

Paper Examples

All the below examples are run with Newton-Krylov. They all converged within 10 outer iterations. The baseline for the cost functional is the problem computed with $\beta = 10^3$. I changed the colormap to fewer colors, so that the differences between the different κ are visible in the initial times, while also scaling the colormap for the overall maximum of ρ over all times and κ . The controls are also scaled for all times and κ (for flow control we use the largest value over all times and κ as the scaling for the arrow).

1 Neumann Source Control

We choose

$$\begin{aligned}\rho_0 &= \frac{1}{4} \\ V_{ext} &= \frac{3}{2} \cos\left(\frac{\pi x_1}{5} - \frac{\pi}{5}\right) \sin\left(\frac{\pi x_2}{5}\right) \\ \hat{\rho} &= \frac{1}{4}(1-t) + t \left(\frac{1}{4} \sin\left(\frac{\pi(x_1-2)}{2}\right) \sin\left(\frac{\pi(x_2-2)}{2}\right) + \frac{1}{4} \right)\end{aligned}$$

We choose the domain $[-1, 1]^2$ with a time horizon $(0, 1)$ and $N = 20$, $n = 11$. For $\beta = 10^{-3}$, for $\kappa = -1$ we have $\mathcal{J}_c = 0.0018$, for $\kappa = 0$ (compared to $\mathcal{J}_{uc} = 0.0274$ from $\beta = 10^3$), $\mathcal{J}_c = 0.0017$ and for $\kappa = 1$, $\mathcal{J}_c = 0.0018$. Each of these computations takes around 200 seconds for 10 outer iterations. The results can be seen in Figures 2, 3 and 4 and the external potential acting on ρ is displayed in Figure 1.

We run the same example with $\beta = 10^{-5}$. This gives for $\kappa = -1$, $\mathcal{J}_c = 8.0673 \times 10^{-4}$, for $\kappa = 0$, $\mathcal{J}_c = 8.1989 \times 10^{-4}$, and for $\kappa = 1$, $\mathcal{J}_c = 8.4241 \times 10^{-4}$. Notably, these calculations only take around 20 seconds. The results are displayed in Figures 5, 6 and 7. The controls are larger, but the difference in dynamics is smaller for different interactions.

2 Dirichlet Source Control

We choose

$$\begin{aligned}\rho_0 &= \frac{1}{4} \cos\left(\frac{\pi x_1}{2}\right) \cos\left(\frac{\pi x_2}{2}\right) + \frac{1}{4} \\ V_{ext} &= 2(1-t) \left(-\cos\left(\frac{\pi x_1}{2}\right) \sin\left(\frac{\pi x_2}{2}\right) + 1 \right) \\ \hat{\rho} &= (1-t) \left(\frac{1}{4} \cos\left(\frac{\pi x_1}{2}\right) \cos\left(\frac{\pi x_2}{2}\right) + \frac{1}{4} \right) - t \left(\frac{1}{4} \sin(\pi x_1) \sin\left(\frac{\pi x_2}{2} - \frac{\pi}{2}\right) + \frac{1}{4} \right)\end{aligned}$$

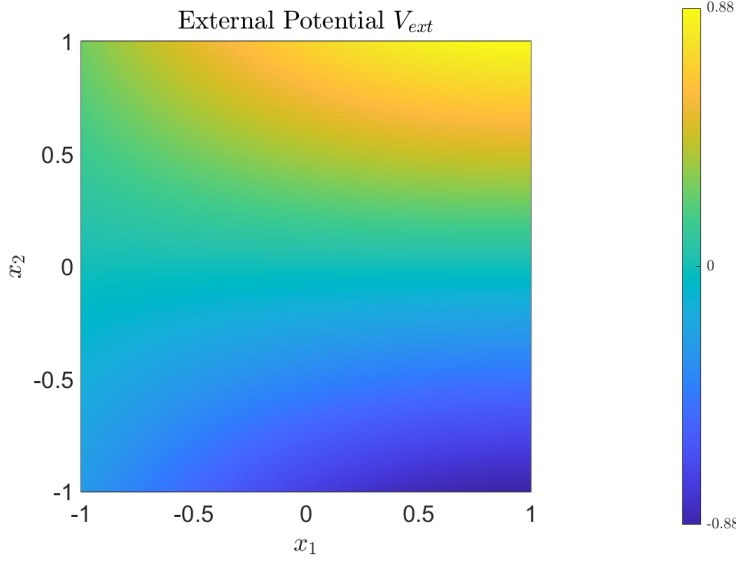


Figure 1: Neumann Source Control: External Potential V_{ext} acting on ρ .

so that the problem has Dirichlet boundary conditions at 0.25 ($\rho = 0.25$ on $\partial\Omega$). We choose the domain $[-1, 1]^2$ with a time horizon $(0, 1)$ and $N = 20$, $n = 11$. For $\beta = 10^{-3}$, for $\kappa = -1$ we have $\mathcal{J}_c = 0.0036$, for $\kappa = 0$ (compared to $\mathcal{J}_{uc} = 0.0219$ from $\beta = 10^3$), $\mathcal{J}_c = 0.0038$ and for $\kappa = 1$, $\mathcal{J}_c = 0.0043$. Each of these computations takes around 70 seconds for 10 outer iterations. The results can be seen in Figures 9, 10 and 11 and the external potential acting on ρ is displayed in Figure 8.

3 Neumann Flow Control

We choose

$$\begin{aligned}\rho_0 &= \frac{1}{4} \\ V_{ext} &= \left((x_1 + 0.3)^2 - 1\right) \left((x_1 - 0.4)^2 - 0.5\right) \left((x_2 + 0.3)^2 - 1\right) \left((x_2 - 0.4)^2 - 0.5\right) \\ \hat{\rho} &= \frac{1}{4}(1 - t) + t \frac{1}{1.3791} \exp \left(-2 \left((x_1 + 0.2)^2 + (x_2 + 0.2)^2 \right) \right)\end{aligned}$$

We choose the domain $[-1, 1]^2$ with a time horizon $(0, 1)$. We have $N = 20$, $n = 11$. For $\beta = 10^{-3}$, $\kappa = 1$ we get $\mathcal{J}_c = 0.0059$ (compare to $\beta = 10^3$ with $\mathcal{J}_{uc} = 0.0336$), for $\kappa = 0$, $\mathcal{J}_c = 0.0043$, and for $\kappa = -1$ we get $\mathcal{J}_c = 0.0030$, (compare to $\beta = 10^3$ with $\mathcal{J}_{uc} = 0.0214$). Each of the problems takes around 180 seconds to solve. The results can be seen in Figures 13,

