PDE solver using optimal transport

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1 Introduction

The back-and-forth method (BFM) is presented as a new solution for partial differential equations[2]. The back-and-forth method (BFM) was originally developed as a solution for the optimal transport problem. However, by extending its application to PDEs through the utilization of optimal transport, BFM becomes a powerful tool for solving PDEs. This solution method is particularly effective for non-linear partial differential equations and is faster than previous methods and does not require stability conditions, allowing a wider range of problems to be solved. This study compares the BFM-based solver with other solvers for the $m = 2$ porous medium equation and shows that under certain conditions, the BFM solver can solve the non-linear porous media equation more efficiently.

2 Background

In this paper, we assume that Ω is a convex and compact subset of $\mathbb{R}^n$. We denote the set of probability measures on Ω, which are non-negative measures with mass 1, as $\mathcal{P}(\Omega)$. Additionally, we represent the space of continuous functions on Ω as $C(\Omega)$. For simplicity, we consider non-negative $L^1(\mathbb{R}^n)$ functions with an integral equal to 1.

The Porous Medium Equation (PME) is expressed as

$$\frac{\partial \rho}{\partial t} = \gamma \Delta(\rho^m)$$

for a fixed $m > 1$. This partial differential equation can be expressed as a Wasserstein gradient flow based on the energy function

$$U(\rho) = \frac{\gamma}{m-1} \int_\Omega \rho^m \, dx.$$

This allows the JKO scheme to find approximate solutions to the porous medium equation by discretizing time using a time step size τ and performing the following iterations based on the variational principle.

$$\rho^{(n+1)} := \underset{\rho}{\operatorname{argmin}}\, U(\rho) + \frac{1}{2\tau} W_2^2(\rho, \rho^{(n)})$$

Here, Kantorovich's dual formula for the 2-Wasserstein distance is expressed as

$$\frac{1}{2\tau} W_2^2(\rho, \mu) = \sup_{(\varphi,\psi)\in C} \left(\int_\Omega \varphi \, d\rho + \int_\Omega \psi \, d\mu \right)$$

where $\mathcal{C}$ is defined by $\mathcal{C} = \{(\varphi, \psi) \in C(\Omega)\times C(\Omega) \mid \varphi(x)+\psi(y) \le \frac{1}{2\tau}|x-y|^2\}$ and τ represents the time step within the scheme. Therefore, the above minimization problem is represented as follows:

$$\min_{\rho\in P} \left(U(\rho) + \frac{1}{2\tau} W_2^2(\rho, \mu) \right) = \sup_{(\varphi,\psi)\in C} \left(\int_\Omega \psi \, d\mu - U^*(-\varphi) \right)$$

Here, $U^*(-\varphi) = \sup_{\rho\in P} \int_\Omega \left(-\frac{\gamma}{m-1}\rho^m + \rho\varphi \right) dx$ is the Legendre-Fenchel transform of U with respect to $-\varphi$.

Furthermore, by using the c-transform defined by $\psi^c(x) = \inf_{y\in\Omega} \left(\frac{1}{2\tau}|x-y|^2 - \psi(y) \right)$, the minimization problem has the following duality:

$$\begin{aligned}
&\min_{\rho\in P} \left(U(\rho) + \frac{1}{2\tau} W_2^2(\rho, \mu) \right) \\
&= \sup \left(\int_\Omega \varphi^c \, d\mu - U^*(-\varphi) \right) =: \sup J \\
&= \sup \left(\int_\Omega \psi \, d\mu - U^*(-\psi^c) \right) =: \sup I
\end{aligned}$$

Also, the solution to the generalized optimal transport problem ρ_* has the following properties:

$$\rho_*(x) = \delta U^*(-\varphi_*),\ \varphi_* \in U(\rho_*),\ \rho_*(x) = T_{\varphi\#}\mu$$

where $T_{\varphi\#}\mu$ is the pushforward measure with T being the map transporting from μ to ρ ($T_{\varphi\#}\mu = \rho$).

3 The back-and-forth method and JKO scheme

BFM is an algorithm that iteratively performs gradient ascent updates in the φ space for the functional $J(\varphi)$ and in the ψ-space for the functional $I(\psi)$. Also, by swapping φ and ψ using the c-transform, it is possible to go back and forth between J and I and find the solution φ_* of the BFM while maintaining symmetry. The algorithm is based on the following ideas:

1. Back-and-forth Scheme: Iteratively alternate between gradient ascent steps in J and I.
2. For the H^1-type norm H in Sobolev space, the gradient ascent steps are given by:
$$\nabla_H J(\varphi) = (\Theta_1 \mathrm{Id} - \Theta_2\Delta)^{-1} \left[\delta U^*(-\varphi) - T_{\varphi\#}\mu\right],$$
$$\nabla_H I(\psi) = (\Theta_1 \mathrm{Id} - \Theta_2\Delta)^{-1} \left[\mu - T_{\psi\#}(\delta U^*(\psi^c))\right].$$
The appropriate choices for Θ_1 and Θ_2 can be found in [2].

Furthermore, utilizing the obtained solution φ_* from BFM, the minimization problem for ρ_* is solved using $\rho_*(x) = \delta U^*(-\varphi)$.

