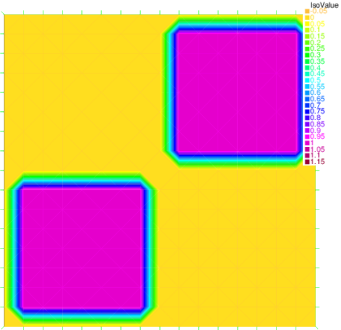
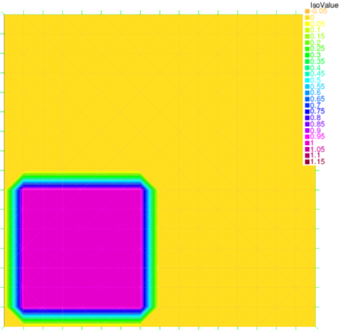
- If $\tilde{c}_1 + \tilde{c}_2 \leqslant 1$, then
$$c_i^{n+1}(x) = \overline{c}_i - \tilde{c}_i,$$
- Otherwise, the constraint is saturated then we write $\tilde{c}_1 = u$ and $\tilde{c}_2 = 1 - u$ where u minimizes
$$\frac{1}{2}\left(|u - \overline{c}_1|^2 + |1 - u - \overline{c}_2|^2\right) + h\left(u(\log(u) + V_1) + (1-u)(\log(1-u) + V_2)\right).$$
And
$$c_1^{n+1}(x) = \overline{c}_1 - u, \qquad c_2^{n+1}(x) = \overline{c}_2 - 1 + u.$$

Simulation



$\rho_1 + \rho_2$



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Thank you for your attention

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