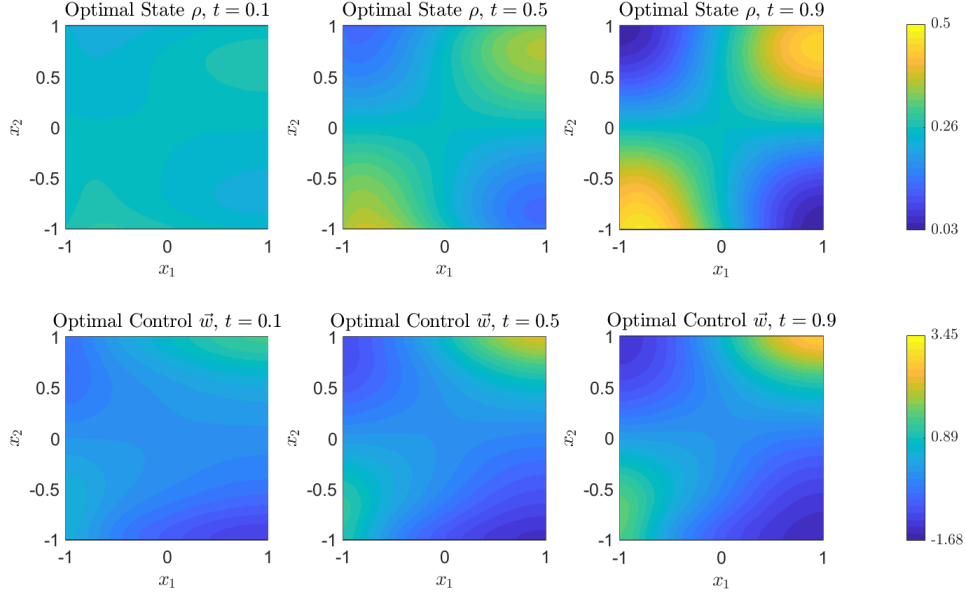


Figure 2: Neumann Source Control: Optimal ρ and optimal control for $\kappa = 0$ and $\beta = 10^{-3}$.

14 and 15 and the external potential associated with it is shown in Figure 12. Note that mass is conserved.

4 Dirichlet Flow Control

I computed the Dirichlet example once with and once without V_{ext} . I think we can just use the one that has V_{ext} included.

4.1 Dirichlet Flow Control without V_{ext}

We choose

$$\rho_0 = \left(\frac{\pi}{4}\right)^2 \cos\left(\frac{\pi x_1}{2}\right) \cos\left(\frac{\pi x_2}{2}\right) + \left(\frac{\pi}{4}\right)^2$$

$$\hat{\rho} = (1-t) \left(\left(\frac{\pi}{4}\right)^2 \cos\left(\frac{\pi x_1}{2}\right) \cos\left(\frac{\pi x_2}{2}\right) + \left(\frac{\pi}{4}\right)^2 \right) + t \left(\left(\frac{\pi}{4}\right)^2 \cos\left(\frac{\pi x_1}{2}\right) \cos\left(\frac{3\pi x_2}{2}\right) + \left(\frac{\pi}{4}\right)^2 \right)$$

We choose the domain $[-1, 1]^2$ with a time horizon $(0, 1)$. We have $N = 20$, $n = 11$. For $\beta = 10^{-3}$, $\kappa = 1$ we get $\mathcal{J}_c = 0.0121$, for $\kappa = 0$, $\mathcal{J}_c = 0.0095$, and for $\kappa = -1$ we get $\mathcal{J}_c = 0.0104$, (compare to $\beta = 10^3$ with $\mathcal{J}_{uc} = 0.5272$). Each of the problems takes around 50 seconds to solve. The results can be seen in Figures 16, 17 and 18.

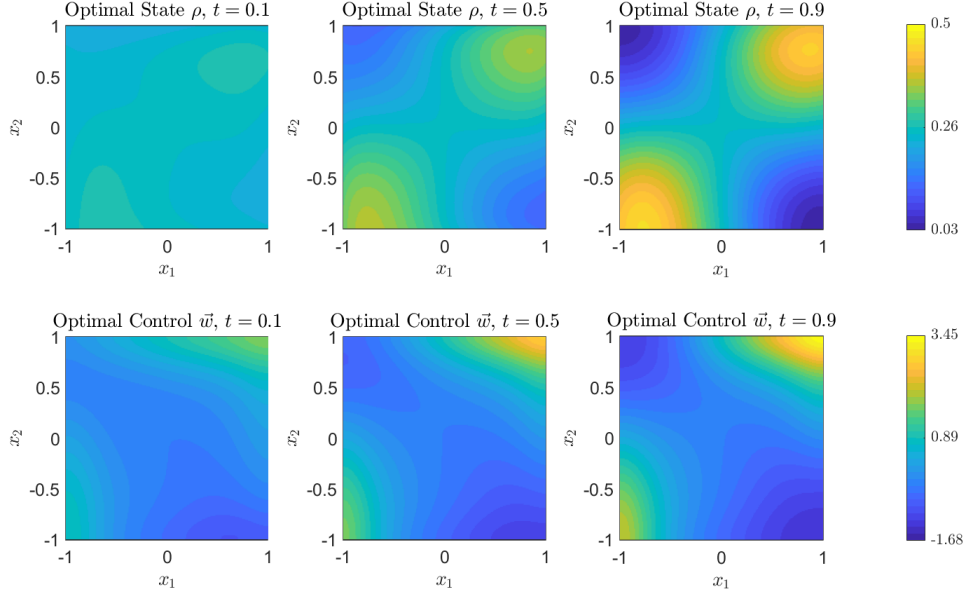


Figure 3: Neumann Source Control: Optimal ρ and optimal control for $\kappa = -1$ and $\beta = 10^{-3}$.