Algorithm 1 The back-and-forth scheme for solving $J(\varphi)$ and $I(\psi)$

Input: μ and φ_0, iterate:

$$\begin{aligned}
\varphi_{k+\frac{1}{2}} &= \varphi_k + \nabla_H J(\varphi_k) \\
\psi_{k+\frac{1}{2}} &= (\varphi_{k+\frac{1}{2}})^c \\
\psi_{k+1} &= \psi_{k+\frac{1}{2}} + \nabla_H I(\psi_{k+\frac{1}{2}}) \\
\varphi_{k+1} &= (\psi_{k+1})^c
\end{aligned}$$

return φ_*

4 Experiments and Results

The porous medium equation (m=2) is solved using two different methods: The BBR scheme proposed by Berger, Brezis, Rogers [1], and the back-and-forth method explained in this paper. The speed and error of the two computational methods are compared with the exact solution, the Barenblatt solution, given by:

$$\rho(t,x) = \max\left(\frac{1}{t^{\frac{1}{3}}}\left(\left(\frac{\sqrt{3}}{16}\right)^{\frac{2}{3}} - \frac{1}{12}\frac{|x|^2}{t^{\frac{2}{3}}}\right), 0\right)$$

Verify under the conditions of a grid size of 512 and $\varepsilon = 10^{-3}$. Graphs for multiple time step sizes τ at times $t = t_0, t_0 + 0.4, t_0 + 0.8, t_0 + 2.0$ are shown in Figures 1 and 2.

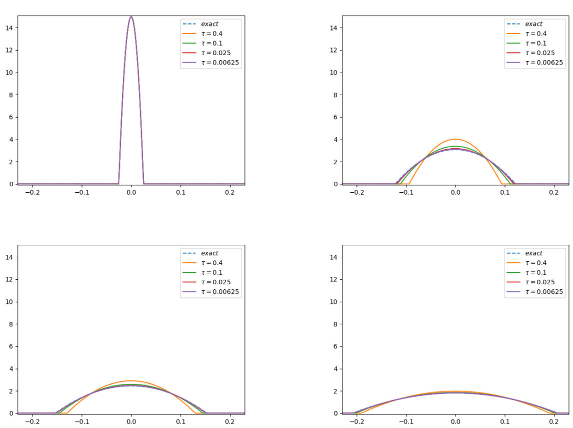

Figure 1: Comparison between the back-and-forth method and the barenblatt solution at times $t = 0, 0.4, 0.8, 2.0$.

5 Conclusion

The main objective of this paper was to explore solutions to nonlinear porous gradient equations, particularly employing the back-and-forth method as a numerical approach for nonlinear partial differential equations.

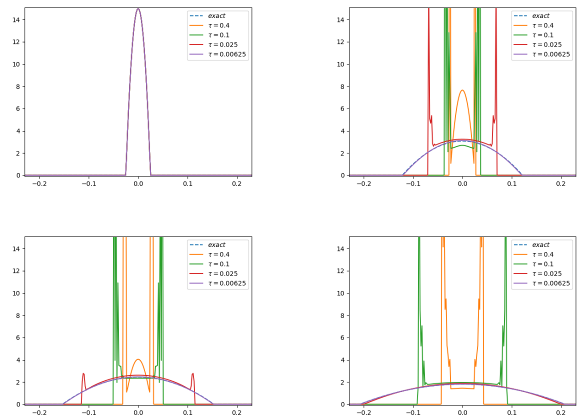

Figure 2: Comparison between the BBR scheme and the barenblatt solution at times $t = 0, 0.4, 0.8, 2.0$.

I also compared the results with other solution methods. The back-and-forth method demonstrated the ability to approximate the solution with minimal errors even for large time step sizes compared to other methods. This is attributed to the reconstruction of ρ through $\rho_*(x) = \delta U^*(-\varphi)$, avoiding shocks at the discontinuous at the boundary of ρ, and the capability to compute without constraints by solving the dual problem.

However, it is essential to choose appropriate time steps, τ, and conditions to exit the iterations of the back-and-forth method, such as $\|\delta U^*(-\varphi) - T_{\varphi\#}\mu\|_{L^1(\Omega)} < \varepsilon$, in alignment with the grid size.

On the other hand, the BBR scheme, as observed in Figure 2, there are discontinuities at the boundary of the support ($\operatorname{supp}\rho = \{x \in \Omega \,|\, \rho(x) > 0\}$) of the evolving function ρ, leading to constraints. Therefore, without choosing an small size for the time step τ, the presence of abrupt changes in the gradient $\nabla\rho$ can result in shocks at the boundary.

Therefore, as long as τ is not chosen too small, the back-and-forth method can accurately simulate the solution compared to other methods.

For future prospects, increasing the value of m in the porous medium gradient equation and exploring scenarios in two or three dimensions are potential directions to consider.

References

[1] Alan E. Berger, Haim Brezis, and Joël C. W. Rogers. A numerical method for solving the problem $u_t - \delta f(u) = 0$. *RAIRO. Analyse numérique*, 13(4):297–312, 1979.

[2] Matt Jacobs, Wonjun Lee, and Flavien Léger. The back-and-forth method for Wasserstein gradient flows. *ESAIM Control Optim. Calc. Var.*, 27:Paper No. 28, 35, 2021.