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Application of Physics-Informed Neural Networks (PINNs) to Solve a Dynamic Model of Drug Abuse

Chyntia Meininda Anjanni

Gadjah Mada University

Sumardi Sumardi

Gadjah Mada University

Fitri Cahyani

Gadjah Mada University

Abstract: Drug abuse remains a complex and persistent issue in Indonesia, requiring a systematic approach to understand its underlying dynamics. This study applies Physics-Informed Neural Networks (PINNs) as an alternative method for solving the nonlinear differential equations of the $S_n S_e IR$ drug abuse dynamics model. The model divides the population into four compartments: susceptible individuals without education (S_n), susceptible individuals with education (S_e), active users (I), and individuals who have quit or completed rehabilitation (R). The focus of this research is the forward problem, in which the solution of the model is approximated using parameter values obtained from the literature. The PINNs framework combines a data loss term, which measures the discrepancy between predicted solutions and synthetic data, and a physics loss term that enforces consistency with the governing differential equations. The performance of PINNs was first validated by comparing its results with synthetic data generated using the classical fourth-order Runge–Kutta (RK4) method. The model was then further tested using additional synthetic datasets to evaluate generalization. The findings demonstrate that PINNs can successfully approximate the solution of the $S_n S_e IR$ model, yielding continuous and mathematically consistent trajectories that align with the system's dynamics. Moreover, the mesh-free nature of PINNs provides flexibility and computational efficiency, highlighting its potential as a promising tool for analysing complex population-based models.

Keywords: Physics-Informed Neural Networks (PINNs), $S_n S_e IR$ model, Differential equations, Drug abuse dynamics, Forward problem;

Introduction

Drug misuse continues to be a significant public health issue with substantial social and economic consequences. Global reports consistently highlight a rising number of drug users. WHO (2024) estimates that psychoactive substances contribute to hundreds of thousands of deaths annually, while UNODC (2024) reports that more than 296 million people worldwide used illicit drugs in 2021. A similar trend is observed in Indonesia. Data from BNN (2025) indicate that the number of drug users has reached several million, accompanied by high mortality rates and an increasing number of drug-related criminal cases. These findings underscore the need for a systematic understanding of the mechanisms that drive drug-use dynamics within a population.

Mathematical modelling provides a structured framework for analysing such dynamics by dividing the population into compartments and representing transitions between them using differential equations (Boyce, 2017). This approach has been widely adopted to study epidemiological and social processes, including addiction-related behaviours. One model particularly relevant to drug misuse is the $S_n S_e IR$ model introduced by Husain et al.

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(2020), which distinguishes between susceptible individuals without education (S_n) and those who receive preventive education (S_e). This structure enables direct evaluation of how educational interventions influence transitions into drug use. Husain et al. (2020) showed that higher levels of public education can reduce the number of active users and lower the system's basic reproduction number. However, due to its nonlinear structure, the model offers limited analytic tractability, and conventional numerical methods may encounter challenges related to discretisation, accuracy, and stability (Ezadi, 2013; Resmawan, 2023).

Advances in machine learning provide promising alternatives for addressing these limitations. Physics-Informed Neural Networks (PINNs), introduced by Raissi et al. (2017), integrate the governing differential equations directly into the training process of neural networks. Rather than relying solely on data, PINNs ensure that the learned solution adheres to the mathematical laws underlying the system. This approach has demonstrated strong performance in producing accurate, mesh-free solutions across various scientific fields, including biological and epidemiological modelling (Karniadakis, 2021; Farea, 2025).

Despite the increasing use of PINNs in scientific computing, their application to drug abuse dynamics models remains limited. In particular, the $S_n S_e IR$ model incorporating educational interventions has rarely been explored using physics-informed learning approaches. Therefore, investigating whether PINNs can accurately approximate the dynamics of this model becomes an important research question.

Building on these developments, the present study applies PINNs to approximate solutions of the $S_n S_e IR$ drug misuse model using a forward-problem formulation. The model parameters are adopted from Husain et al. (2020). The accuracy of the PINNs approximation is first assessed using synthetic data generated with the classical fourth-order Runge–Kutta (RK4) method (Burden, 2011), followed by additional evaluation using synthetic observational datasets. Overall, this study aims to demonstrate the capability of PINNs as an efficient and flexible tool for analysing complex social dynamics governed by nonlinear differential equations.

