Report 23/04/2020

Quick observation: When relaxing the tolerances, we need to check the exact solutions. For example in FixPt, when we set the ODE tolerance to 10^{-7}, the consistency error in w is larger than 10^{-4}, so we need to adapt that. This is less of an issue in the way that Multiple Shooting consistency errors are calculated because they are added and not multiplied.

Generally we will have $n = 61$, $N = 60$, ODE Tols $= 10^{-8}$, Consistency Tols $= 10^{-4}$, $\lambda = 0.01$, solver FixPt and $\gamma = 1$ repulsive, $\gamma = -1$ attractive.

1 Interacting Problems - static target 1

The considered problem is the following:

$$\partial_t \rho = D_0 \Delta \rho - \nabla \cdot (\rho w) + \gamma \nabla \cdot \int_\Omega \rho \rho' \nabla V_2 dr,$$

with $w = 0$ in the forward case, but flow control in the optimization problem. There is no force term involved and mass is conserved. The initial condition for ρ is:

$$\rho_{IC} = 0.5,$$

such that $\int_{-1}^{1} \rho_{IC} = 1$. The first choice of $\hat{\rho}$ is:

$$\hat{\rho} = \frac{1}{4}\cos(\pi y + \pi) + \frac{1}{2}$$
$$\int_{-1}^{1} \frac{1}{4}\cos(\pi y + \pi) + \frac{1}{2} dy = 1,$$

see Figure 1.
Using 'FixPt' and looking at $\beta = 10^{-1}$ we get the following results: First consider $\gamma = 1$. Then the forward and optimal solutions can be seen in Figure 2. The optimal control can also be seen in Figure 2. $J_{FW} = 0.0193$ and $J_{Opt} = 0.0164$.
For $\gamma = -1$, the situation is a little different, see Figure 3. When $\gamma = 1$, the interaction is driving towards the desired state, when $\gamma = -1$, it is driving away from it. $J_{FW} = 0.0488$ and $J_{Opt} = 0.0392$.
When setting $\beta = 10$ for both $\gamma = 1$ and $\gamma = -1$, the algorithm solves the problem in 300 to 400 iterations ($\beta = 10^{-1}$ needs 700 to 800 iterations). Then J is more or less the same in the forward and optimal case, as expected.
The case $\beta = 10^{-3}$ is a bit more tricky. Both for $\gamma = 1$ and $\gamma = -1$, the algorithm diverges.
Choose $\gamma = 0.5$ and $\beta = 10^{-3}$, then it diverges at 0.00061179, however, while $J_{FW} = 0.0247$, $J_{Opt} = 0.0019$, so the overall cost is already lowered, see Figure 4. Choosing $\gamma = -0.5$, the

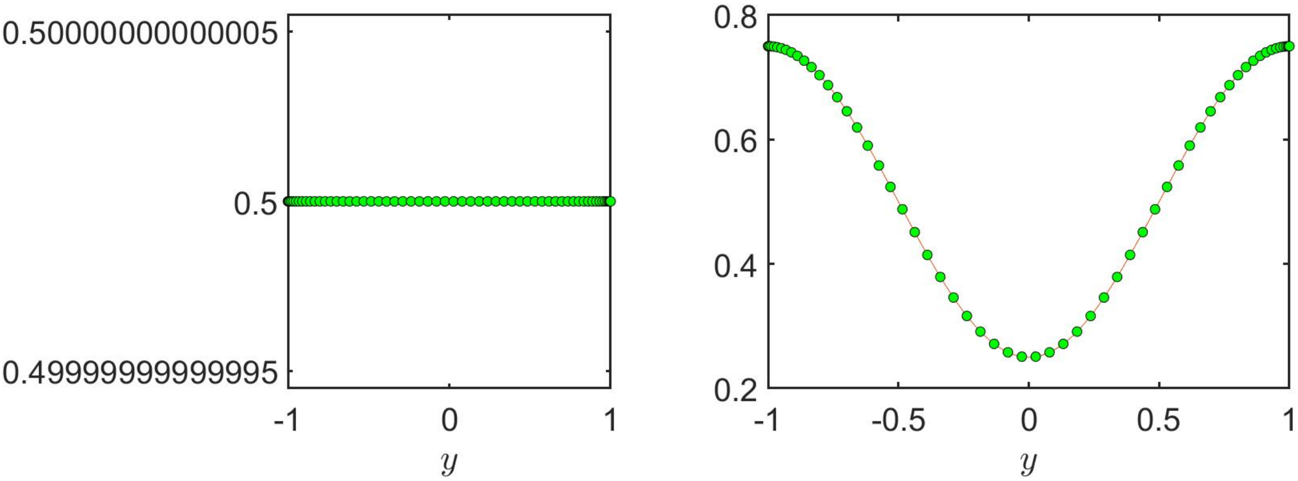

Figure 1: First Choice of ρ_{IC} and $\hat{\rho}$.

algorithm diverges at 0.00055109, however, the solution is already improved, $J_{FW} = 0.0329$, $J_{Opt} = 0.0023$, see Figure 5. The two figures (4 and 5) look very similar.
My theory is that for small β, the advection term is allowed to get very large, which causes problems for the solution of the equation. Looking at Figures 5 and 4 seem to confirm this: While ρ is around 0.5, w is around 10.

1.1 Diffusion vs advection term

If we change the diffusion coefficient in this problem, we can see whether this theory is true. Changing D_0 to 2, for $\gamma = -0.5$, shows that it now diverges at 0.00011836. This is a bit later than before. When we choose $D_0 = 3$, the problem converges, with $J_{FW} = 0.0339$, $J_{Opt} = 0.0096$ within 787 iterations, see Figure 6.
The same thing works for $\gamma = 0.5$, $J_{FW} = 0.0287$ and $J_{Opt} = 0.0085$, see Figure 7. In fact $\gamma = -1$ converges with $D_0 = 2$, but $\gamma = 1$ diverges with $D_0 = 2$, but converges with $D_0 = 5$. I conclude that the issue of convergence has to do with the strength of the advection term in comparison to the other terms in the equation.

2 Interacting Problems - static target 2

Investigating a similar problem but this time the target is:

$$\hat{\rho} = \frac{1}{4}\cos(\pi y) + \frac{1}{2}$$
$$\int_{-1}^{1} \frac{1}{4}\cos(\pi y) + \frac{1}{2} dy = 1,$$

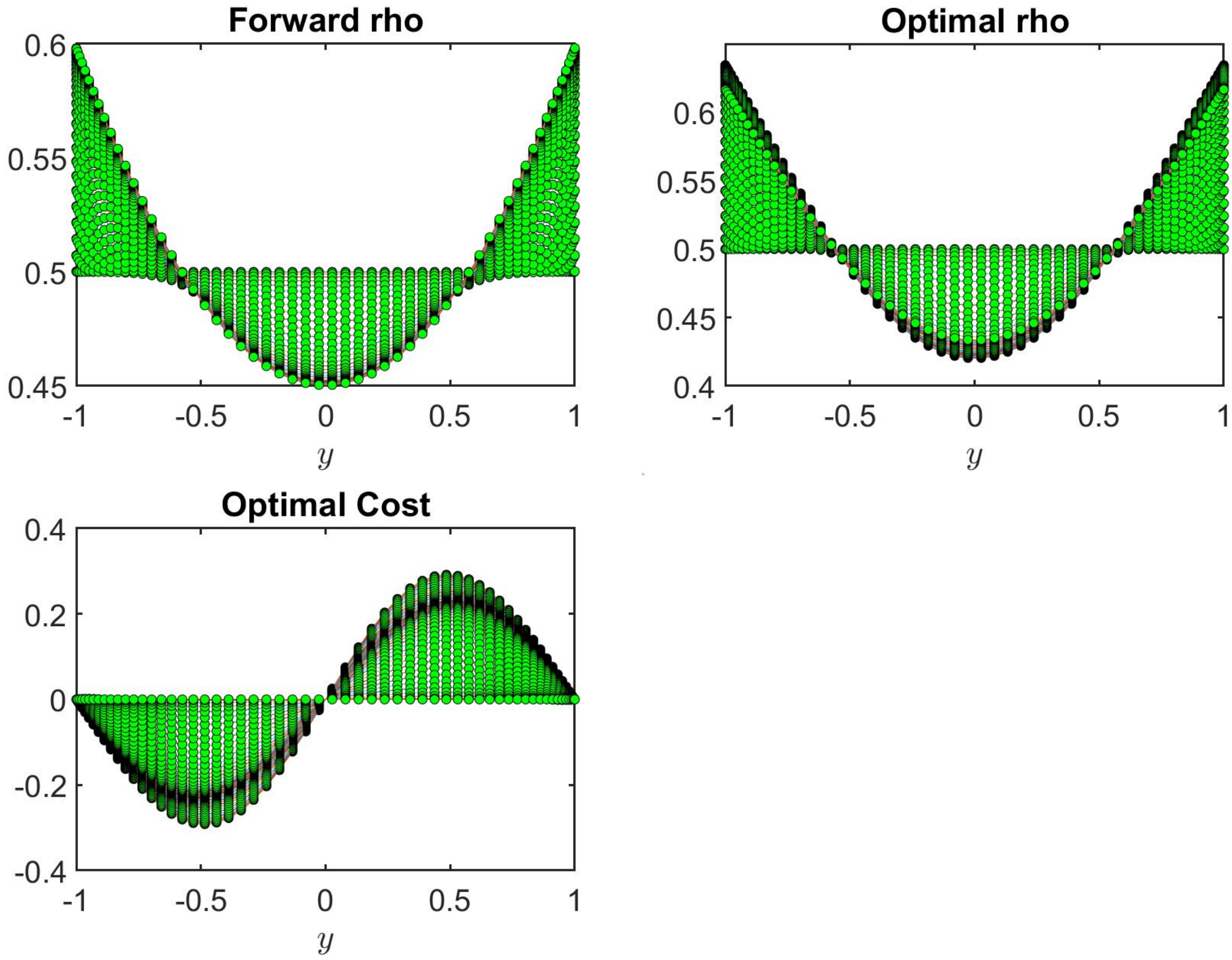

Figure 2: Solutions ρ_{FW} and ρ_{Opt} and Optimal control w, $\gamma = 1$, $\beta = 10^{-1}$.