4.2 Dirichlet Flow Control with V_{ext}

We add the following external potential to the above problem, see Figure 19

$$V_{ext} = 10 \sin\left(\frac{\pi x_1}{2}\right) \sin\left(\frac{\pi x_2}{3} - \frac{\pi}{2}\right)$$

For $\beta = 10^{-3}$, $\kappa = 1$ we get $\mathcal{J}_c = 0.0130$, for $\kappa = 0$, $\mathcal{J}_c = 0.0106$, and for $\kappa = -1$ we get $\mathcal{J}_c = 0.0113$. (Compare these to $\beta = 10^3$ with $\mathcal{J}_{uc} = 0.0898$) Each of the problems takes around 50 seconds to solve. The results can be seen in Figures 20, 21 and 22.

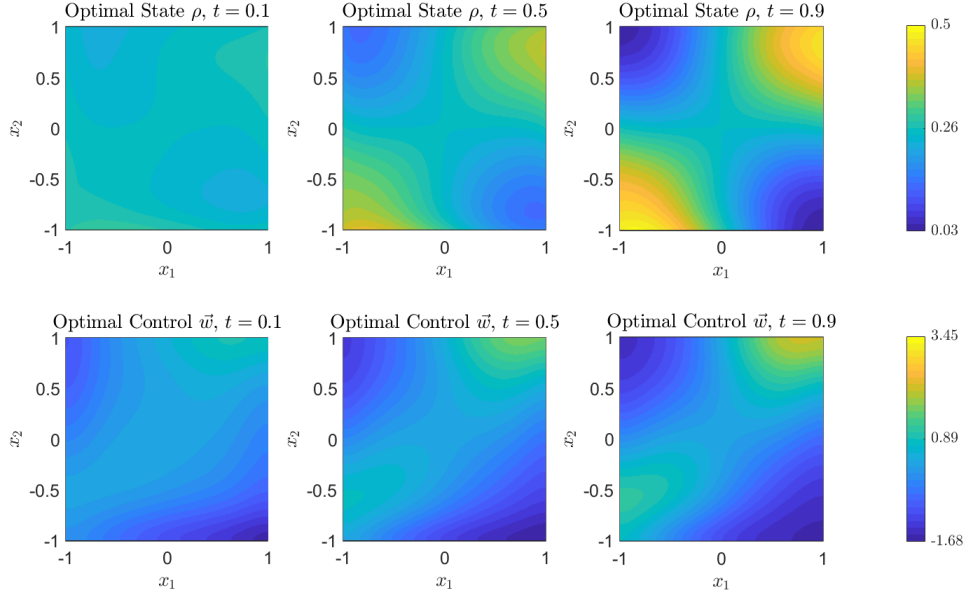


Figure 4: Optimal ρ and optimal control for $\kappa = 1$ and $\beta = 10^{-3}$.

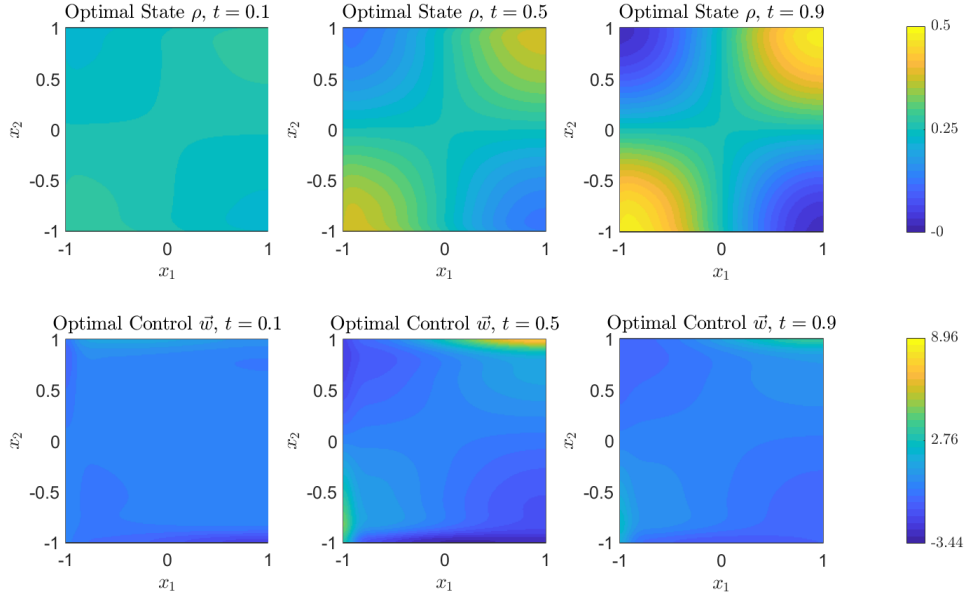


Figure 5: Neumann Source Control: Optimal ρ and optimal control for $\kappa = 0$ and $\beta = 10^{-5}$.

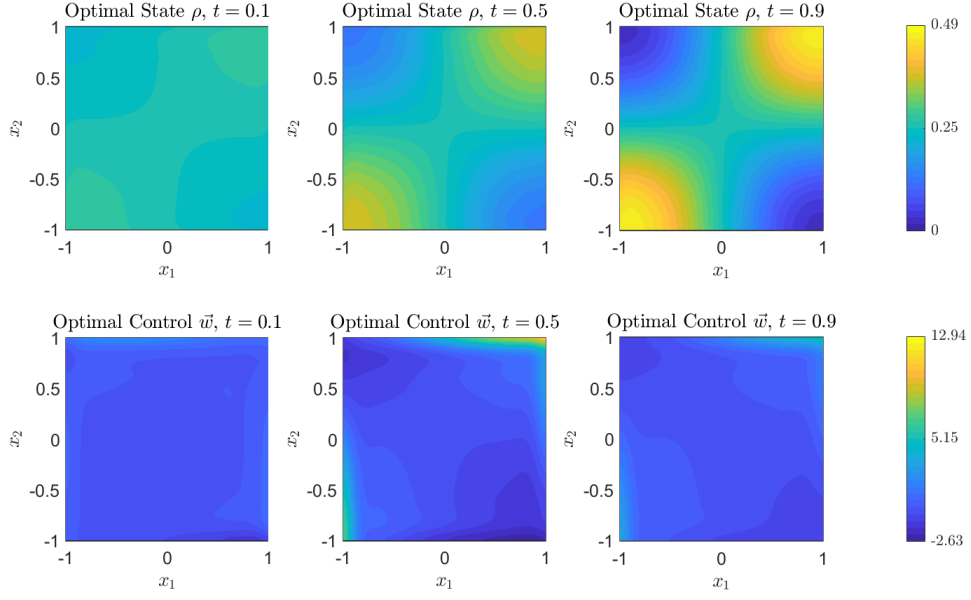


Figure 6: Neumann Source Control: Optimal ρ and optimal control for $\kappa = -1$ and $\beta = 10^{-5}$.