Model Formulation

Compartmental models, including the classical Susceptible–Infected–Recovered (SIR) framework introduced by Kermack and McKendrick (1927), have long been used to describe the spread of infectious diseases and other social processes with similar dynamic patterns. While the SIR model provides a fundamental foundation, it does not distinguish different levels of susceptibility nor incorporate preventive interventions. To address these limitations, this study adopts the $S_n S_e IR$ model proposed by Husain et al. (2020), which extends the classical structure by including the influence of educational programs within the susceptible population.

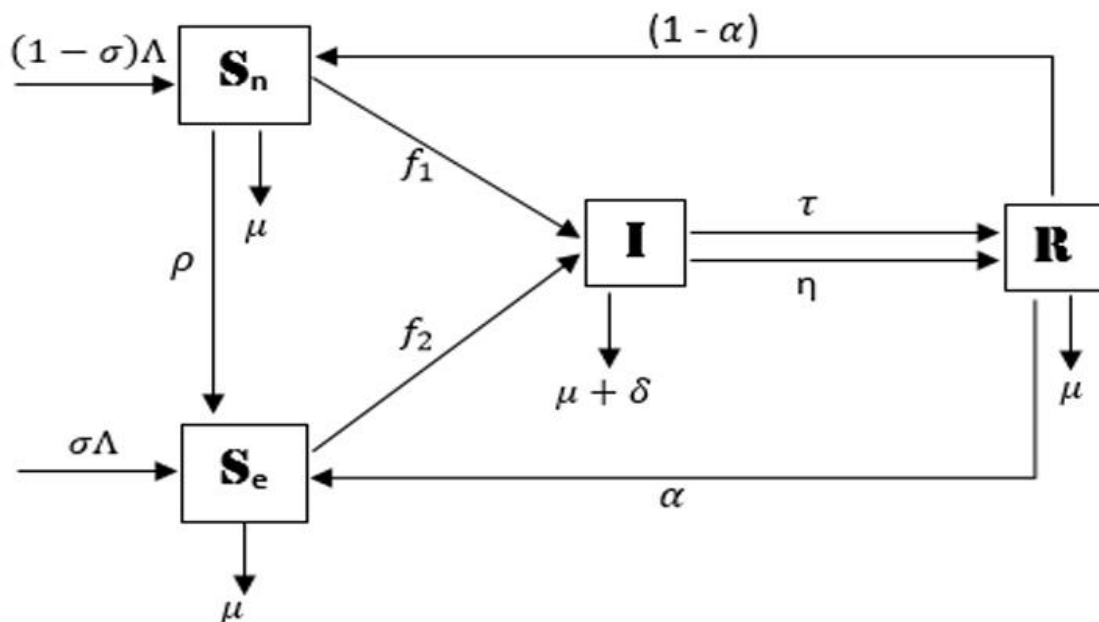


Figure 1. Schematic diagram of the drug-use transmission model
Source: Husain et al. (2020)

To provide a clearer understanding of how individuals transition between compartments, the interaction patterns in the $S_n S_e IR$ model are illustrated through a compartmental diagram. The schematic representation outlines the movement of individuals among susceptible groups (with and without education), active drug users, and those who have recovered or undergone rehabilitation. It also highlights the mechanisms of education, relapse, treatment, and mortality that drive the system's dynamics over time. This diagram serves as a visual guide for interpreting the mathematical relationships that will be formalized in the subsequent differential equations.

The diagram illustrates the flow of individuals among four compartments: susceptible without education (S_n), susceptible with education (S_e), active users (I), and recovered or rehabilitated individuals (R). Recruitment enters the susceptible population with proportions $(1 - \sigma)\Lambda$ for uneducated individuals and $\sigma\Lambda$ for educated individuals. Transitions from S_n to S_e occur at rate ρ , while interactions with active users lead to new users through the incidence terms f_1 and f_2 . Individuals in the I compartment may stop using drugs through voluntary cessation (τ) or rehabilitation (η), moving into the recovery compartment R . A fraction α of those recovered may return to the educated susceptible group, while the remaining $(1 - \alpha)$ re-enter the uneducated susceptible group. All compartments experience natural mortality at rate μ , with an additional mortality rate δ applied to active users. The structure summarizes how educational efforts, relapse, treatment, and behavioral transitions jointly influence the dynamics of drug misuse.

Model Structure

The population is divided into four compartments:

- $S_n(t)$: susceptible individuals without education
- $S_e(t)$: susceptible individuals who have received drug-prevention education
- $I(t)$: active drug users who may influence others
- $R(t)$: individuals who have quit drug use or completed rehabilitation

The total population $N(t)$ is assumed to remain constant, leading to the relationship:

$$S_n(t) = N(t) - (S_e(t) + I(t) + R(t))$$

Table 1. Variables of the $S_n S_e IR$ Model

Variables	Description
$S_n(t)$	Susceptible individuals without education
$S_e(t)$	Susceptible individuals with education
$I(t)$	Active drug users
$R(t)$	Recovered/rehabilitated individuals

Parameters

The model incorporates demographic processes, educational intervention, transmission dynamics, and relapse mechanisms. Parameter definitions are summarised below.