so that the particles are supposed to go to the middle, see Figure 8.
Starting with $\beta = 10^{-1}$ and $\gamma = -1$, we have $J_{FW} = 0.0179$ and $J_{Opt} = 0.0146$, see Figure 9. As expected, in comparison to the other example, w is pushing the solution inwards (while in the above example, it pushed the particles outwards).With $\gamma = 1$, $J_{FW} = 0.0466$ and $J_{Opt} = 0.032$, see Figure 10. We can observe that the order of magnitude of w is around the same for both γ (restricted by J/ β?), but the results aren't as close to $\hat{\rho}$, since the interactions are working against the target (interactions repulsive).
Checking $\beta = 10^{-3}$ next, expecting a similar result as above. As expected, the case with $\gamma = -1$ diverges at 0.00051689. $J_{FW} = 0.0179$ and $J_{Opt} = 0.0013$, see Figure 11. Choosing $\gamma = 1$ surprisingly converges in 778 iterations. $J_{FW} = 0.0466$, $J_{Opt} = 0.0031$, see Figure 12. It is especially surprising given that the particle interactions are repulsive, while the target is in the middle of the domain. A theory could be that the particle interaction is in the 'opposite

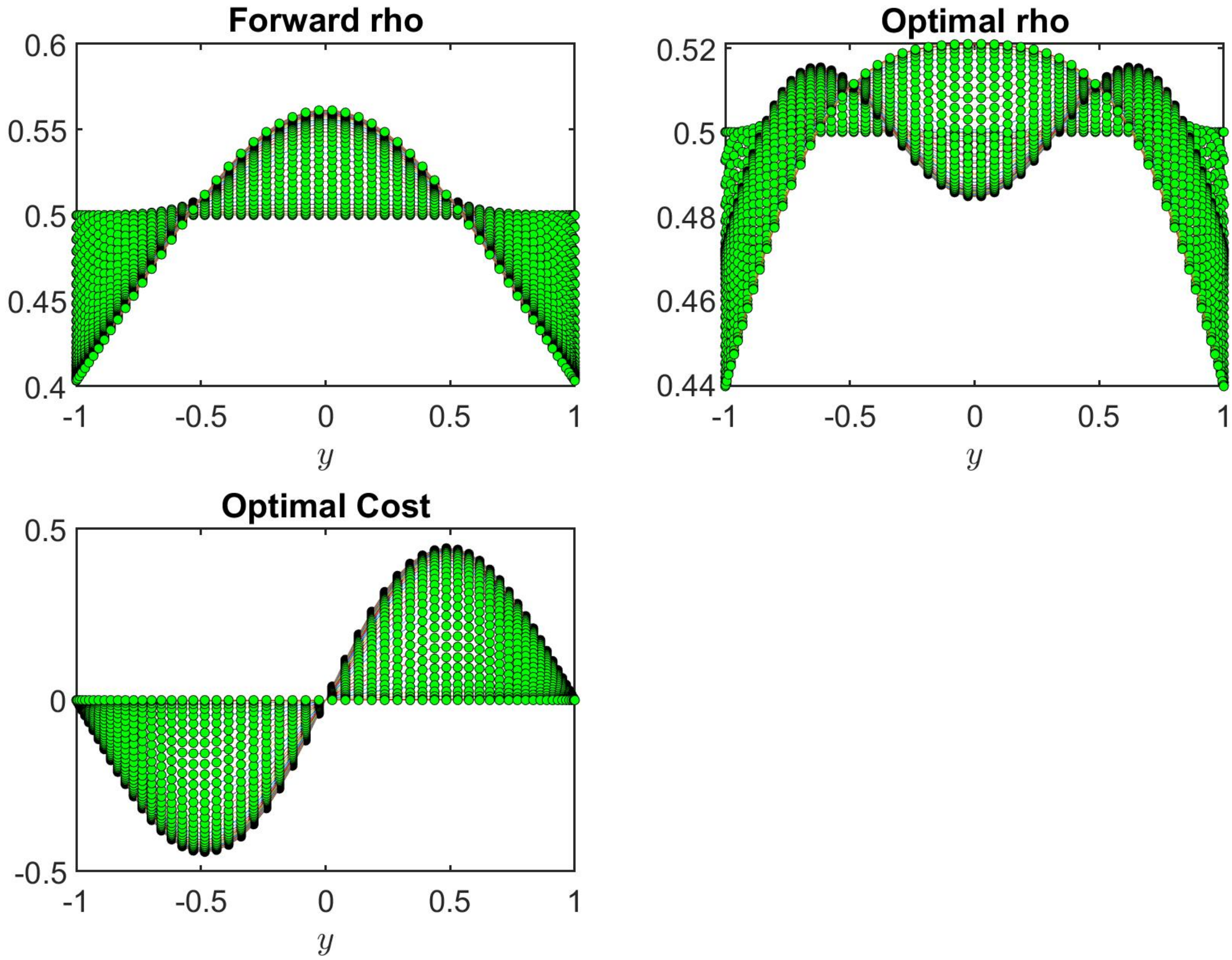

Figure 3: Solutions ρ_{FW} and ρ_{Opt} and Optimal control w, $\gamma = -1$, $\beta = 10^{-1}$.

direction' to the advection and therefore it isn't as advection dominated as the problem with attractive particles?
Checked both $\gamma = 1$ and $\gamma = -1$ with $\beta = 10$, which converges and doesn't seem to pose a problem.

2.1 Diffusion vs advection term

As for the other example, we can try to increase the diffusion to confirm that a large advection term is the problem. Choosing $\beta = 10^{-3}$, $\gamma = -1$ and $D_0 = 3$. This converges in 789 iterations, $J_{FW} = 0.0262$ and $J_{Opt} = 0.0074$, see Figure 13. We can conclude that this again is an issue of advection dominance. However, it is interesting that the $\gamma = 1$ case worked for $D_0 = 1$.

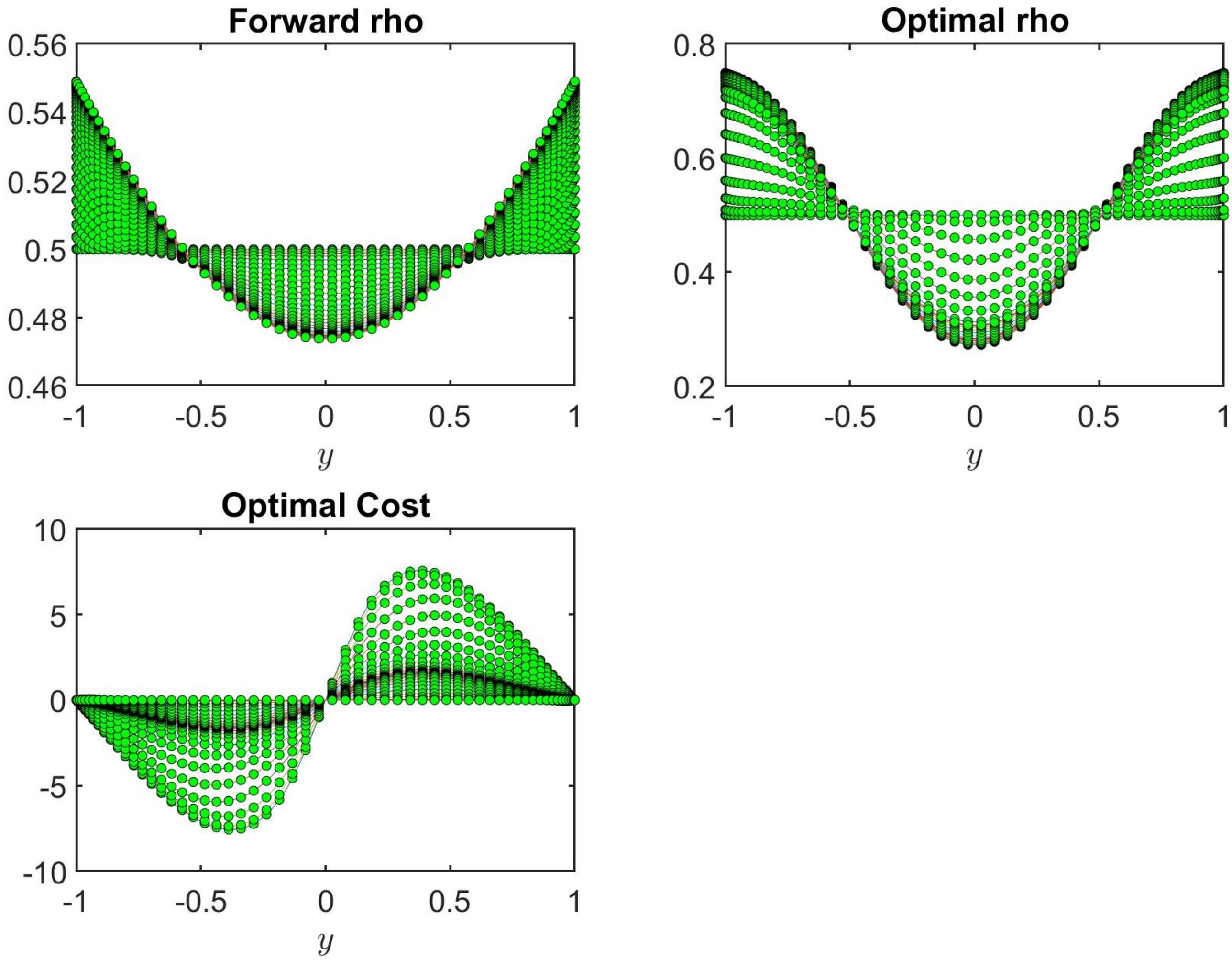

Figure 4: Solutions ρ_{FW} and ρ_{Opt} and Optimal control w, $\gamma = 0.5$, $\beta = 10^{-3}$.

3 Interacting Problems - moving target 1

The target is now

$$\hat{\rho} = (1-t)0.5 + t\frac{1}{4}(\cos(\pi y) + 2),$$

see Figure 14.

Choosing $\beta = 10^{-1}$, $\gamma = -1$, $D_0 = 1$, this converges in 637 iterations, $J_{FW} = 0.0041$ and $J_{Opt} = 0.0033$. Choosing $\gamma = 1$ also converges with $J_{FW} = 0.0195$ and $J_{Opt} = 0.0164$.

Try $\beta = 10$, converges for both $\gamma = 1$, $\gamma = -1$, J_{FW} and J_{Opt} basically identical. As perhaps expected, $\beta = 10^3$ converges within one iteration for both choices of γ.