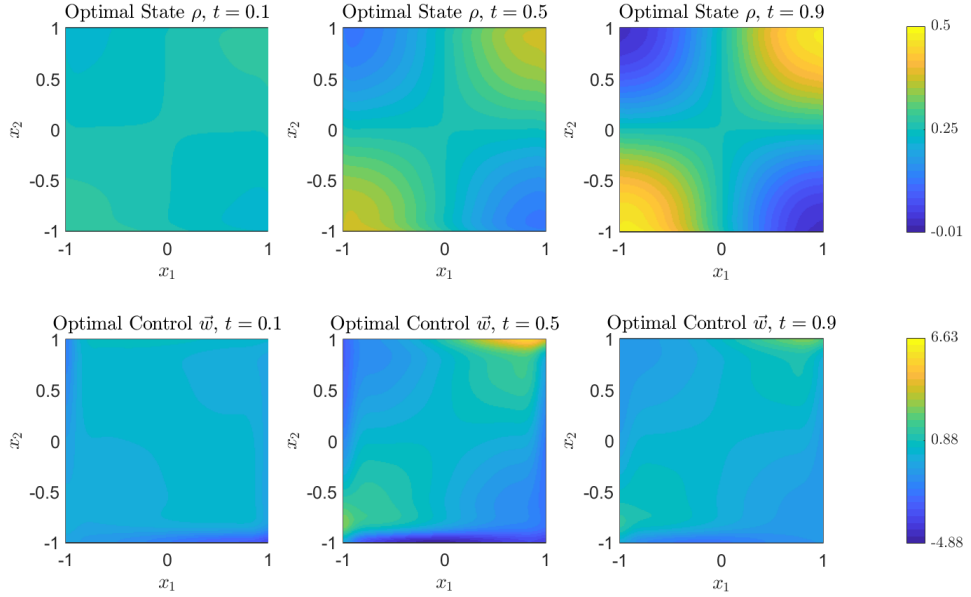


Figure 7: Neumann Source Control: Optimal ρ and optimal control for $\kappa = 1$ and $\beta = 10^{-5}$.

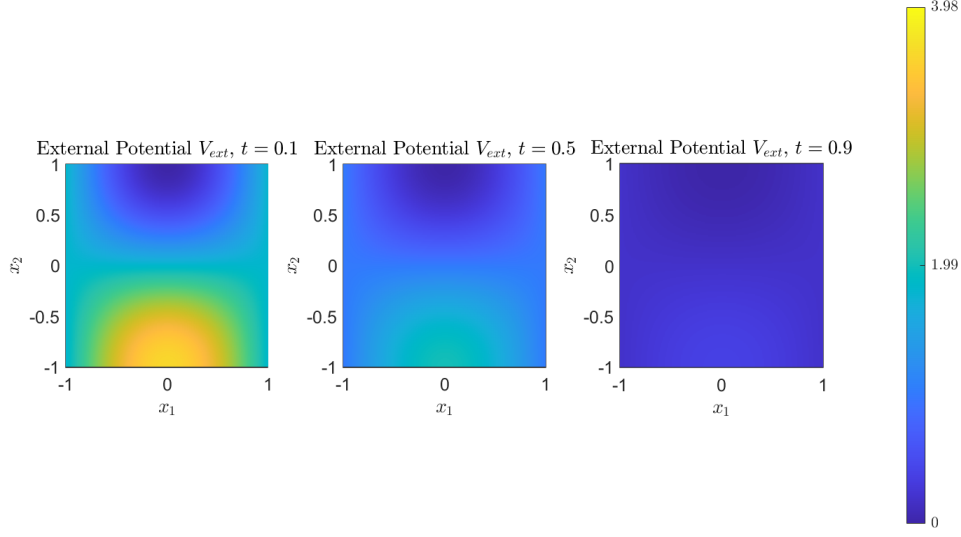


Figure 8: Dirichlet Source Control: External Potential V_{ext} acting on ρ .

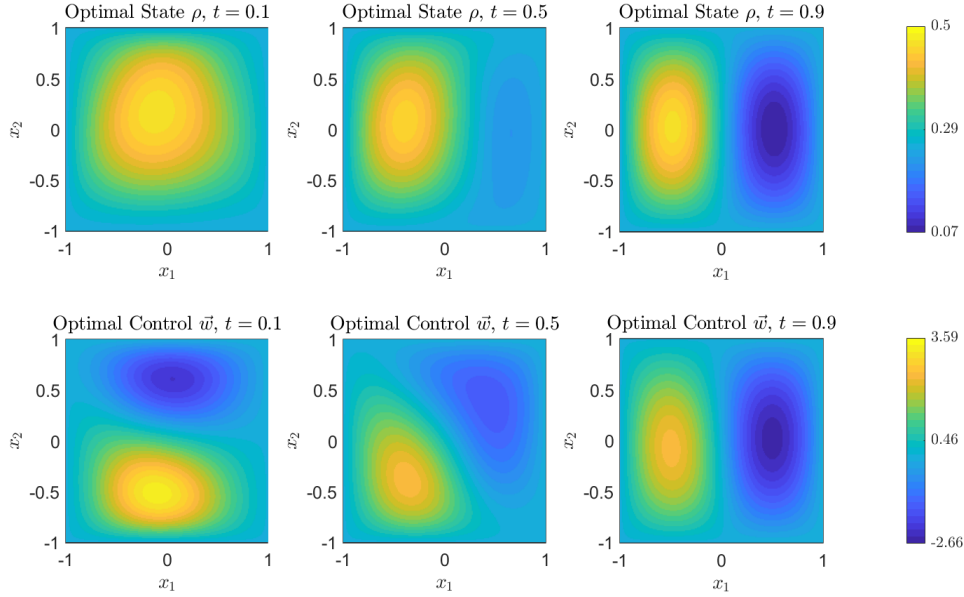


Figure 9: Dirichlet Source Control: Optimal ρ and optimal control for $\kappa = 0$ and $\beta = 10^{-3}$.

