Efficient algorithms for infectious disease resource allocation model

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Algorithm 1 Physics-Informed Neural Network (PINN) Training for Epidemic Modeling

Require: Training data tensors S_{data}, I_{data}, R_{data}, Time tensor t_{data}, Population N, Neural Network NN with weights w and biases b

Ensure: Preprocessed tensors on the same device

Initialize NN with Xavier initialization for weights w and biases b
Define early stopping criteria with patience and delta
Set learning rate lr and regularization parameters λ, p
for each epoch up to num_epochs **do**
    Compute predictions: S_{pred}, I_{pred}, $R_{pred} \leftarrow NN(t_{data})$
    Compute time derivatives of S_{pred}, I_{pred}, R_{pred} via autograd
    Calculate residuals using SIR model equations:

$$\frac{dS}{dt} = -\beta\frac{S_{pred}I_{pred}}{N}$$
$$\frac{dI}{dt} = \beta\frac{S_{pred}I_{pred}}{N} - \gamma I_{pred}$$
$$\frac{dR}{dt} = \gamma I_{pred}$$

    Compute loss function components:
    $MSE_{SIR} \leftarrow \frac{1}{q}\sum_{i=1}^{q}\left[(S_i - S_{pred_i})^2 + (I_i - I_{pred_i})^2 + (R_i - R_{pred_i})^2\right]$
    $MSE_{residuals} \leftarrow \frac{1}{q}\sum_{i=1}^{q}\left[\left(\frac{dS_i}{dt} - \frac{dS_{pred_i}}{dt}\right)^2 + \left(\frac{dI_i}{dt} - \frac{dI_{pred_i}}{dt}\right)^2 + \left(\frac{dR_i}{dt} - \frac{dR_{pred_i}}{dt}\right)^2\right]$
    $Loss \leftarrow MSE_{SIR} + MSE_{residuals} + \lambda \cdot \text{Regularization}(NN)$
    Update NN parameters via backpropagation and optimization step
    Adjust learning rate with learning rate scheduler if needed
    Check for early stopping, break if condition is met
end for
Output: Trained PINN model NN

The SIR model is described by the following set of differential equations:

$$\frac{dS}{dt} = -\beta\frac{SI}{N}, \tag{1}$$
$$\frac{dI}{dt} = \beta\frac{SI}{N} - \gamma I, \tag{2}$$
$$\frac{dR}{dt} = \gamma I, \tag{3}$$

where S is the number of susceptible individuals, I is the number of infectious individuals, R is the number of recovered individuals, and N is the total population.

Parameter	Definition
β	Transmission rate
γ	Recovery rate

Algorithm 2 Training of Physics-Informed Neural Network (PINN) for Epidemic Modeling

Require: Training data tensors S_{data}, I_{data}, R_{data}, time tensor t_{data}, population size N, initial learning rate lr, regularization parameters λ_{reg}, p_{reg}, and number of epochs num_epochs.

Ensure: All tensors are on the computational device, e.g., GPU.

Initialize PINN NN with weights w and biases b using Xavier initialization.
Define EarlyStopping class with patience, delta, and verbose output.
Set up the Adam optimizer with learning rate lr and weight decay.
Set up learning rate scheduler with reduction factor and patience.
for $epoch = 1$ to num_epochs **do**
    Compute predictions S_{pred}, I_{pred}, R_{pred} from $NN(t_{data})$.
    Compute gradients $\frac{dS_{pred}}{dt}$, $\frac{dI_{pred}}{dt}$, $\frac{dR_{pred}}{dt}$ with respect to t_{data} using automatic differentiation.
    Define the SIR model's theoretical dynamics:

$$\frac{dS}{dt} = -\beta\frac{SI}{N},$$
$$\frac{dI}{dt} = \beta\frac{SI}{N} - \gamma I,$$
$$\frac{dR}{dt} = \gamma I.$$