Setting $\beta = 10^{-3}$, $\gamma = 1$, the algorithm converges as well, $J_{FW} = 0.0195$, $J_{Opt} = 0.0011$. Choosing $\gamma = -1$ diverges at 0.00011435, $J_{FW} = 0.0041$, $J_{Opt} = 2.1312 \times 10^{-4}$, see Figure 15. This is the same observation as above, advection and interaction work in the same direction,

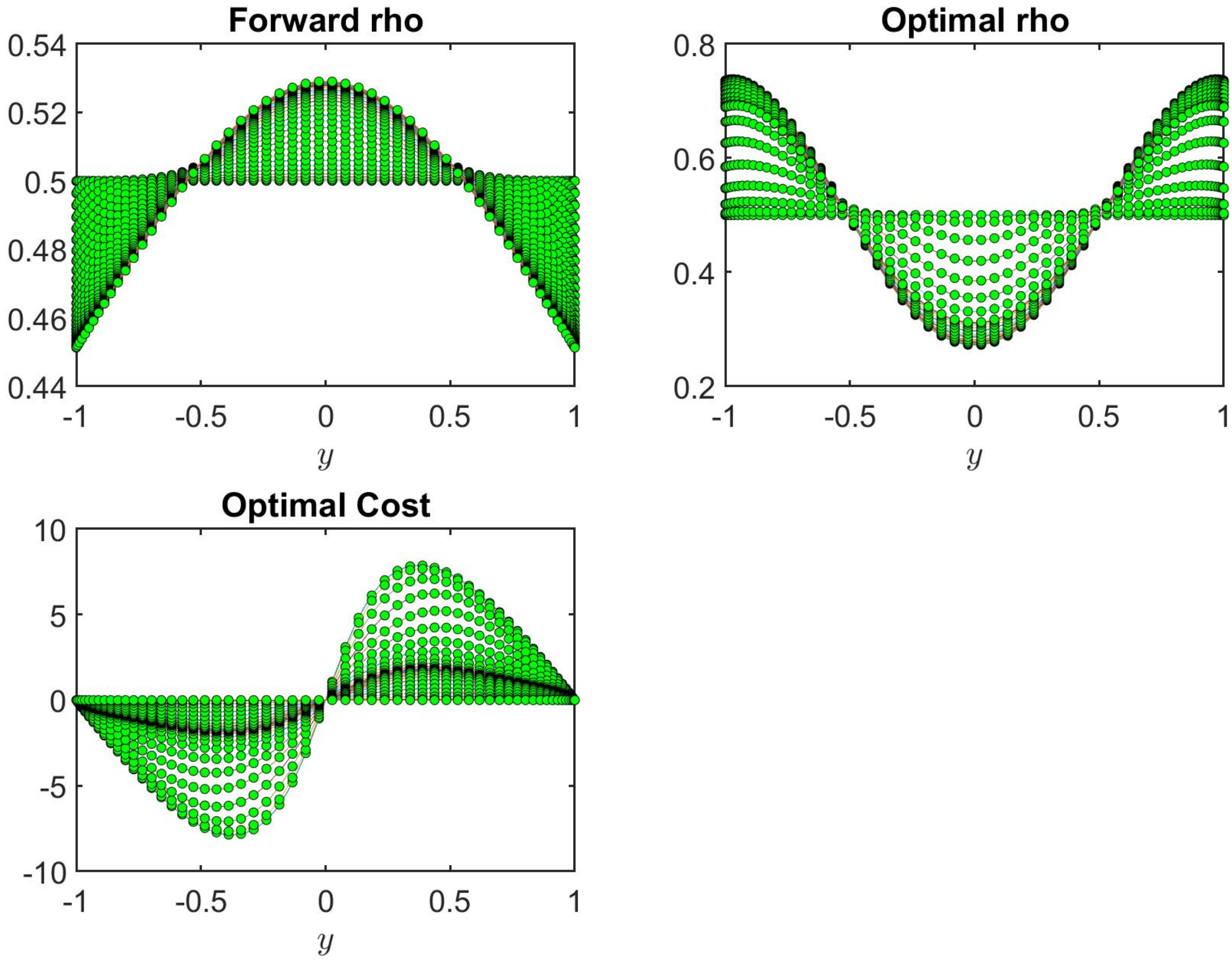

Figure 5: Solutions ρ_{FW} and ρ_{Opt} and Optimal control w, $\gamma = -0.5$, $\beta = 10^{-3}$.

so it is a harder problem? Choosing $\gamma = -0.9$ instead of $\gamma = -1$ converges, $J_{FW} = 0.0045$, $J_{Opt} = 2.3514 \times 10^{-4}$.

3.1 Diffusion vs advection term

Setting $D_0 = 2$, $\beta = 10^{-3}$ and $\gamma = -1$ converges. This again suggests that the diffusion advection interaction is influencing the stability of the code.

4 Interacting Problems - moving target 2

The target is now

$$\hat{\rho} = (1-t)0.5 + t\frac{1}{4}(\cos(\pi y + \pi) + 2),$$

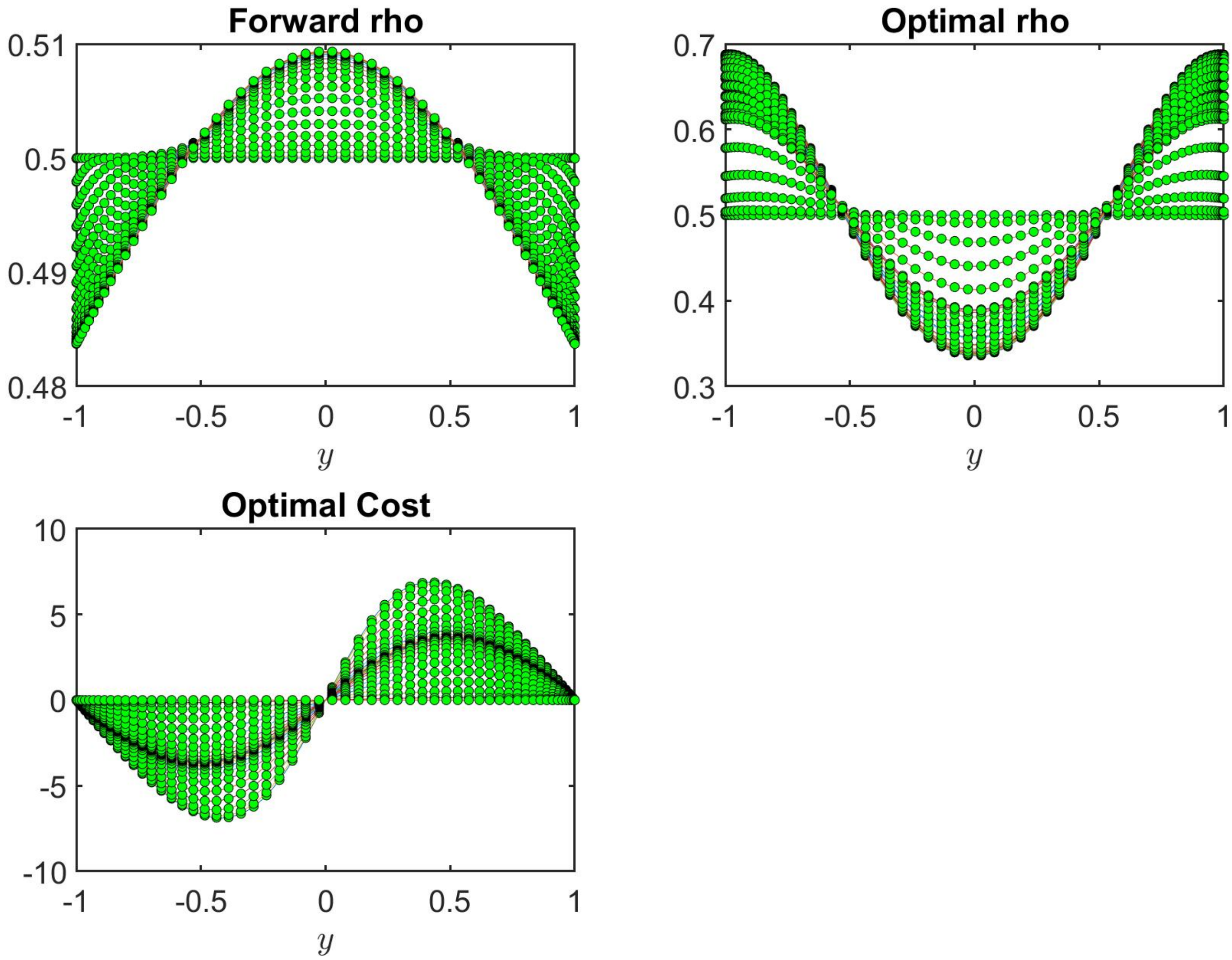

Figure 6: Solutions ρ_{FW} and ρ_{Opt} and Optimal control w, $\gamma = -0.5$, $\beta = 10^{-3}$, with $D_0 = 3$.

see Figure 17.
First try $\beta = 10^{-1}$, $\gamma = 1$, which converges in 651 iterations, $J_{FW} = 0.0047$, $J_{Opt} = 0.0040$. Then choosing $\gamma = -1$, converges with $J_{FW} = 0.0209$ and $J_{Opt} = 0.0168$.
Try $\beta = 10$, converges for both $\gamma = 1$, $\gamma = -1$, J_{FW} and J_{Opt} basically identical. As perhaps expected, $\beta = 10^3$ converges within one iteration for both choices of γ.
Try $\beta = 10^{-3}$ and $\gamma = 1$. This converges in 625 iterations, $J_{FW} = 0.0047$ and $J_{Opt} = 3.4051 \times 10^{-4}$, see Figure 18. Looking at $\gamma = -1$, this converges as well, $J_{FW} = 0.0209$, $J_{Opt} = 8.9783 \times 10^{-4}$, see Figure 19. One question is now why this works for this example, but not for the one above, given that they are very similar in nature.