Table 2. Parameters of the $S_n S_e IR$ model

Parameter	Description
Λ	Recruitment rate into the susceptible population
σ	Fraction of newly recruited individuals receiving education
μ	Natural death rate
δ	Additional death rate in the user compartment
ρ	Rate of transition from uneducated to educated susceptibles
β_1	Contact rate between (S_n) and (I)
β_2	Contact rate between (S_e) and (I)
η	Rehabilitation rate of active users
τ	Rate at which users stop using drugs (voluntary cessation)
α	Fraction of recovered individuals returning to (S_e)

Source: Husain et al. (2020)

Following the mass-action incidence formulation described by Hethcote (2000), the contact terms are defined as:

$$f_1 = \beta_1 \frac{S_n I}{N}, f_2 = \beta_2 \frac{S_e I}{N}$$

Educational intervention and relapse dynamics follow the formulation of Li et al. (2018). Recovered individuals may return either to the educated susceptible group S_e with proportion α or to the uneducated group S_n with proportion $1 - \alpha$.

Model Equations

Combining the demographic, educational, transmission, recovery, and relapse mechanisms, the population dynamics are governed by the following nonlinear ordinary differential equations (Husain et al., 2020):

$$\begin{aligned} \frac{dS_n}{dt} &= (1 - \sigma)\Lambda + (1 - \alpha)R - \beta_1 \frac{S_n I}{N} - \rho S_n - \mu S_n, \\ \frac{dS_e}{dt} &= \sigma\Lambda + \rho S_n + \alpha R - \beta_2 \frac{S_e I}{N} - \mu S_e, \\ \frac{dI}{dt} &= \beta_1 \frac{S_n I}{N} + \beta_2 \frac{S_e I}{N} - (\eta + \tau + \mu + \delta)I, \\ \frac{dR}{dt} &= (\eta + \tau)I - \alpha R - \mu R - (1 - \alpha)R. \end{aligned}$$

The resulting system forms a nonlinear ODE model describing the impact of education, interaction rates, cessation, rehabilitation, and relapse on the spread of drug misuse within a population.

Method

This study employs Physics-Informed Neural Networks (PINNs) to approximate the solution of the nonlinear differential equations governing the $S_n S_e I R$ drug misuse model. The methodology consists of several stages: formulation of the compartmental model, generation of synthetic data using a conventional numerical method, construction of the PINNs framework, and validation of the results.

Formulation of the $S_n S_e I R$ Model

The mathematical model used in this study is based on the compartmental formulation developed by Husain et al. (2020). The population is divided into four groups: susceptible individuals without education (S_n), susceptible individuals with education (S_e), active drug users (I), and recovered or rehabilitated individuals (R). The dynamics of each compartment are described by a system of nonlinear ordinary differential equations incorporating recruitment, education, interaction rates, recovery, relapse, and mortality. The complete formulation has been presented in Section 2. This model constitutes the physical law that must be satisfied by the PINNs approximation through its physics-informed loss component.

Synthetic Data Generation Using RK4

Before applying PINNs, synthetic data were generated to serve as reference trajectories for the system. The fourth-order Runge–Kutta (RK4) method was selected because of its stability and accuracy in solving nonlinear differential equations. Using parameter values adopted from Husain et al. (2020), the model was simulated over a fixed time interval with initial conditions chosen to reflect realistic population proportions. The resulting trajectories for $S_n(t)$, $S_e(t)$, $I(t)$, and $R(t)$ were then used both as training supervision, where selected RK4 points contributed to the data-loss term, and as a validation benchmark, where the complete RK4 solution was used to evaluate the accuracy of the PINNs approximation.

Model Parameters

To generate the synthetic data used for training and validating the PINNs model, the $S_n S_e IR$ model system was simulated using a set of parameter values adapted from Husain et al. (2020) and supplemented with reasonable assumptions commonly used in compartmental modelling. These parameters govern the recruitment rate, education effect, transmission intensity, recovery mechanisms, and mortality processes within the population. Since this study focuses exclusively on the forward problem, all parameters remain fixed during the PINNs training phase and are not subject to estimation.