    Compute the loss components:

$$MSE_{SIR} = \frac{1}{q}\sum_{i=1}^{q}\left[(S_i - S_{pred_i})^2 + (I_i - I_{pred_i})^2 + (R_i - R_{pred_i})^2\right],$$

$$MSE_{residuals} = \frac{1}{q}\sum_{i=1}^{q}\left[\left(\frac{dS_{pred_i}}{dt} + \beta\frac{S_{pred_i}I_{pred_i}}{N}\right)^2 + \left(\frac{dI_{pred_i}}{dt} - \beta\frac{S_{pred_i}I_{pred_i}}{N} + \gamma I_{pred_i}\right)^2 + \left(\frac{dR_{pred_i}}{dt} - \right.\right.$$

    Compute regularization term (if L2 regularization is used):

$$Reg_{L2} = \lambda_{reg}\sum_{w}\|w\|^{p_{reg}}.$$

    Compute total loss:

$$Loss = MSE_{SIR} + MSE_{residuals} + Reg_{L2}.$$

    Perform backpropagation and update PINN parameters using the optimizer.
    Update learning rate with scheduler based on the validation loss.
    if EarlyStopping condition is met **then**
        break
    end if
    if $(epoch + 1) \mod 100 = 0$ or $epoch = 0$ **then**
        Log current epoch and loss for monitoring.
    end if
end for
Output: Trained PINN NN.

Algorithm 3 Physics-Informed Neural Network (PINN) for SIR Dynamics

Require: Training dataset $\mathcal{D} = \{(t_i, S_i, I_i, R_i)\}_{i=1}^{N}$, where t_i denotes time, and S_i, I_i, R_i represent susceptible, infected, and recovered individuals at time t_i, respectively.

Data Preprocessing:

Convert $\mathcal{D}$ into tensors: $\mathbf{S}, \mathbf{I}, \mathbf{R} \in \mathbb{R}^{N\times 1}$ and $\mathbf{t} \in \mathbb{R}^{N\times 1}$.

Neural Network Architecture:

Define a fully connected neural network $\mathcal{N}(\mathbf{t}; \theta)$ with input $\mathbf{t}$, parameters θ, hidden layers, and Tanh activation functions. The network predicts $\hat{\mathbf{S}}, \hat{\mathbf{I}}, \hat{\mathbf{R}}$ at times $\mathbf{t}$.

Loss Function:

The loss function $\mathcal{L}(\theta)$ consists of two parts: the prediction loss and the differential equation loss.

Prediction loss: $\mathcal{L}_{\text{pred}} = \frac{1}{N}\sum_{i=1}^{N}\left(||\hat{\mathbf{S}}_i - \mathbf{S}_i||^2 + ||\hat{\mathbf{I}}_i - \mathbf{I}_i||^2 + ||\hat{\mathbf{R}}_i - \mathbf{R}_i||^2\right)$.

DE loss: Compute the gradients $\frac{d\hat{\mathbf{S}}}{dt}, \frac{d\hat{\mathbf{I}}}{dt}, \frac{d\hat{\mathbf{R}}}{dt}$ using automatic differentiation. Use these to define the SIR model's dynamics:

$$\begin{aligned}
\frac{dS}{dt} &= -\beta\frac{SI}{N}, \\
\frac{dI}{dt} &= \beta\frac{SI}{N} - \gamma I, \\
\frac{dR}{dt} &= \gamma I.
\end{aligned}$$

$\mathcal{L}_{\text{DE}} = \frac{1}{N}\sum_{i=1}^{N}\left(||\frac{d\hat{\mathbf{S}}_i}{dt} + \beta\frac{\hat{\mathbf{S}}_i\hat{\mathbf{I}}_i}{N}||^2 + ||\frac{d\hat{\mathbf{I}}_i}{dt} - \beta\frac{\hat{\mathbf{S}}_i\hat{\mathbf{I}}_i}{N} + \gamma\hat{\mathbf{I}}_i||^2 + ||\frac{d\hat{\mathbf{R}}_i}{dt} - \gamma\hat{\mathbf{I}}_i||^2\right)$.