Test $\beta = 10^{-3}$, $\gamma = -1$ with Picard. It converges in 619 iterations but is considerably slower than FixPt. $J_{FW} = 0.0209$ and $J_{Opt} = 8.9784 \times 10^{-4}$ are basically the same values as with

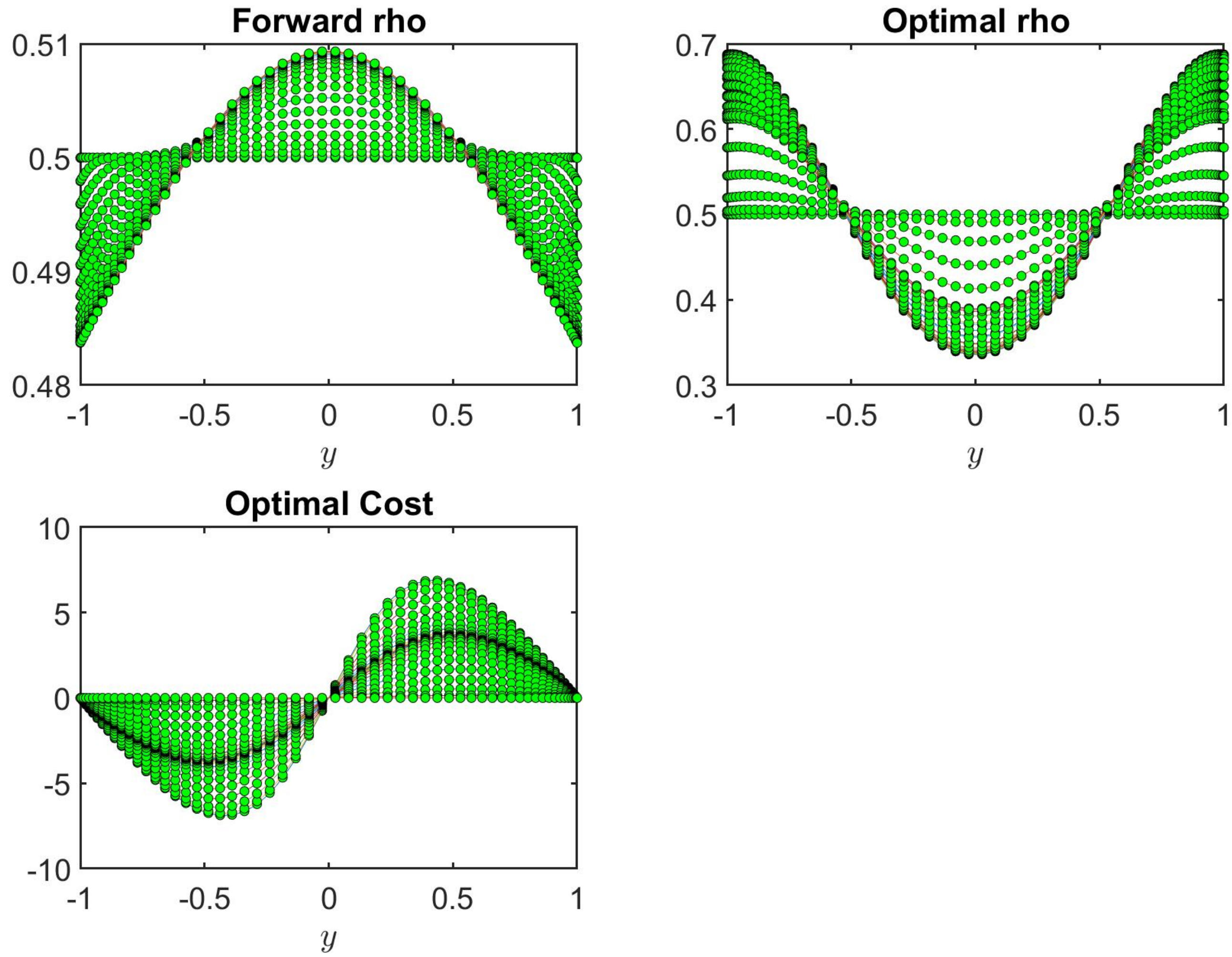

Figure 7: Solutions ρ_{FW} and ρ_{Opt} and Optimal control w, $\gamma = -0.5$, $\beta = 10^{-3}$, with $D_0 = 3$.

FixPt. For $\gamma = 1$ it also converges and we have $J_{FW} = 0.0047$ and $J_{Opt} = 3.4041 \times 10^{-4}$, which is again very close to the values with FixPt.

4.1 Diffusion vs advection term

We can try to break this example by decreasing the diffusion coefficient. Choosing $\gamma = 1$, since this works in the same direction as the advection. Interestingly, I can lower the diffusion coefficient to $D_0 = 0.17$ and the algorithm converges. At $D_0 = 0.16$ it diverges in 4 Iterations. $D_0 = 0.1699$ diverges at a consistency of 0.00011768 in 474 iterations, see Figure 20 and compare to the case with $D_0 = 1$ in Figure 18. In Figure 20 the optimal cost is of order 0.5, while in Figure 18 the cost is of order 2. Already at $D_0 = 0.01695$, the algorithm diverges in 9 iterations.

Trying to break $\gamma = -1$ seems to be easier. Choosing $D_0 = 0.5$, the algorithm diverges at 0.00271887 in 342 iterations, however $D_0 = 0.51$ converges.

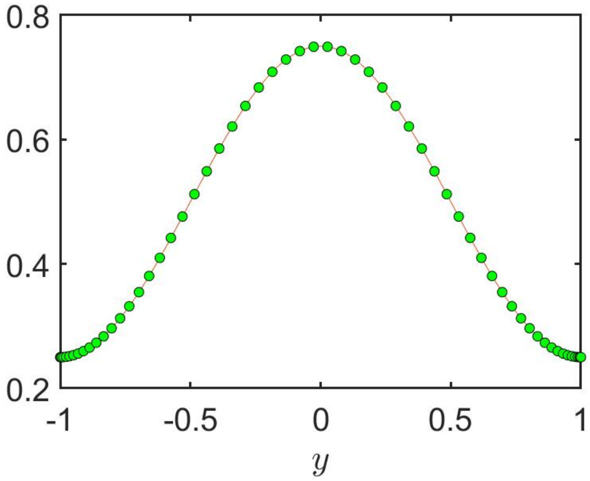

Figure 8: $\hat{\rho}$ 2.

5 $\gamma = 0$ case

As a comparison, this is moving target 1 with $\gamma = 0$ and $\beta = 10^{-3}$, see Figure 21. $J_{FW} = 0.0104$, $J_{Opt} = 5.4136 \times 10^{-4}$. $\gamma = -1$ gives lower J, $\gamma = 1$ higher J.
This is moving target 2 with $\gamma = 0$ and $\beta = 10^{-3}$, see Figure 22. $J_{FW} = 0.0104$, $J_{Opt} = 5.4136 \times 10^{-4}$. $\gamma = 1$ gives lower J, $\gamma = -1$ higher J, which is the opposite of the problem with moving target 1 and absolutely expected.

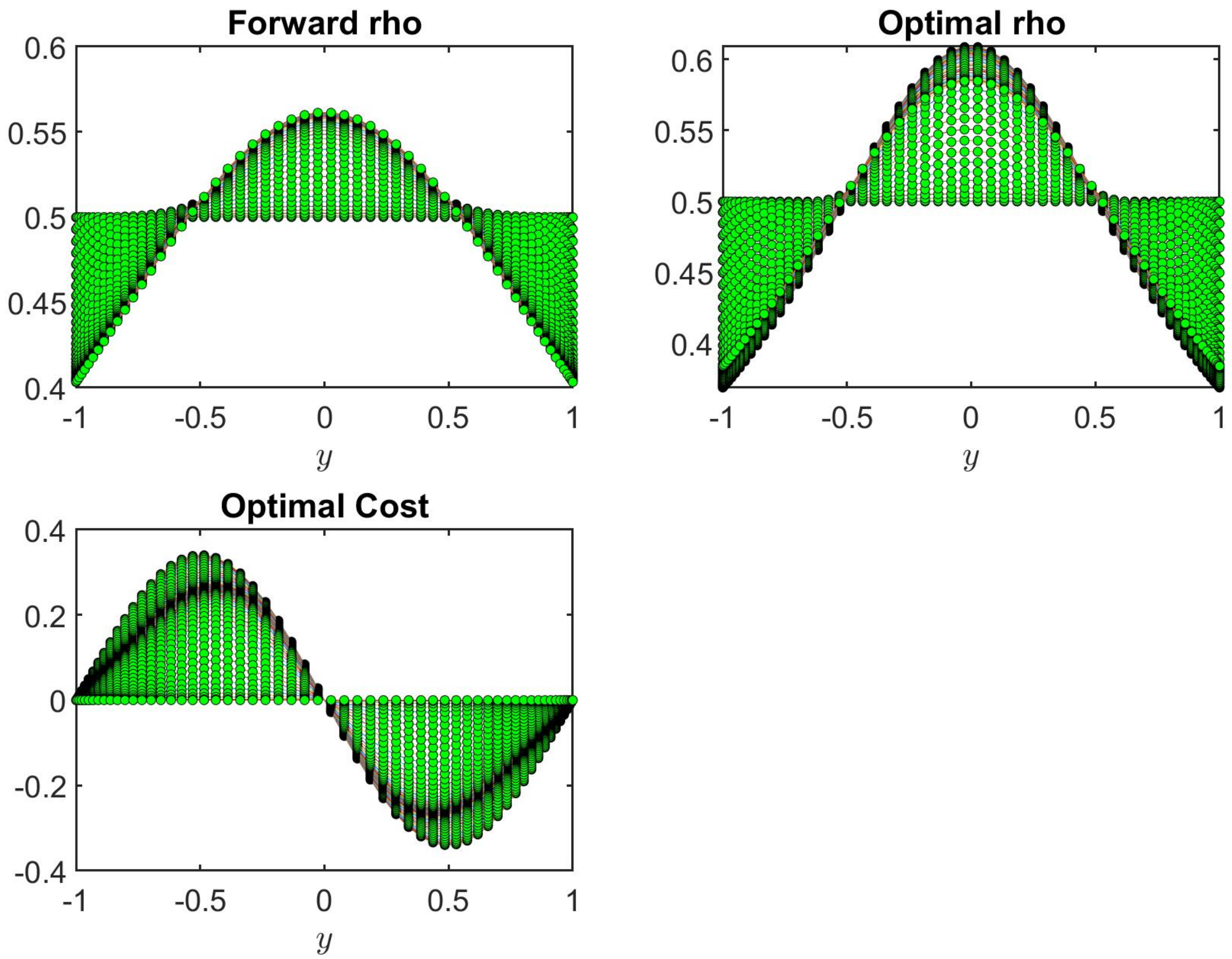

Figure 9: Solutions ρ_{FW} and ρ_{Opt} and Optimal control w, $\gamma = -1$, $\beta = 10^{-1}$, with $D_0 = 1$.