The initial conditions for the simulation were set to

$$S_n(0) = 250, S_e(0) = 200, I(0) = 50, R(0) = 0,$$

representing the initial distribution of individuals across the four compartments. The complete set of parameters used in the simulations is summarised in Table 3.

Table 3. Parameter values used in the simulation of the $S_n S_e IR$ model

Parameter	Description	$R_0 < 1$	$R_0 > 1$	Source
σ	Fraction of new individuals receiving education	0.20	0.40	Assumed
ρ	Education rate from S_n to S_e	0.10	0.10	Assumed
μ	Natural death rate	0.02	0.02	Burattini et al. (1998)
β_1	Transmission rate for S_n	0.12	0.20	Nyabadza dan Musekwa (2010)
β_2	Transmission rate for S_e	0.12	0.20	Nyabadza dan Musekwa (2010)
τ	Voluntary cessation rate	0.01	0.008	Assumed
δ	Additional death rate in I	0.03	0.02	Burattini et al. (1998)
Λ	Recruitment rate	10	14	Assumed
α	Fraction of recovered individuals returning to S_e	0.09	0.09	Assumed
η	Rehabilitation rate	0.15	0.07	Nyabadza dan Musekwa (2010)

Source: Husain et al. (2020)

These parameters determine the qualitative behaviour of the model, including the rate at which individuals transition between susceptibility, education, active use, and recovery. The two parameter sets correspond to scenarios with $R_0 < 1$ and $R_0 > 1$, allowing the system to exhibit different dynamic regimes. In this study, the PINNs framework is evaluated under these fixed parameter configurations to analyse its ability to approximate the forward solution of the model.

PINNs Architecture

The architecture of the Physics-Informed Neural Networks (PINNs) used in this study follows the general formulation for forward problems as presented by Farea et al. (2025). In this framework, the neural network is trained to approximate the solution of a system of nonlinear differential equations while respecting the governing physical laws represented by the mathematical model.

Consider a general ordinary differential equation of the form

$$\frac{dx}{dt} = f(t, x)$$

In the PINNs framework, the unknown solution $x(t)$ is approximated by the output of a neural network defined as

$$\hat{x}(t) = f_N(t; \theta)$$

where θ represents the parameters of the neural network consisting of weights and biases.

Because the governing equation involves derivatives with respect to time, the derivative of the neural network output must also be computed. In PINNs, this derivative is obtained using automatic differentiation as

$$\frac{d\hat{x}(t)}{dt}$$

Based on this formulation, the residual of the differential equation is defined as

$$r(t) = \frac{d\hat{x}(t)}{dt} - f(t, \hat{x}(t))$$

The residual measures how well the neural network prediction satisfies the governing differential equation. If the residual approaches zero, the neural network output satisfies the mathematical structure of the system.

To enforce this condition, the residual is incorporated into the physics-informed loss function defined as

$$\mathcal{L}_f = \frac{1}{N_f} \sum_{i=1}^{N_f} |r(t_i)|^2$$

where N_f denotes the number of collocation points.

In this study, the neural network receives the time variable $t \in [0, T]$ as input and produces a four-dimensional vector representing the approximate solution of the $S_n S_e IR$ system

$$\hat{X}(t) = (\hat{S}_n(t), \hat{S}_e(t), \hat{I}(t), \hat{R}(t))$$

The time derivatives of the network output are computed as

$$\frac{d\hat{X}}{dt}(t) = \left(\frac{d\hat{S}_n}{dt}, \frac{d\hat{S}_e}{dt}, \frac{d\hat{I}}{dt}, \frac{d\hat{R}}{dt} \right)$$

These derivatives are compared with the right-hand side of the dynamical system

$$F(\hat{X}(t)) = (f_{S_n}(t), f_{S_e}(t), f_I(t), f_R(t))$$

The residual of the system at a collocation point t_i is defined as

$$r(t_i) = \frac{d\hat{X}}{dt}(t_i) - F(\hat{X}(t_i))$$

The physics loss is therefore given by

$$\mathcal{L}_f = \frac{1}{N_f} \sum_{i=1}^{N_f} |r(t_i)|^2$$

In addition to the physics loss, the network is trained using synthetic data generated by the classical fourth-order Runge–Kutta (RK4) method. If $X(t_j)$ denotes the reference solution at time t_j , the data loss is defined as

$$\mathcal{L}_d = \frac{1}{N_d} \sum_{j=1}^{N_d} \|\hat{X}(t_j) - X(t_j)\|^2$$

Finally, the total loss minimized during training is expressed as

$$\mathcal{L}_{total} = \lambda_f \mathcal{L}_f + \lambda_d \mathcal{L}_d$$

where λ_f and λ_d are weighting parameters that balance the contribution of the physics loss and the data loss.