Total loss: $\mathcal{L} = \mathcal{L}_{\text{pred}} + \mathcal{L}_{\text{DE}}$.

Training:

Use gradient descent to minimize $\mathcal{L}(\theta)$ with respect to θ.

Apply early stopping based on validation loss to prevent overfitting.

Evaluation:

Evaluate the trained model $\mathcal{N}(\mathbf{t}; \theta^*)$ on test data to predict $\hat{\mathbf{S}}, \hat{\mathbf{I}}, \hat{\mathbf{R}}$.

Compare predictions with actual data to assess model performance.

Algorithm 4 PINNs used to determine simultaneously the parameters of the neural network and the embedded SIR model.

Require: Time points t, initial susceptible S^0, infected I^0, and recovered R^0 populations.

Randomly initialize weights w, biases b, and dynamics parameters β, γ;
for each epoch in epochs **do**
    The values of each compartment of the SIR model can be obtained from the forward propagation of the neural network with the input as t:
    $S, I, R = NN(t)$;
    Evaluate the composed loss function, including the data loss (with s to be the number of observations in each compartment, thus the number of time points collected):
    $MSE_{SIR} = \frac{1}{s}\sum_{i=1}^{s}((S_i - S_i^0)^2 + (I_i - I_i^0)^2 + (R_i - R_i^0)^2)$, denoting the mismatch of the output of the neural network and observation data.
    Here the residual loss:
    $MSE_{residuals} = \frac{1}{q}\sum_{i=1}^{q}\left(\left|\left|\frac{dS_i}{dt_i} + \frac{\beta S_i I_i}{N}\right|\right|^2 + \left|\left|\frac{dI_i}{dt_i} - \frac{\beta S_i I_i}{N} + \gamma I_i\right|\right|^2 + \left|\left|\frac{dR_i}{dt_i} - \gamma I_i\right|\right|^2\right)$,
    stands for the sum of the residual errors for each compartment of the SIR model.
    Thus, the total loss function can be obtained:
    $Loss = MSE_{SIR} + MSE_{residuals}$;
    The Adam Optimizer toolkit in Pytorch is utilized to update the weights w and biases b, as well as β and γ by minimizing the loss function.
end for

Algorithm 5 Training PINN for SIR Model

Require: Time points t, initial susceptible S_0, infected I_0, recovered R_0, population N.

Randomly initialize neural network parameters θ.
for each epoch **do**
    Obtain S, I, R from neural network: $S, I, R = \mathcal{N}(t; \theta)$.
    Calculate data loss MSE_{SIR}:
    $MSE_{SIR} = \frac{1}{N}\sum_{i=1}^{N}((S_i - S_{0i})^2 + (I_i - I_{0i})^2 + (R_i - R_{0i})^2)$.
    Compute residuals $\frac{dS}{dt}, \frac{dI}{dt}, \frac{dR}{dt}$ via autodiff.
    Calculate SIR model loss $MSE_{residuals}$:
    $MSE_{residuals} = \frac{1}{N}\sum_{i=1}^{N}\left(\left|\frac{dS_i}{dt} + \beta\frac{S_i I_i}{N}\right|^2 + \left|\frac{dI_i}{dt} - \beta\frac{S_i I_i}{N} + \gamma I_i\right|^2 + \left|\frac{dR_i}{dt} - \gamma I_i\right|^2\right)$.
    Total loss $Loss = MSE_{SIR} + MSE_{residuals}$.
    Update θ using optimizer to minimize $Loss$.
    Implement early stopping if validation loss does not improve.
end for

Algorithm 6 Streamlined PINN Algorithm for SIR Model

Require: Time points t, initial conditions S_0, I_0, R_0, total population N.