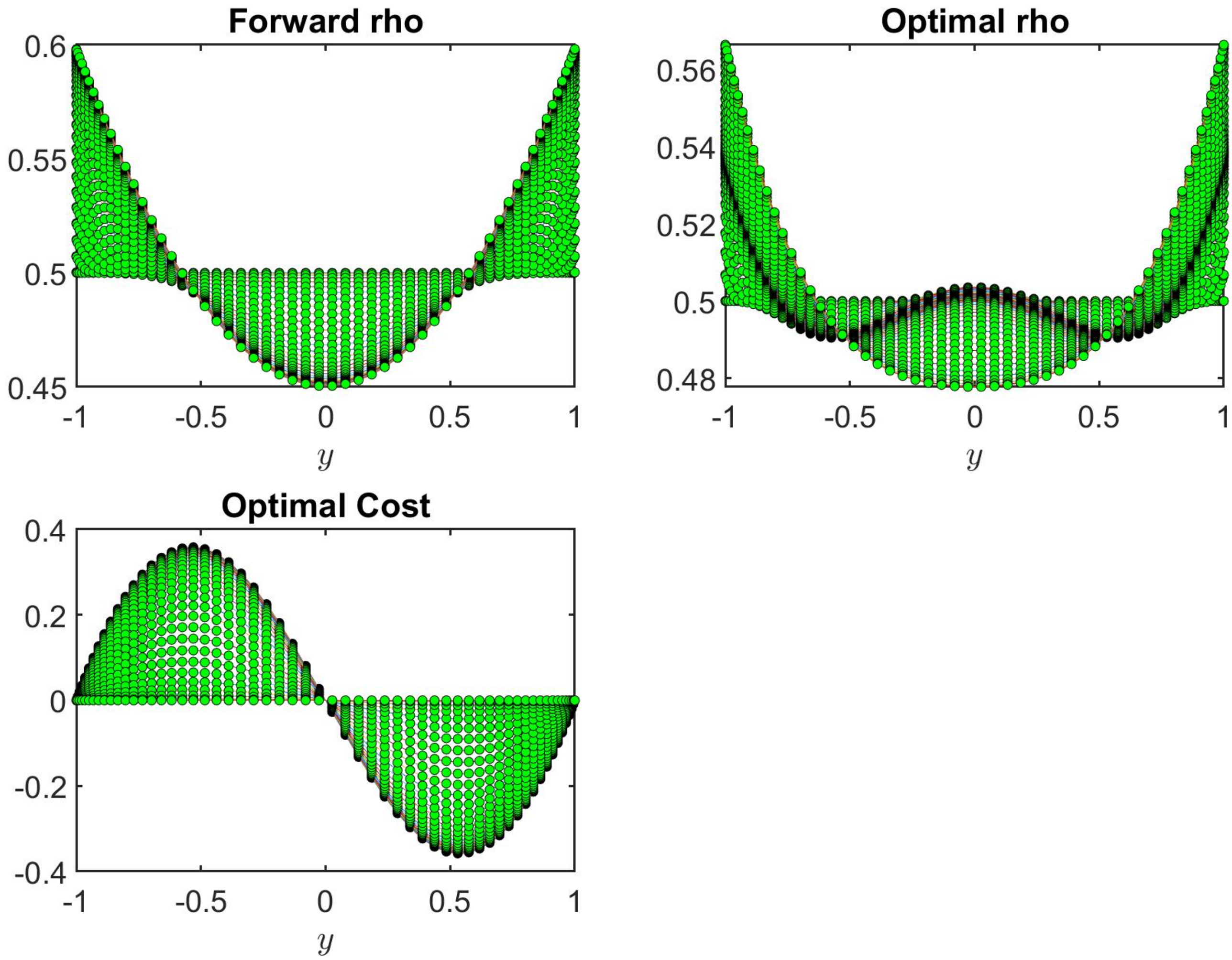

Figure 10: Solutions ρ_{FW} and ρ_{Opt} and Optimal control w, $\gamma = 1$, $\beta = 10^{-1}$, with $D_0 = 1$.

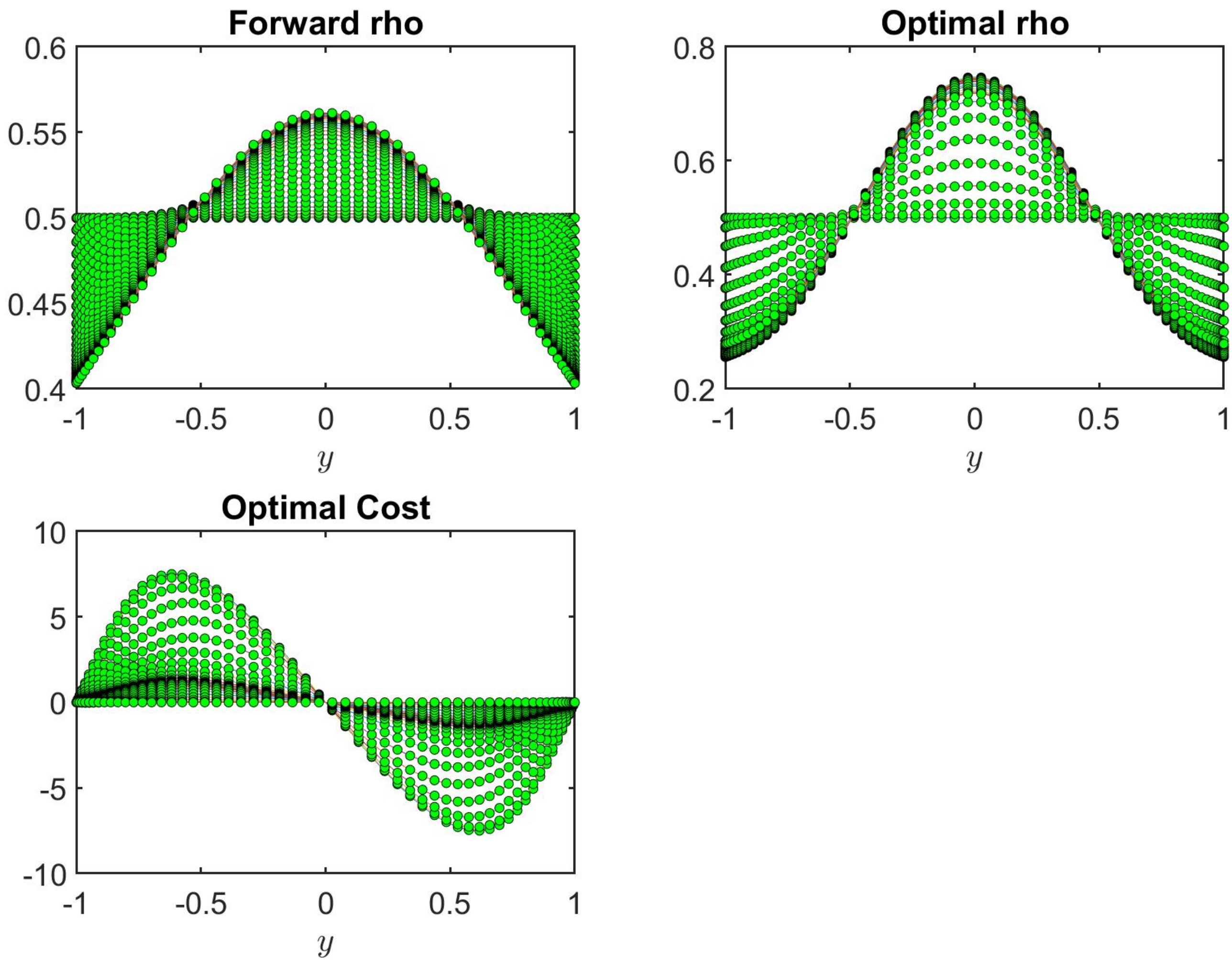

Figure 11: Solutions ρ_{FW} and ρ_{Opt} and Optimal control w, $\gamma = -1$, $\beta = 10^{-3}$, with $D_0 = 1$.

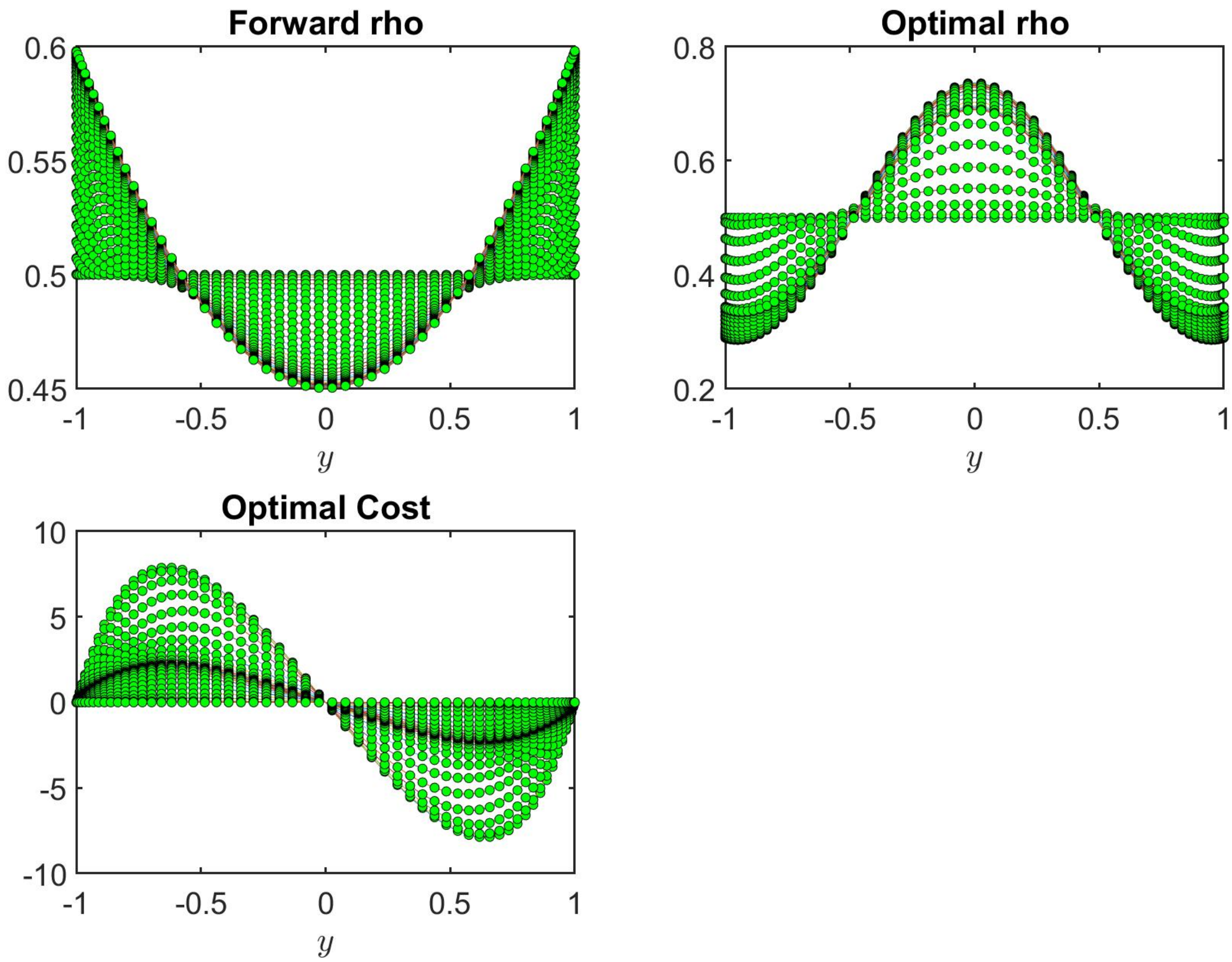

Figure 12: Solutions ρ_{FW} and ρ_{Opt} and Optimal control w, $\gamma = 1$, $\beta = 10^{-3}$, with $D_0 = 1$.