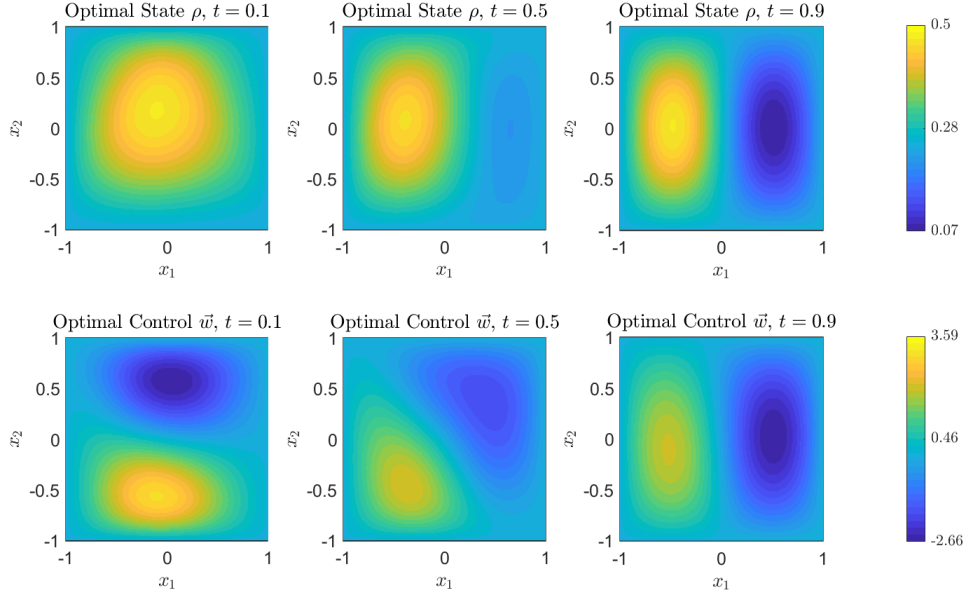


Figure 10: Dirichlet Source Control: Optimal ρ and optimal control for $\kappa = -1$ and $\beta = 10^{-3}$.

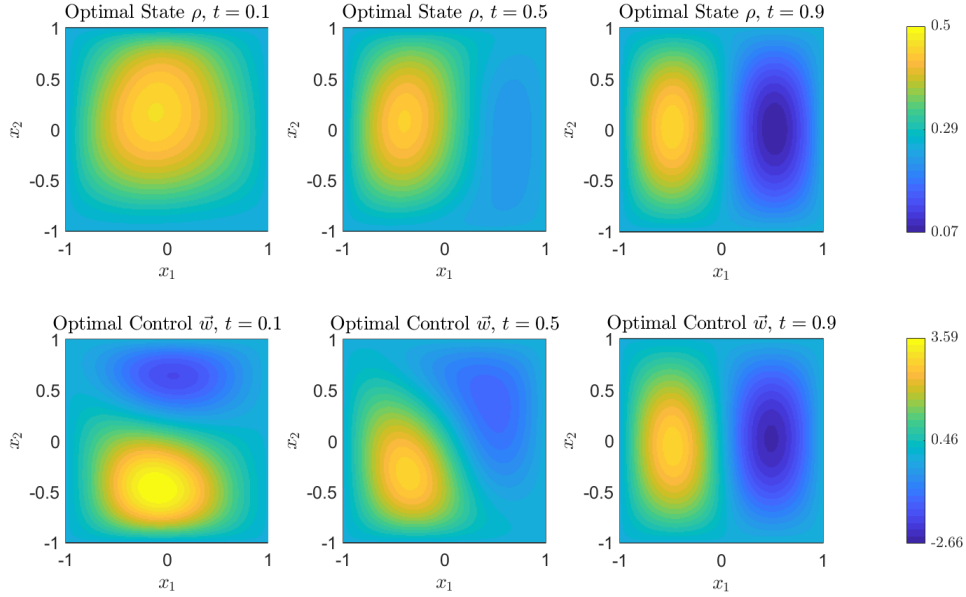


Figure 11: Dirichlet Source Control: Optimal ρ and optimal control for $\kappa = 1$ and $\beta = 10^{-3}$.

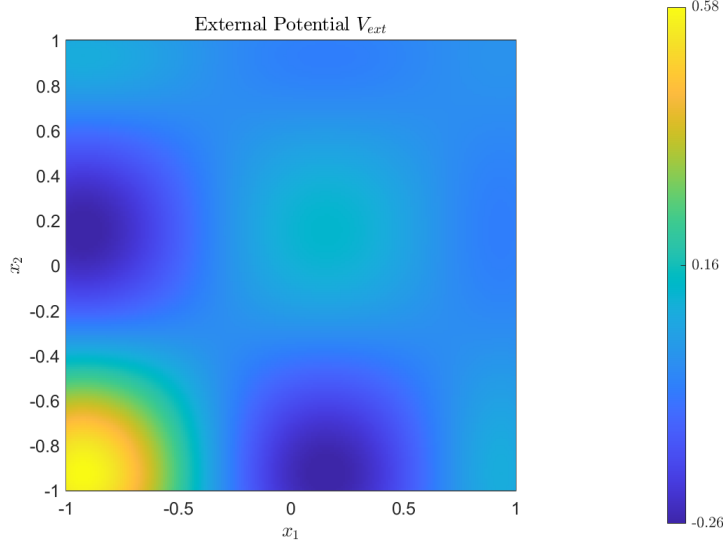


Figure 12: Neumann Flow Control: External Potential V_{ext} acting on ρ .