Randomly initialize network parameters θ and disease parameters β, γ.
for each epoch **do**
    Propagate t through network to get $S, I, R = \mathcal{N}(t; \theta)$.
    Compute data fidelity loss MSE_{SIR}:
    $MSE_{SIR} = \frac{1}{N}\sum_{i=1}^{N}\left((S_i - S_{0i})^2 + (I_i - I_{0i})^2 + (R_i - R_{0i})^2\right)$.
    Derive SIR dynamics residuals via autodiff:
    $MSE_{residuals} = \frac{1}{N}\sum_{i=1}^{N}\left(\left|\frac{dS_i}{dt} + \beta\frac{S_iI_i}{N}\right|^2 + \left|\frac{dI_i}{dt} - \beta\frac{S_iI_i}{N} + \gamma I_i\right|^2 + \left|\frac{dR_i}{dt} - \gamma I_i\right|^2\right)$.
    Define total loss $Loss = MSE_{SIR} + MSE_{residuals}$.
    Minimize $Loss$ to update θ, β, and γ with optimizer.
    Apply early stopping based on validation loss.
end for

Algorithm 7 Parameter Estimation for SEIRD Model via Differential Equation Learning

Require: Time series data, population data, initial infected and death counts.

Normalize and partition data for model inputs.
Initialize model states $u(t_0) = [S_0, E_0, I_0, R_0, D_0]$.
Discretize time domain into $t_1, t_2, \ldots, t_n$.
Construct neural networks $NN_\beta(t; \theta_\beta)$, $NN_\gamma(t; \theta_\gamma)$, $NN_\delta(t; \theta_\delta)$, $NN_\alpha(t; \theta_\alpha)$ with parameters θ_β, θ_γ, θ_δ, θ_α.
Define the SEIRD differential equations with learned parameters:
function SEIRD($\dot{u}, u, \theta, t$)
    $\beta(t), \gamma(t), \delta(t), \alpha(t) \leftarrow |NN_\beta(t; \theta_\beta)|, |NN_\gamma(t; \theta_\gamma)|, |NN_\delta(t; \theta_\delta)|, |NN_\alpha(t; \theta_\alpha)|$
    $\dot{S}, \dot{E}, \dot{I}, \dot{R}, \dot{D} \leftarrow$ transitions based on SEIRD dynamics and $\beta(t), \gamma(t), \delta(t), \alpha(t)$
end function
Formulate the initial value problem (IVP) using $u(t_0)$ and SEIRD dynamics.
Define loss function $\mathcal{L}(\theta)$ combining prediction errors and parameter trajectory regularizations.
Minimize $\mathcal{L}(\theta)$ using gradient-based optimization with callbacks to monitor convergence.
Evaluate model fit with metrics such as MSE, MAE, MAPE, RMSE.

The SEIRD model extends the SIR model by including compartments for exposed (E) and dead (D) individuals:

$$\frac{dS}{dt} = -\beta \frac{SI}{N}, \tag{4}$$

$$\frac{dE}{dt} = \beta \frac{SI}{N} - \delta E, \tag{5}$$

$$\frac{dI}{dt} = \delta E - (\gamma + \alpha) I, \tag{6}$$

$$\frac{dR}{dt} = \gamma I, \tag{7}$$

$$\frac{dD}{dt} = \alpha I, \tag{8}$$

where E represents the exposed individuals who are infected but not yet infectious, and D represents the deceased individuals.

Parameter	**Definition**
β	Transmission rate
δ	Rate at which exposed individuals become infectious
γ	Recovery rate
α	Mortality rate