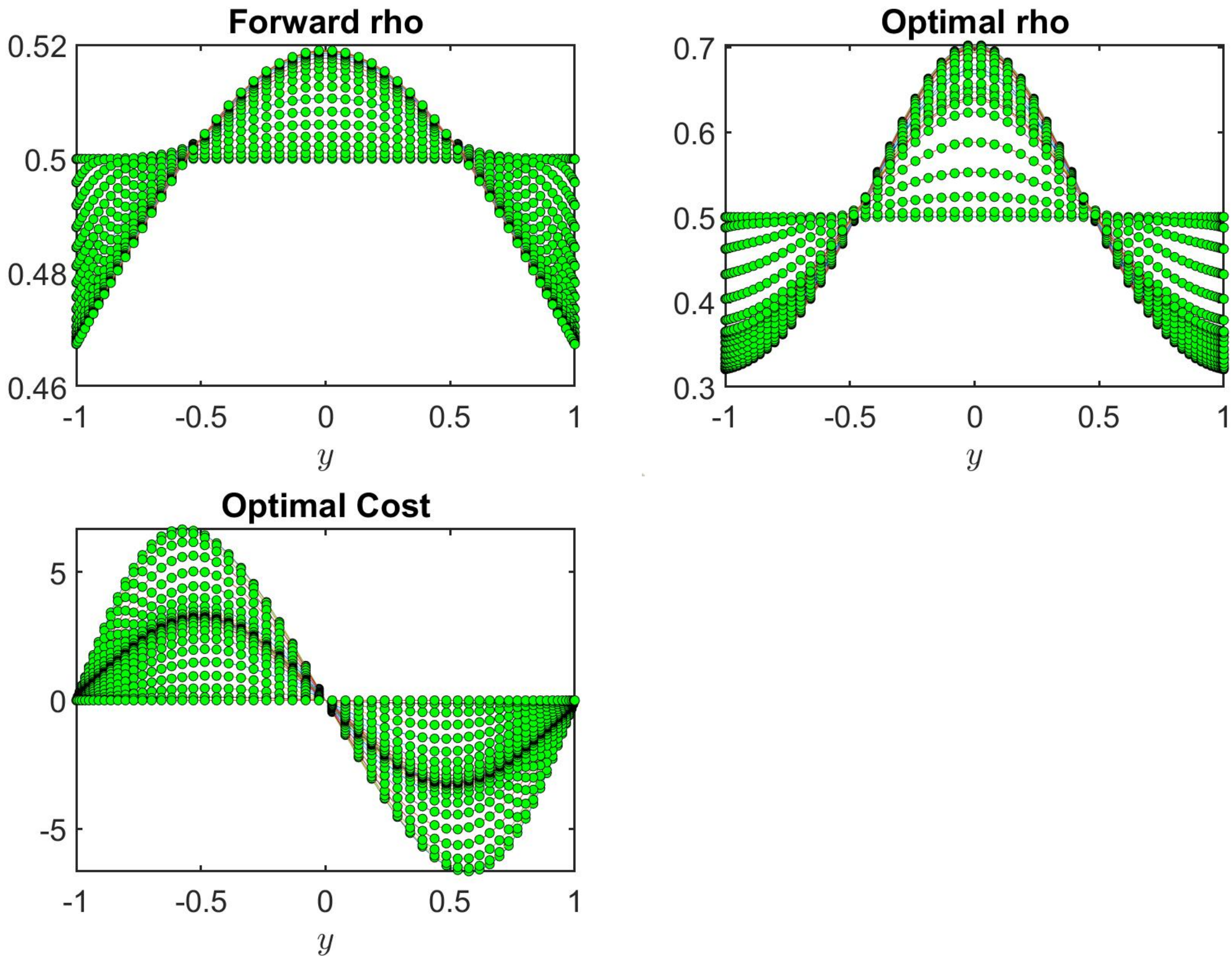

Figure 13: Solutions ρ_{FW} and ρ_{Opt} and Optimal control w, $\gamma = -1$, $\beta = 10^{-3}$, with $D_0 = 3$.

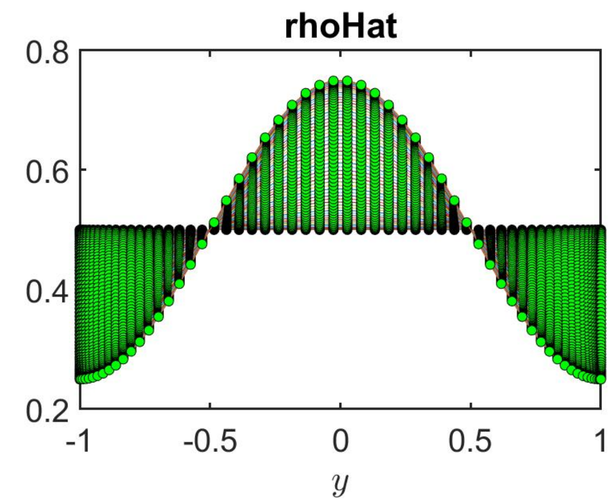

Figure 14: Moving target 1.

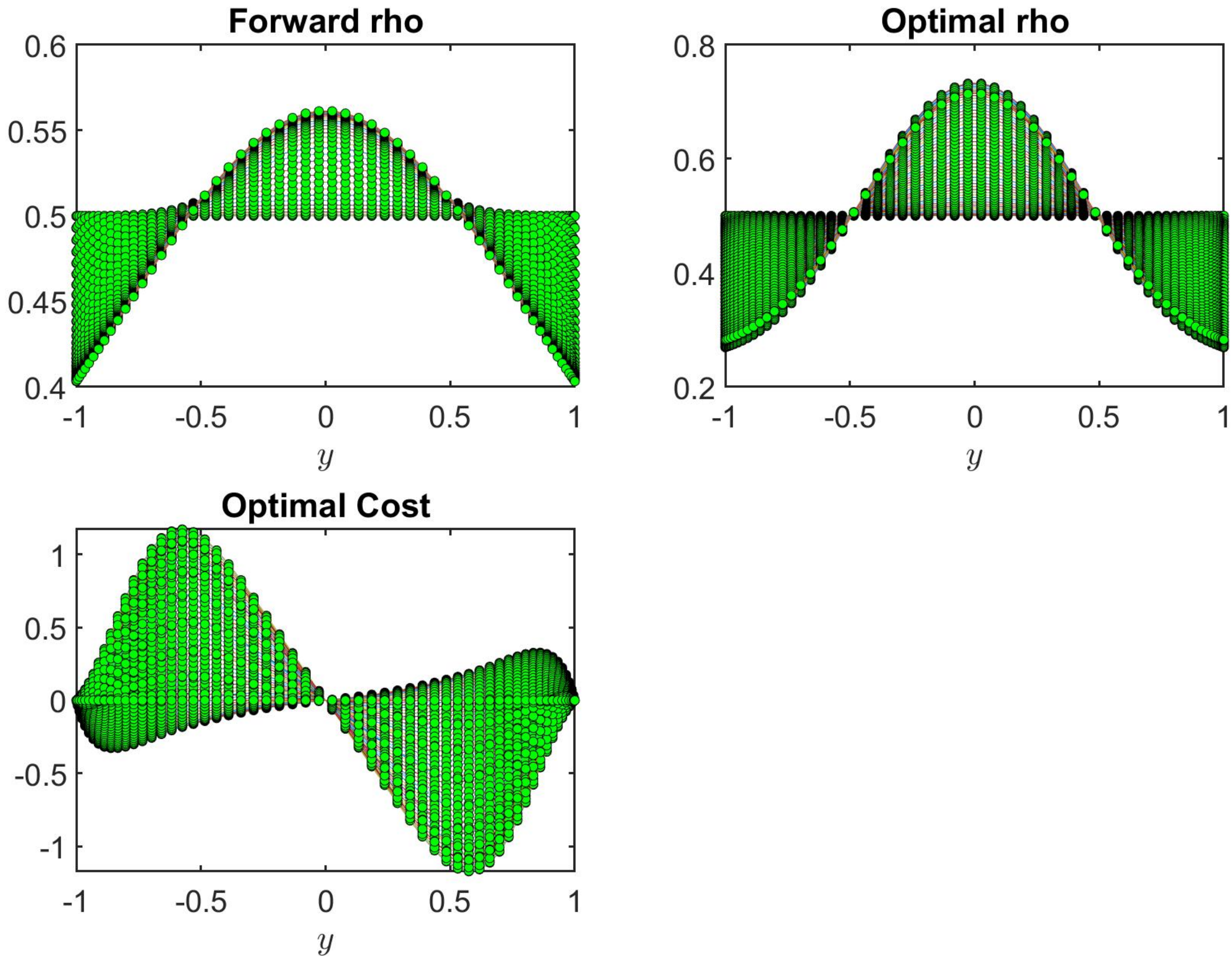

Figure 15: Solutions ρ_{FW} and ρ_{Opt} and Optimal control w, $\gamma = -1$, $\beta = 10^{-3}$, with $D_0 = 1$.