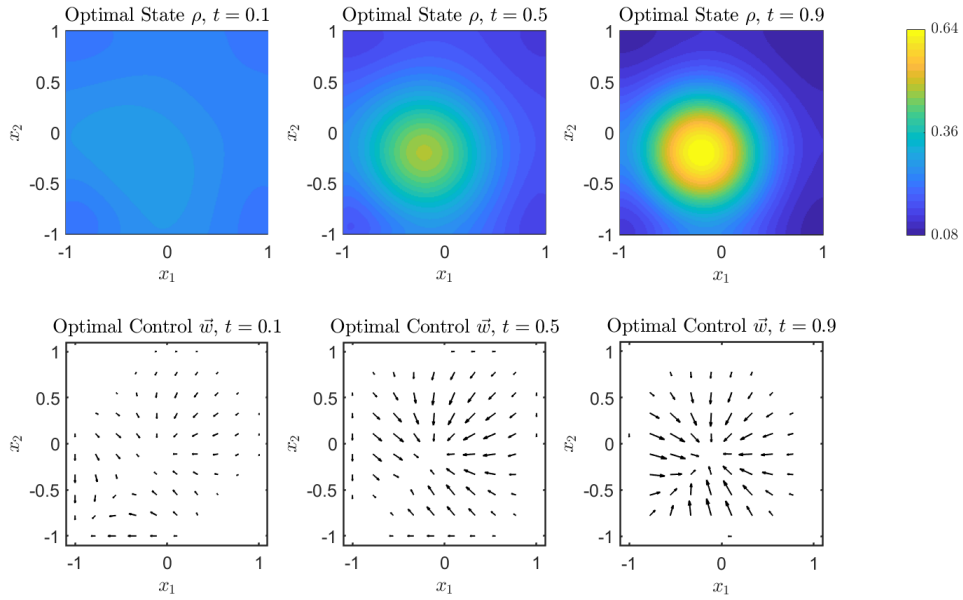


Figure 13: Neumann Flow Control: Optimal ρ and optimal control for $\kappa = 0$ and $\beta = 10^{-3}$.

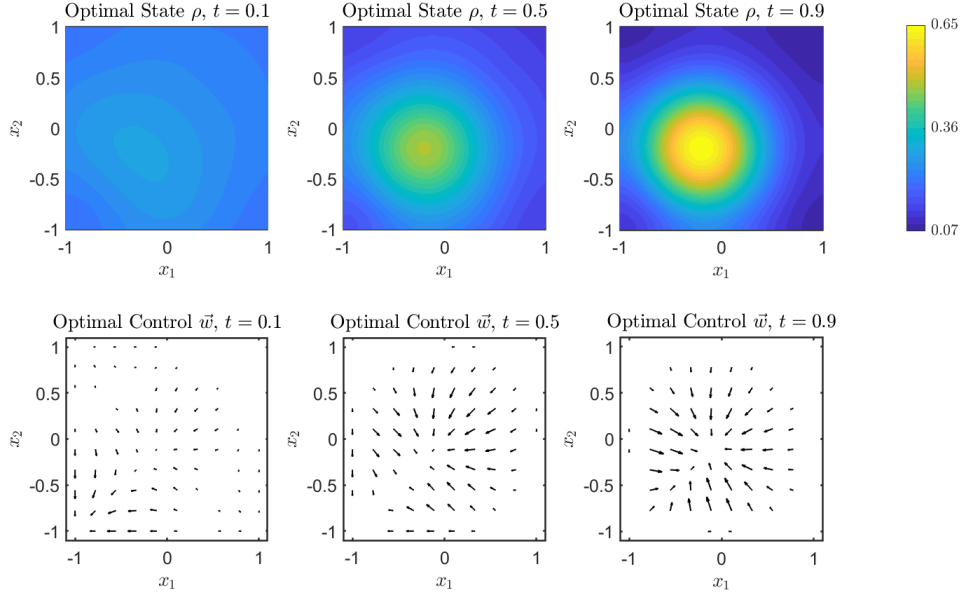


Figure 14: Neumann Flow Control: Optimal ρ and optimal control for $\kappa = -1$ and $\beta = 10^{-3}$.

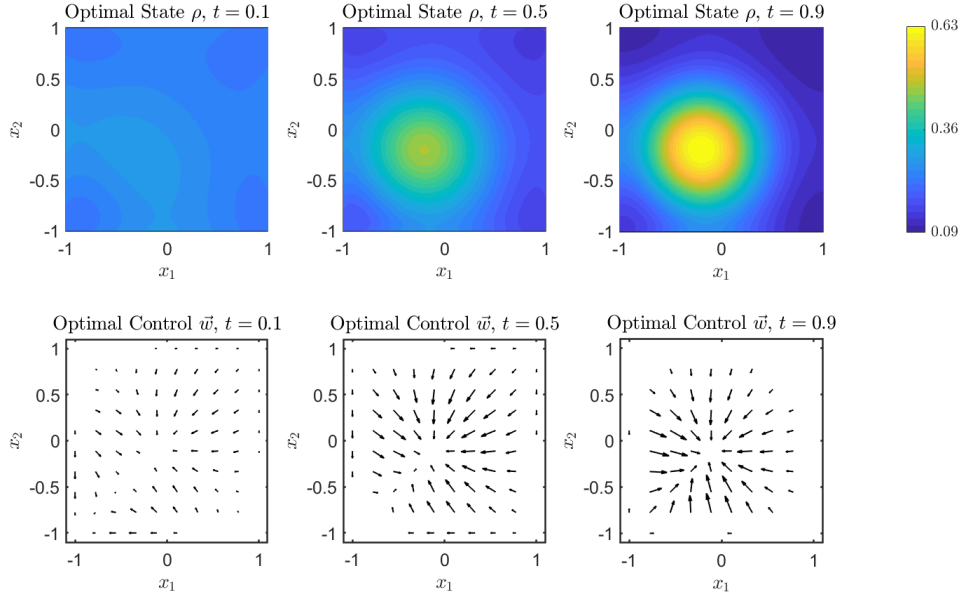


Figure 15: Neumann Flow Control: Optimal ρ and optimal control for $\kappa = 1$ and $\beta = 10^{-3}$.

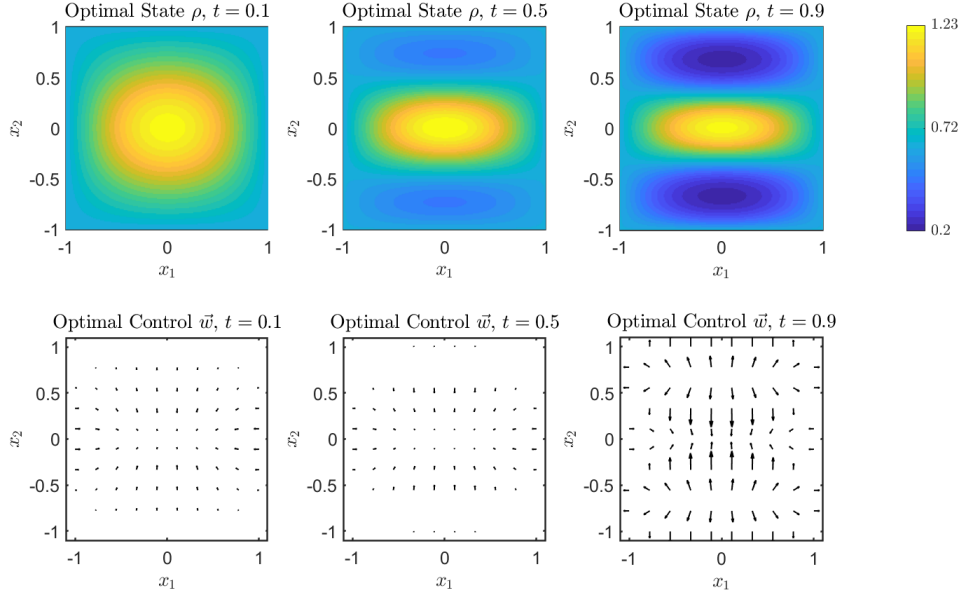


Figure 16: Dirichlet Flow Control: Optimal ρ and optimal control for $\kappa = 0$ and $\beta = 10^{-3}$.