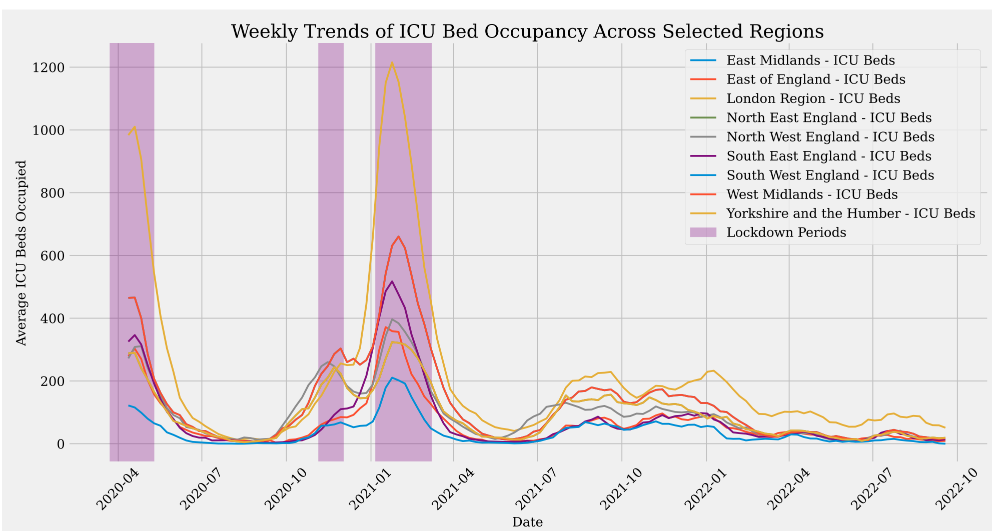

Figure 1: weekly ICU bed occupancy across NHS regions.

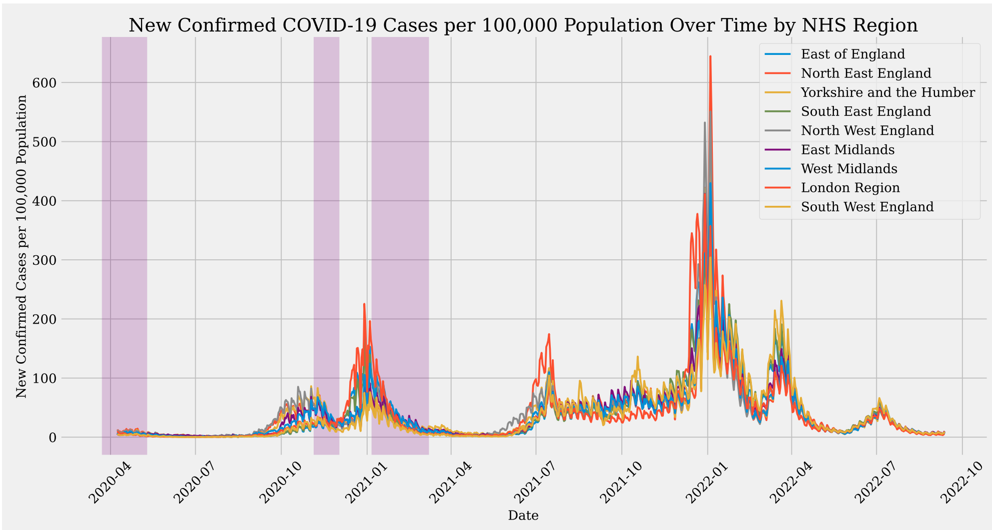

Figure 2: new confirmed COVID-19 cases per 100k people overtime by NHS regions.