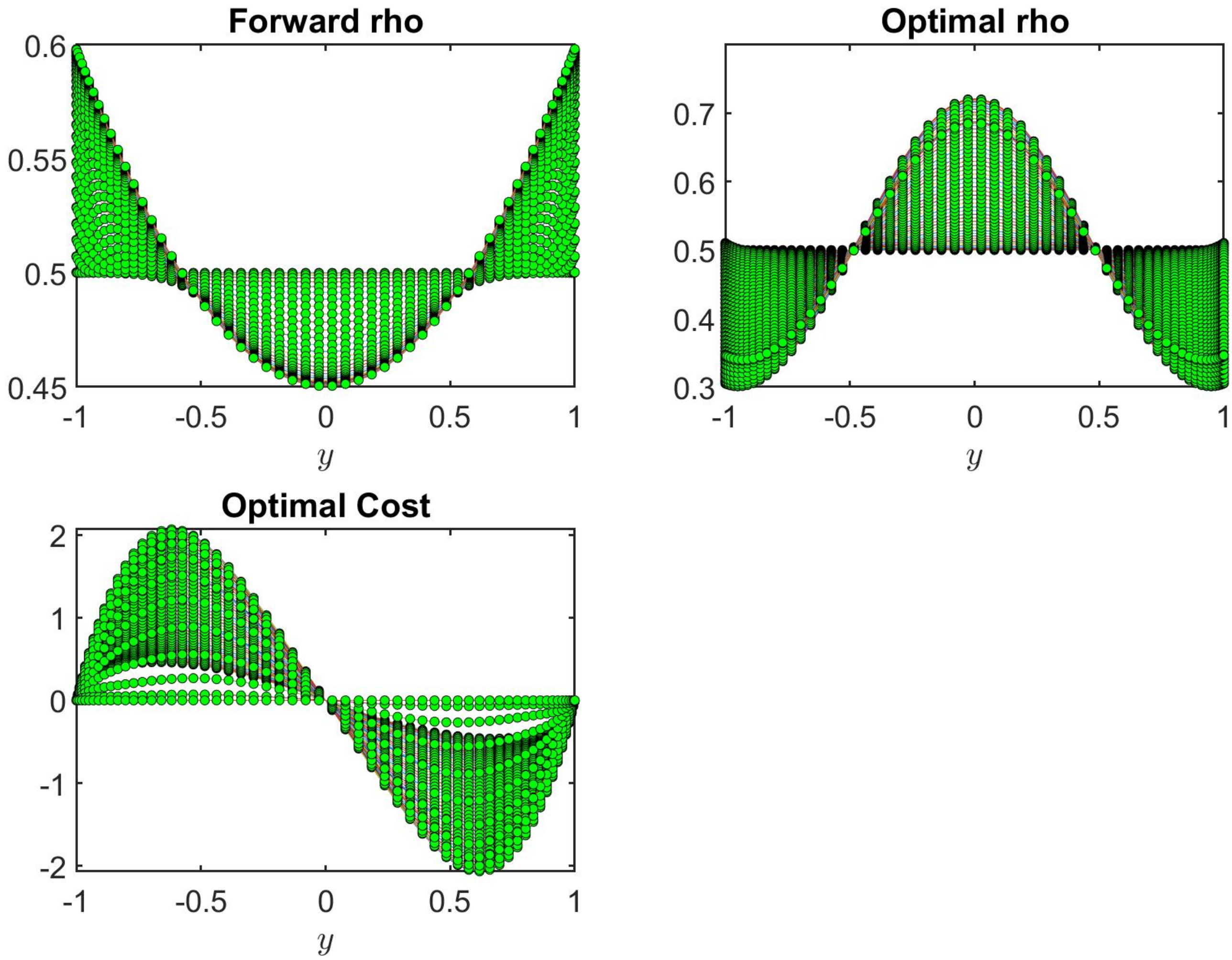

Figure 16: Solutions ρ_{FW} and ρ_{Opt} and Optimal control w, $\gamma = 1$, $\beta = 10^{-3}$, with $D_0 = 1$.

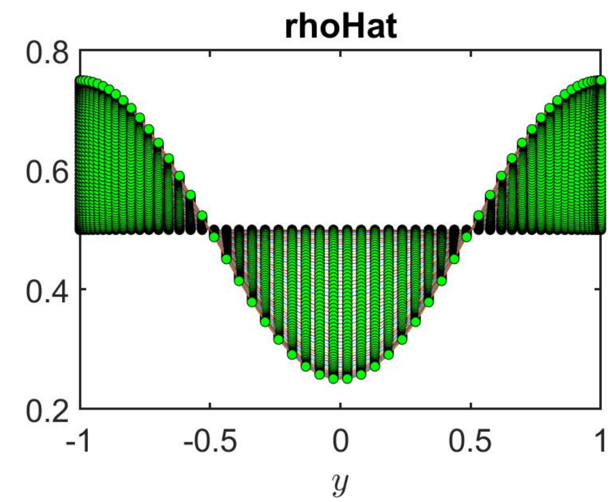

Figure 17: Moving target 2.

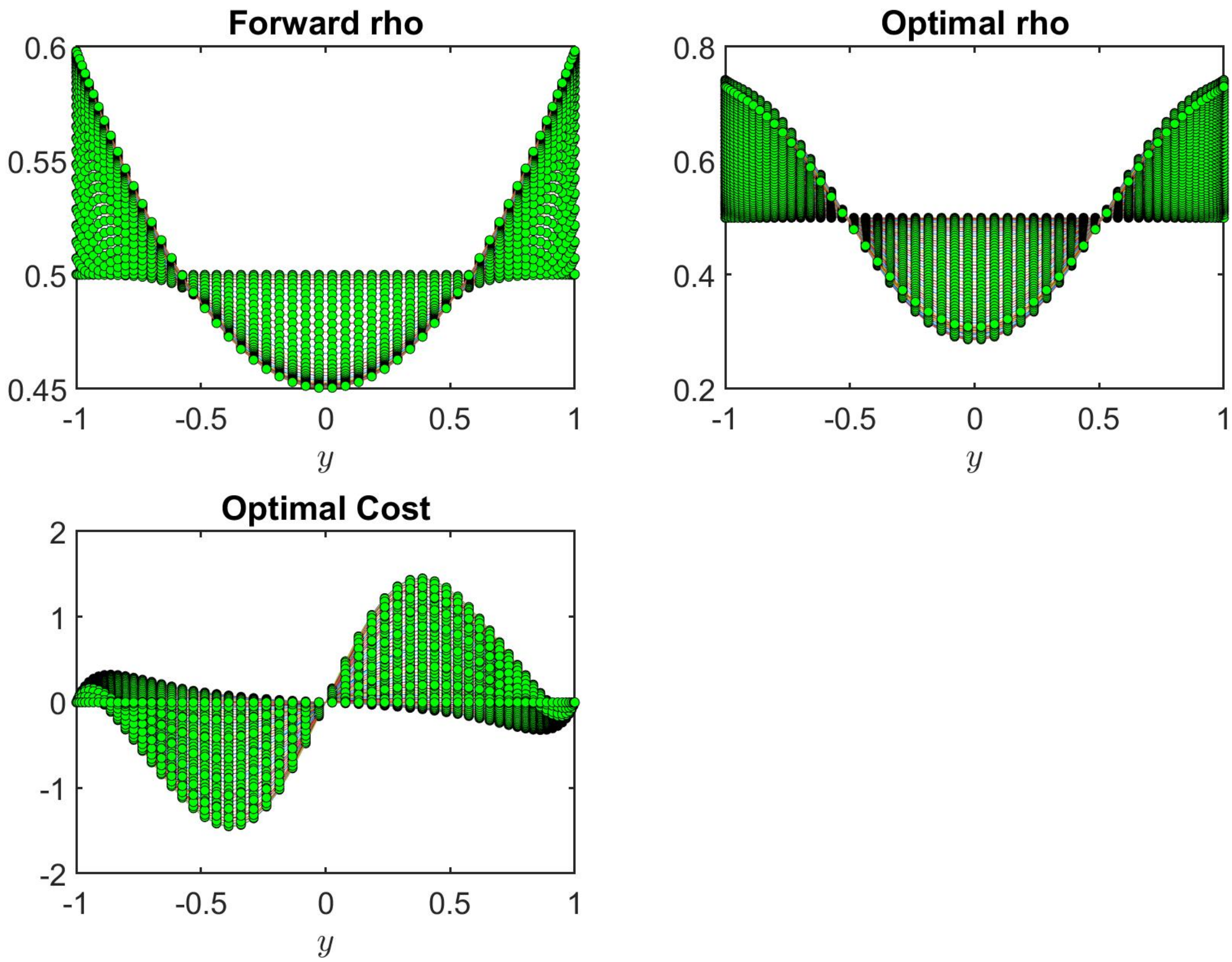

Figure 18: Solutions ρ_{FW} and ρ_{Opt} and Optimal control w, $\gamma = 1$, $\beta = 10^{-3}$, with $D_0 = 1$.