The optimisation process is carried out using the Adam optimizer to minimise the total loss function. At each iteration, the parameters of the neural network are updated using gradient-based optimisation computed through automatic differentiation. The training process continues until the loss value converges and the neural network provides a stable approximation of the solution of the $S_n S_e IR$ model.

Collocation Point Selection

Collocation points were placed within the time domain to ensure that the neural network solution adhered to the structure of the differential equations. In this study, the points were selected uniformly across the simulation interval so that the dynamics of the $S_n S_e IR$ system were represented throughout the entire time range. Although the model may contain periods where changes occur more rapidly, especially in the active user compartment $I(t)$, the use of a uniform distribution helps maintain numerical stability during training. When necessary, additional points can be introduced in regions where the solution varies more sharply to improve the accuracy of the residual evaluation.

Training Procedure

The training process was carried out using the Adam optimizer to minimize the total loss function. During each iteration, the parameters of the neural network were updated through gradient-based optimization using automatic differentiation. This process allows the derivatives of the network output with respect to time to be computed accurately and incorporated into the physics-informed loss function. Because this study focuses solely on the forward problem, all model parameters were kept fixed during the training process. The optimization was therefore directed entirely toward learning a continuous approximation of the solution trajectories $S_n(t)$, $S_e(t)$, $I(t)$, and $R(t)$. The training procedure continued until the total loss function reached a stable value and the residuals of the governing differential equations became sufficiently small, indicating that the neural network solution satisfied both the data and the physical constraints of the $S_n S_e IR$ model.

Validation and Evaluation

The performance of the PINNs model was evaluated by comparing its predicted trajectories with the reference solutions obtained from the classical fourth-order Runge–Kutta (RK4) numerical method. The trajectories produced by the neural network were plotted together with the RK4 solutions to examine the level of agreement between the two approaches across the entire simulation interval.

Since this study relies exclusively on synthetic data and does not involve real observational data, the evaluation focuses on how accurately the PINNs approximation reproduces the reference RK4 solution. This comparison allows the reliability of the PINNs method to be assessed in capturing the nonlinear dynamics of the $S_n S_e IR$ model. A close agreement between the predicted trajectories and the RK4 solutions indicates that the PINNs framework is capable of accurately approximating the forward solution of the governing system of differential equations.

Results and Discussion

This section presents the numerical results obtained from applying Physics-Informed Neural Networks (PINNs) to approximate the forward solution of the $S_n S_e IR$ model under two parameter regimes: $R_0 > 1$ and $R_0 < 1$. The accuracy of the method is evaluated by comparing the predicted trajectories with the synthetic benchmark produced using the classical Runge–Kutta fourth-order (RK4) method.

Training Behaviour

The training process was carried out using the Adam optimizer to minimize the total loss function. The total loss decreased smoothly during the training process using the Adam optimizer and reached stable values of

approximately 10^{-4} . This behaviour indicates that the neural network successfully minimized both the data loss and the physics loss while capturing the nonlinear structure of the underlying system of differential equations. The stable convergence also demonstrates that the PINNs framework maintained numerical stability throughout the optimisation process. The small residual values indicate that the neural network solution satisfies the governing differential equations with high accuracy, demonstrating the effectiveness of the physics-informed constraint during the training process.

Results for the $R_0 > 1$ Scenario

When $R_0 > 1$, the system exhibits growth-dominated behaviour in which drug use initially increases before approaching equilibrium. This case presents a more complex transient structure, making it an appropriate test for evaluating the expressive capability of PINNs.

Active Users $I(t)$ and Recovered Individuals $R(t)$

The comparison between PINNs and RK4 for $I(t)$ shows that the network accurately reproduces the initial rise in the number of active users, followed by the gradual decline toward steady state. The early growth reflects the high transmission rates in the $R_0 > 1$ setting, whereas the subsequent decrease corresponds to recovery and mortality processes. The PINNs trajectory closely follows the RK4 solution throughout the simulation, including the peak region where the curve is highly nonlinear. A similar level of agreement is observed for the recovered population $R(t)$. The initial increase in $R(t)$ is captured with precision, illustrating the network's ability to track rapid transitions associated with intensified rehabilitation and cessation. As the system stabilises, the predicted curve remains nearly identical to the RK4 reference, confirming that PINNs can represent long-term behaviour accurately.