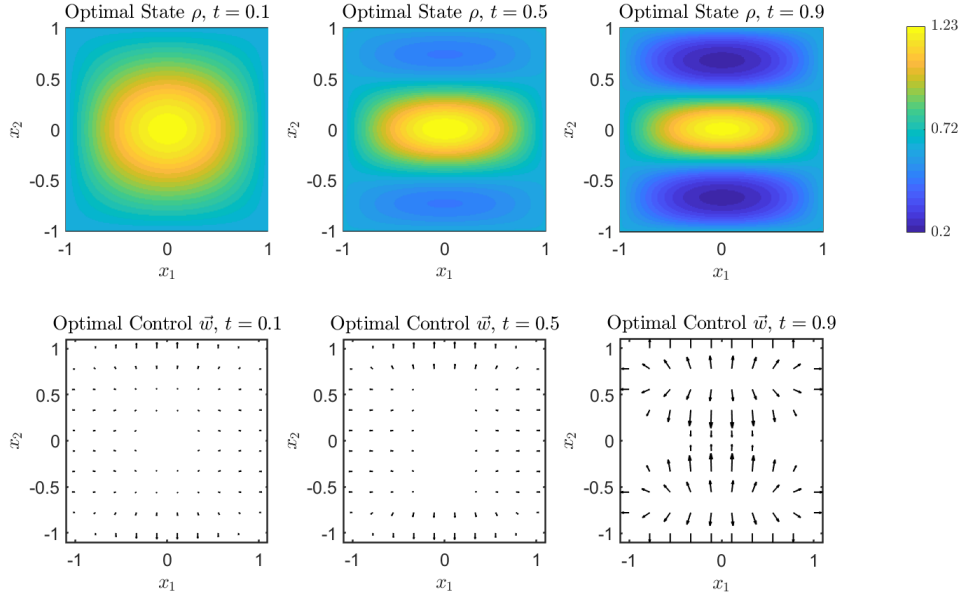


Figure 17: Dirichlet Flow Control: Optimal ρ and optimal control for $\kappa = -1$ and $\beta = 10^{-3}$.

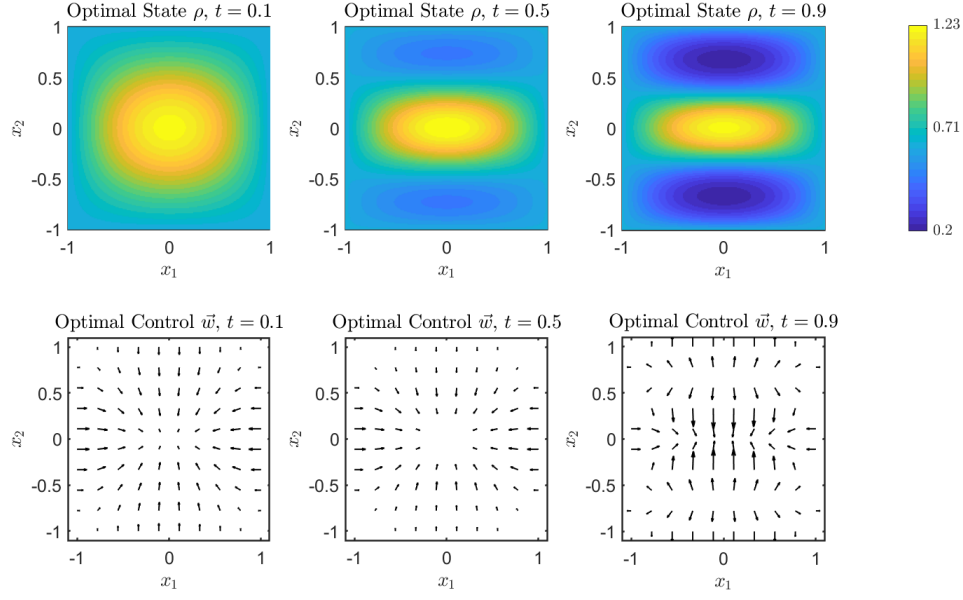


Figure 18: Dirichlet Flow Control: Optimal ρ and optimal control for $\kappa = 1$ and $\beta = 10^{-3}$.

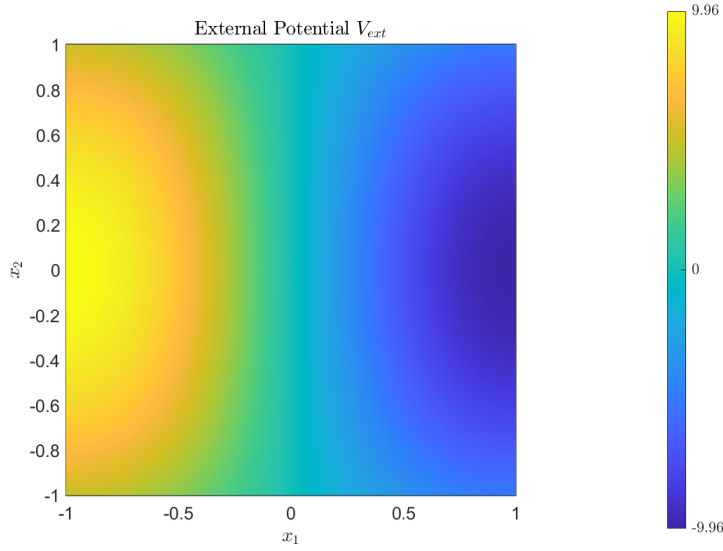


Figure 19: Dirichlet Flow Control 2: External Potential V_{ext} acting on ρ .