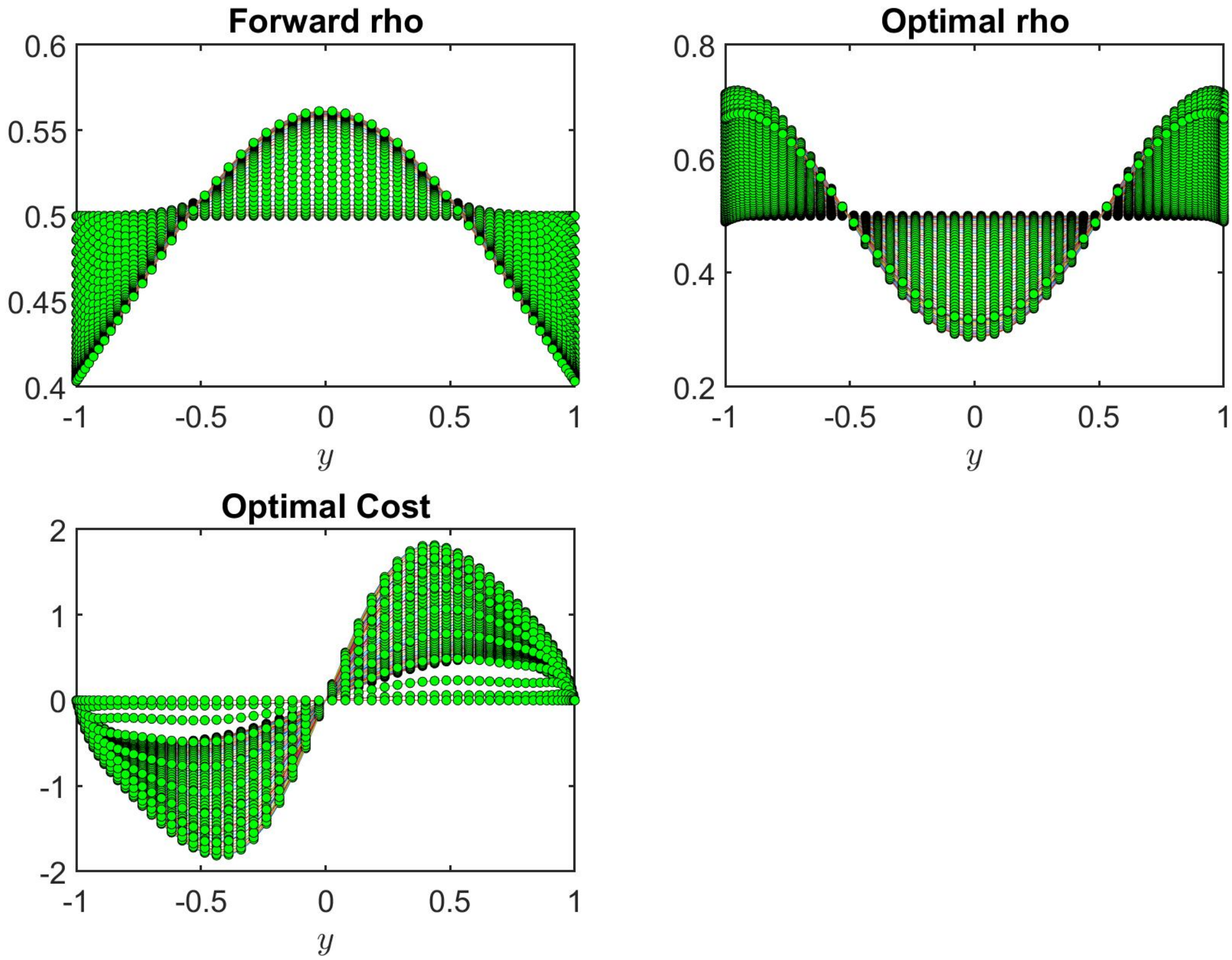

Figure 19: Solutions ρ_{FW} and ρ_{Opt} and Optimal control w, $\gamma = -1$, $\beta = 10^{-3}$, with $D_0 = 1$.

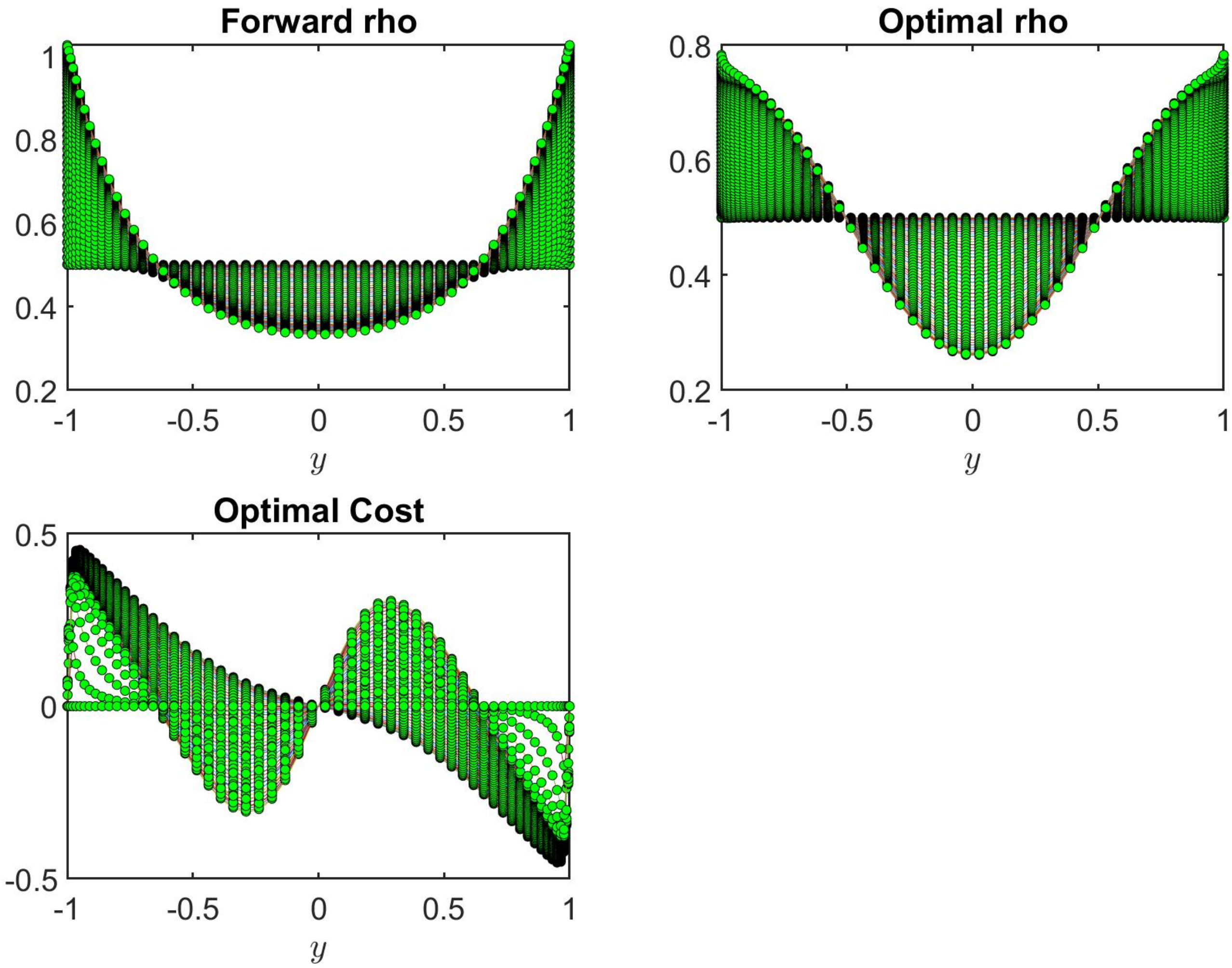

Figure 20: Solutions ρ_{FW} and ρ_{Opt} and Optimal control w, $\gamma = 1$, $\beta = 10^{-3}$, with $D_0 = 0.1699$.

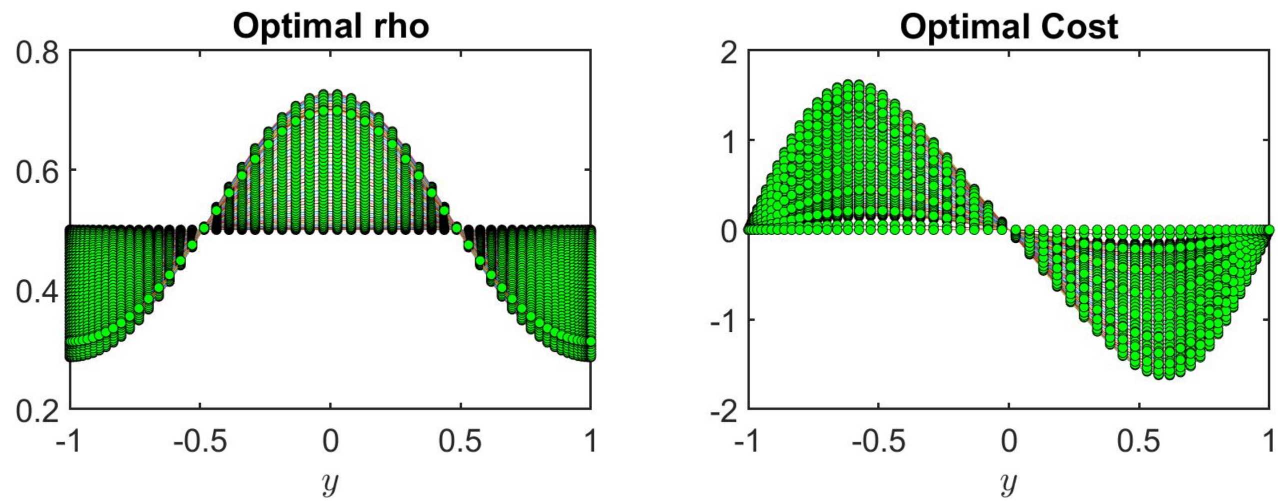

Figure 21: Solution ρ_{Opt} and Optimal control w, $\gamma = 0$, $\beta = 10^{-3}$, with $D_0 = 1$.

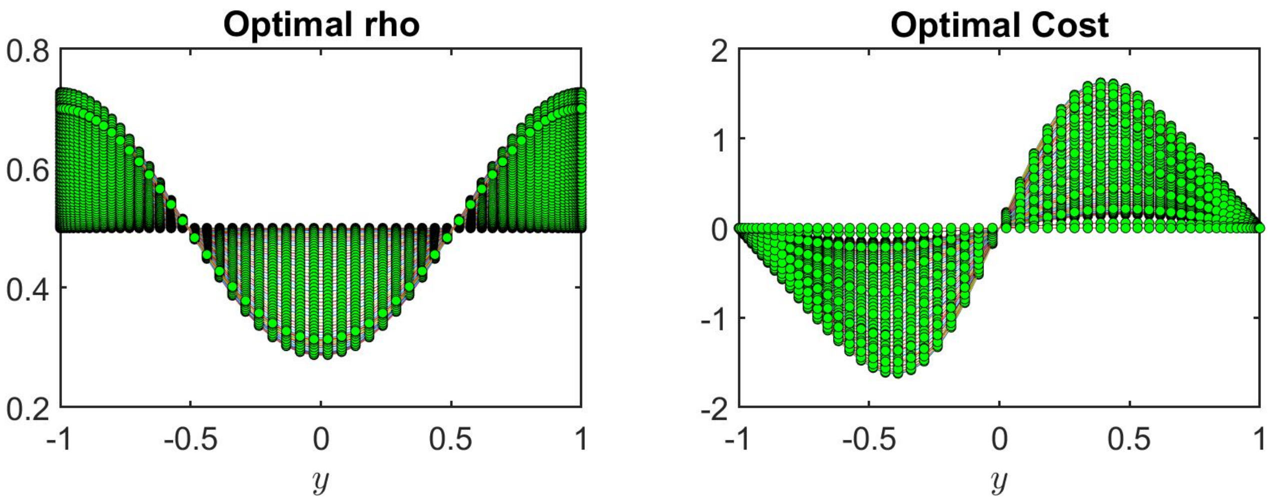

Figure 22: Solution ρ_{Opt} and Optimal control w, $\gamma = 0$, $\beta = 10^{-3}$, with $D_0 = 1$.