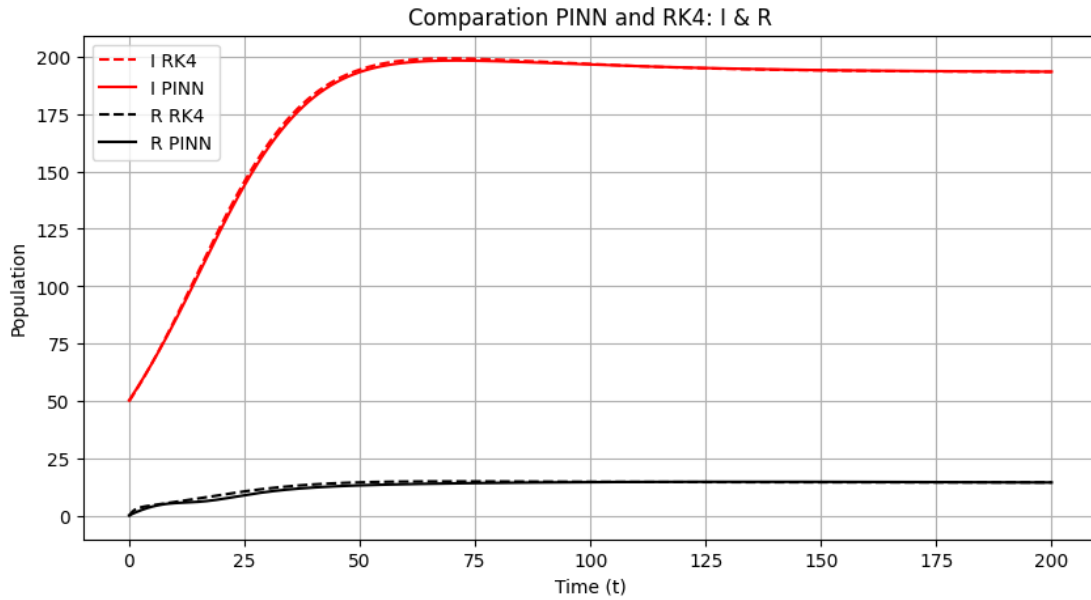


Figure 2. PINNs and RK4 solutions for $I(t)$ and $R(t)$ when $R_0 > 1$

Susceptible Populations $S_n(t)$ and $S_e(t)$

The uneducated susceptible population $S_n(t)$ decreases sharply at the beginning of the simulation due to its interactions with active users. PINNs successfully matches this sharp decline and continues to follow the RK4 curve closely as the system approaches equilibrium. For the educated susceptible group $S_e(t)$, both methods display an initial rapid increase followed by a gradual decrease toward a stable long-term value. This behaviour reflects the strong influence of education-related transitions in the $R_0 > 1$ regime. The close overlap between the two methods shows that PINNs can capture the full trajectory, including its transient rise and asymptotic decline.