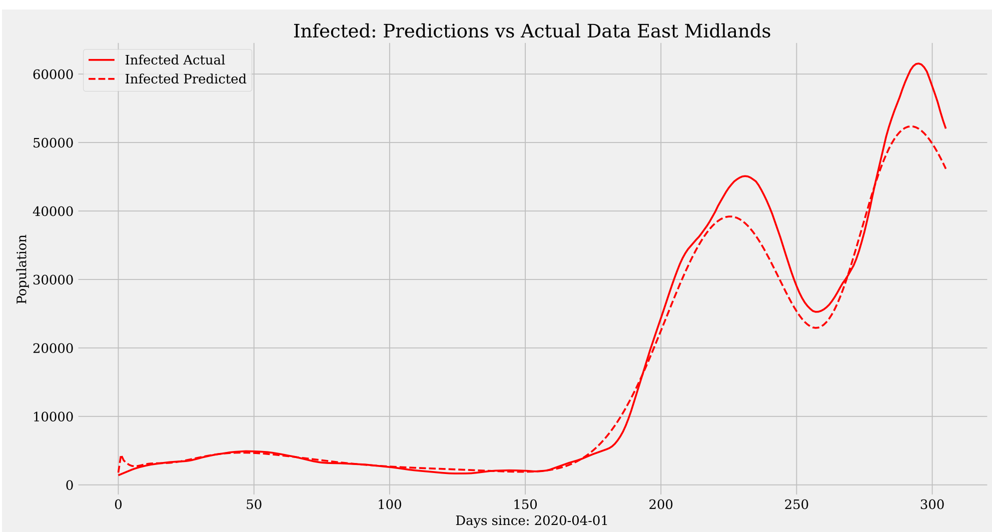

Figure 3: Predicted number of infectious individuals in the East Midlands region.

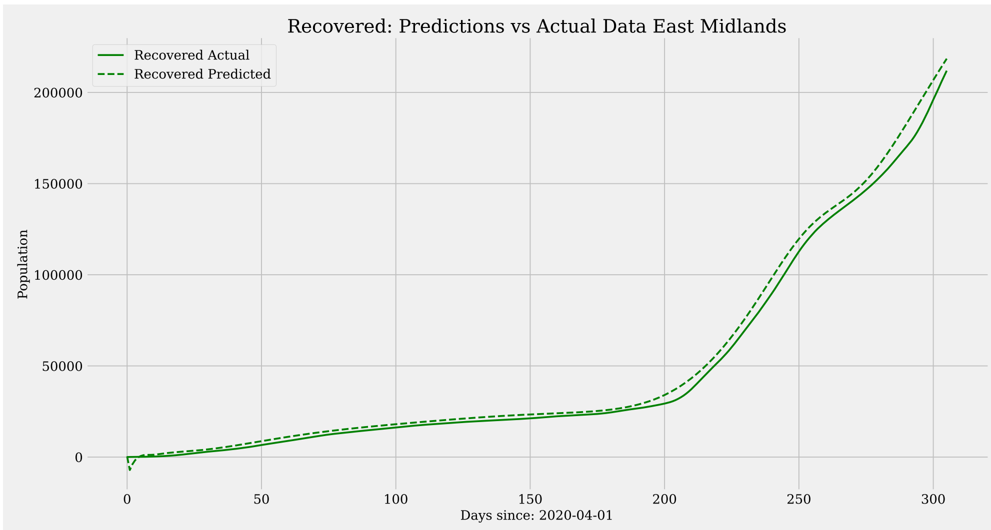

Figure 4: Predicted number of recovered individuals in the East Midlands region.

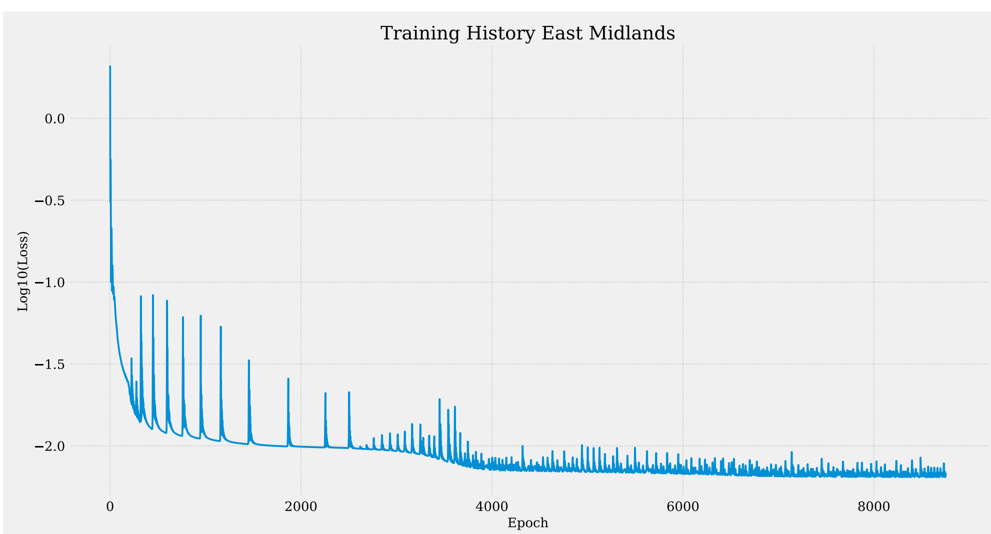

Figure 5: Training history of the PINN model for the East Midlands region.