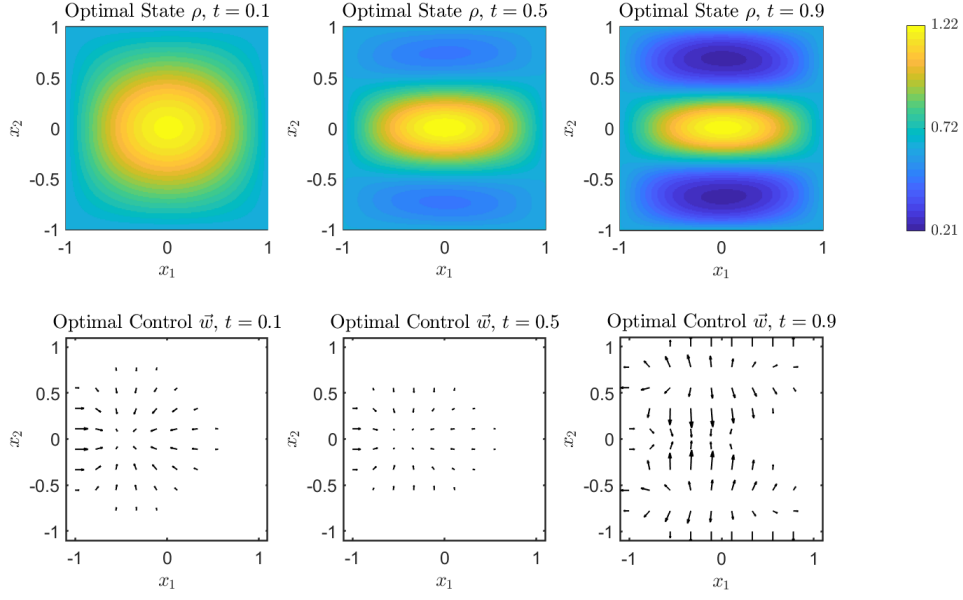


Figure 20: Dirichlet Flow Control 2: Optimal ρ and optimal control for $\kappa = 0$ and $\beta = 10^{-3}$.

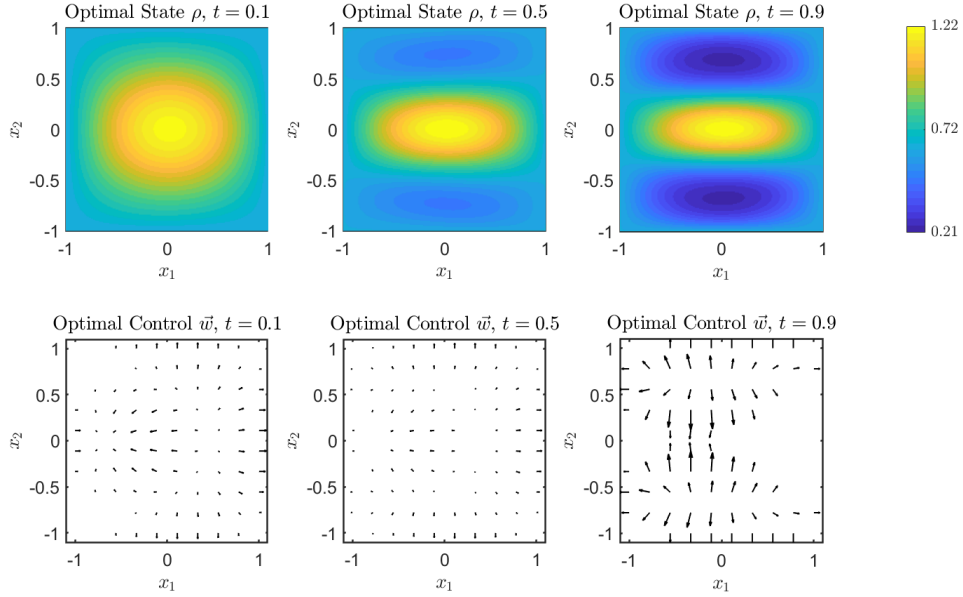


Figure 21: Dirichlet Flow Control 2: Optimal ρ and optimal control for $\kappa = -1$ and $\beta = 10^{-3}$.

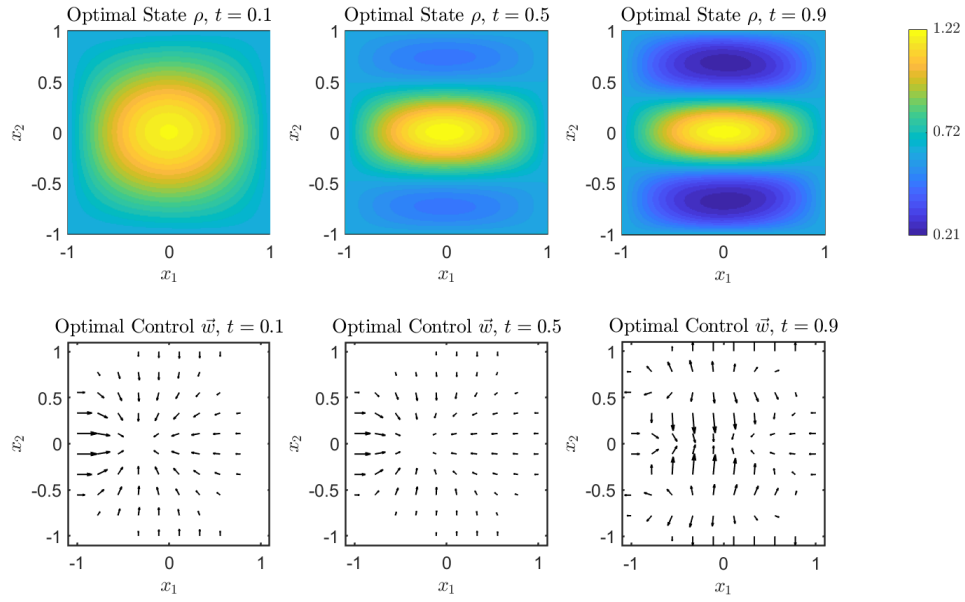


Figure 22: Dirichlet Flow Control 2: Optimal ρ and optimal control for $\kappa = 1$ and $\beta = 10^{-3}$.