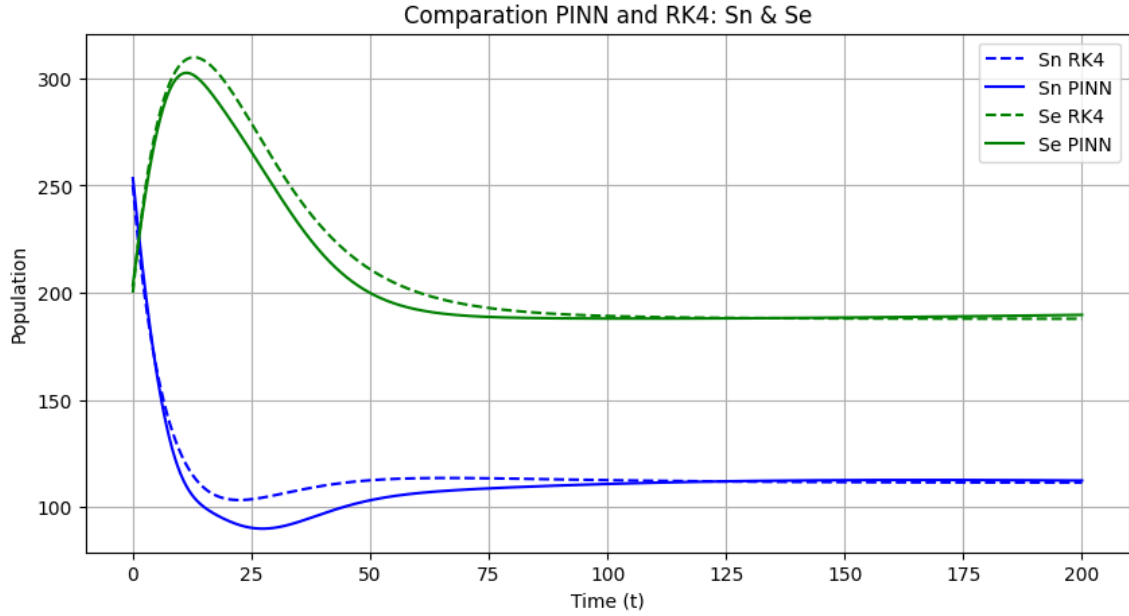


Figure 3. PINNs and RK4 solutions for $S_n(t)$ and $S_e(t)$ when $R_0 > 1$

Interpretation for the $R_0 > 1$ Case

Overall, the $R_0 > 1$ results reveal a system that experiences an early escalation in drug use, accompanied by substantial changes in the susceptible and recovered populations. PINNs is able to replicate these dynamics with a high degree of accuracy. The nearly perfect alignment of the predicted curves with the RK4 solutions suggests that the method is capable of learning both the rapid transient phase and the eventual stabilisation of the system.

Results for the $R_0 < 1$ Scenario

The $R_0 < 1$ regime represents a decay-dominated system in which drug use diminishes over time. This case is useful for assessing the network's ability to capture rapid decreases and long-term convergence toward a drug-free equilibrium.

Active Users $I(t)$ and Recovered Individuals $R(t)$

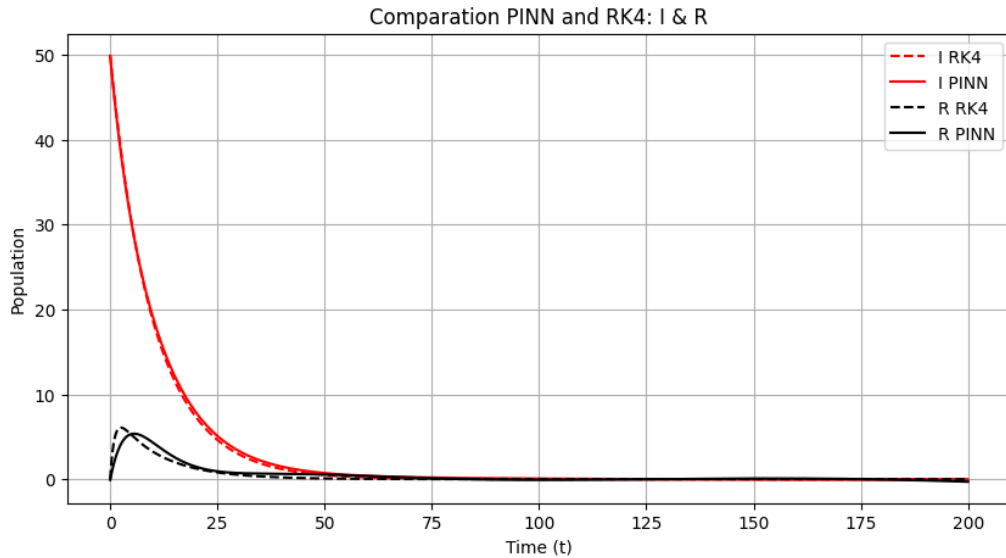


Figure 4. PINNs and RK4 solutions for $I(t)$ and $R(t)$ when $R_0 < 1$

In this scenario, $I(t)$ declines very rapidly from the initial condition. The PINNs approximation mirrors this steep exponential decline almost exactly, demonstrating the network's ability to reproduce fast transitions without numerical oscillation. As $I(t)$ approaches zero, the two solutions remain indistinguishable. For the recovered population $R(t)$, both methods show a small increase at early times followed by a gradual descent toward equilibrium. The PINNs curve matches the RK4 reference throughout the entire time domain, capturing both the mild curvature of the early phase and the smooth long-term behaviour.

Susceptible Populations $S_n(t)$ and $S_e(t)$

The behaviour of the susceptible populations reflects the decaying influence of drug users. The uneducated susceptible group $S_n(t)$ decreases quickly at first and then rises slowly as the number of active users approaches zero. PINNs reproduces this transition without deviation from the RK4 curve. The educated susceptible population $S_e(t)$ shows a modest initial increase followed by gradual convergence to a stable value, and the PINNs approximation remains consistent with the RK4 solution across the entire interval.

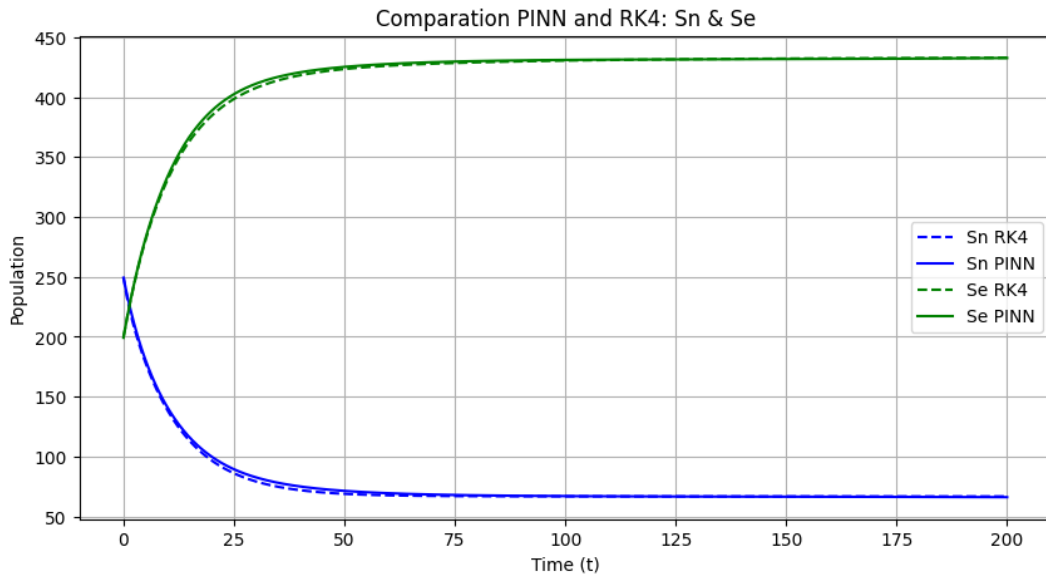


Figure 5. PINNs and RK4 solutions for $S_n(t)$ and $S_e(t)$ when $R_0 < 1$

Interpretation for the $R_0 < 1$ Case

The results for $R_0 < 1$ illustrate a system in which drug use declines rapidly and eventually disappears. All compartments move smoothly toward equilibrium as the influence of active users diminishes. The PINNs solutions are virtually identical to the RK4 benchmarks, indicating that the method is able to approximate decay-dominated dynamics with high precision.

The results demonstrate that the PINNs model successfully reproduces the RK4 numerical solutions for all compartments under both dynamic regimes. In the $R_0 > 1$ scenario, the network accurately captures the initial growth of active drug users followed by stabilization toward equilibrium. In contrast, when $R_0 < 1$, the system exhibits a rapid decay of the active user population toward a drug-free equilibrium. The close agreement between the PINNs predictions and the RK4 solutions confirms that the proposed approach can effectively approximate the nonlinear dynamics of the model.

Conclusion

This study applied Physics-Informed Neural Networks (PINNs) to approximate the forward solution of the $S_n S_e I R$ drug-misuse model and evaluated their performance using synthetic data generated through the classical fourth-order Runge–Kutta method. The results demonstrate that PINNs are capable of reconstructing the system's nonlinear dynamics with high accuracy across both parameter regimes considered, namely $R_0 > 1$ and $R_0 < 1$.

The predicted trajectories closely match the RK4 benchmark for all compartments, including those exhibiting rapid transitions such as the active-user population. The network produced smooth and dynamically consistent solutions while maintaining numerical stability throughout the optimisation process. These findings confirm that PINNs can faithfully integrate the governing differential equations into their learning process, enabling them to capture both transient behaviour and long-term equilibrium in a mesh-free manner. Given their ability to approximate complex dynamical systems with limited data, PINNs offer a promising alternative to traditional numerical solvers for modelling population-based social or epidemiological processes.

Future work may extend this framework to the inverse problem setting, allowing the estimation of key model parameters from real observational data, or explore broader applications that incorporate uncertainty quantification and more complex intervention structures.

Scientific Ethics Declaration

* The authors declare that the scientific ethical and legal responsibility of this article published in EPSTEM Journal belongs to the authors.

Conflict of Interest

* The authors declare that they have no conflicts of interest

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Author(s) Information

Chyntia Meininda Anjanni

Gadjah Mada University
Yogyakarta, Indonesia

*Contact e-mail: chyntiameinindaanjanni@mail.ugm.ac.id
ORCID iD: <https://orcid.org/0009-0002-5108-6759>

Sumardi Sumardi

Gadjah Mada University
Yogyakarta, Indonesia

ORCID iD: <https://orcid.org/0000-0002-7925-9351>

Fitri Cahyani

Gadjah Mada University
Yogyakarta, Indonesia

ORCID iD: <https://orcid.org/0009-0006-8290-6763>

* Corresponding author(s) email

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