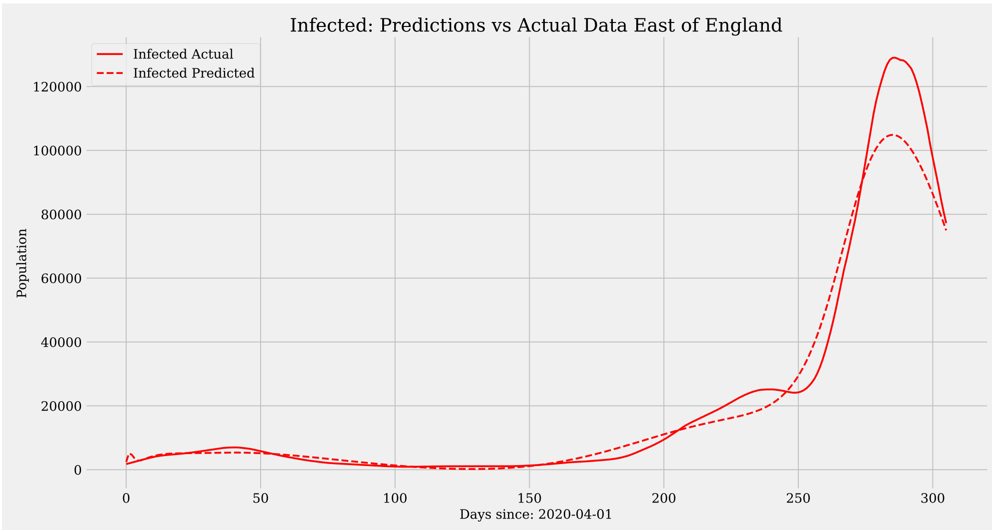

Figure 6: Predicted number of infectious individuals in the East of England region.

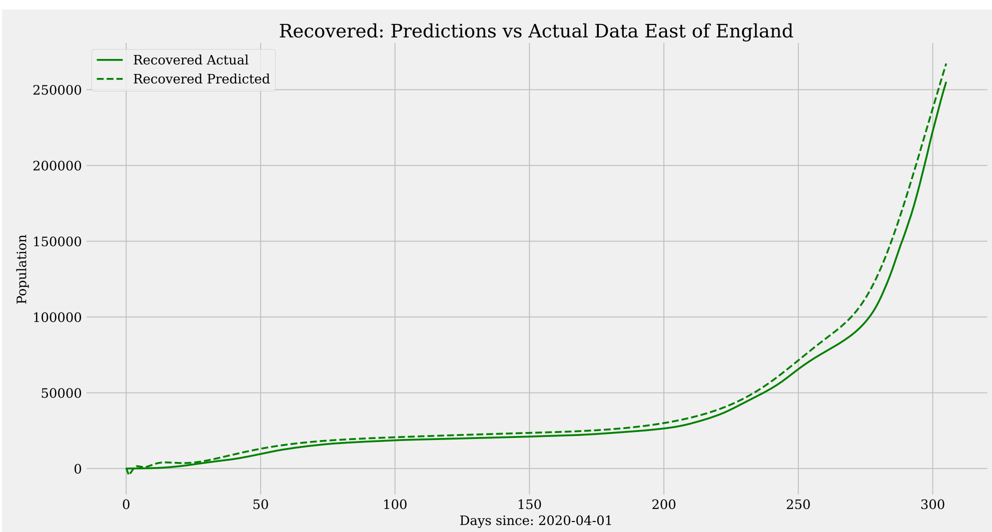

Figure 7: Predicted number of recovered individuals in the East of England region.

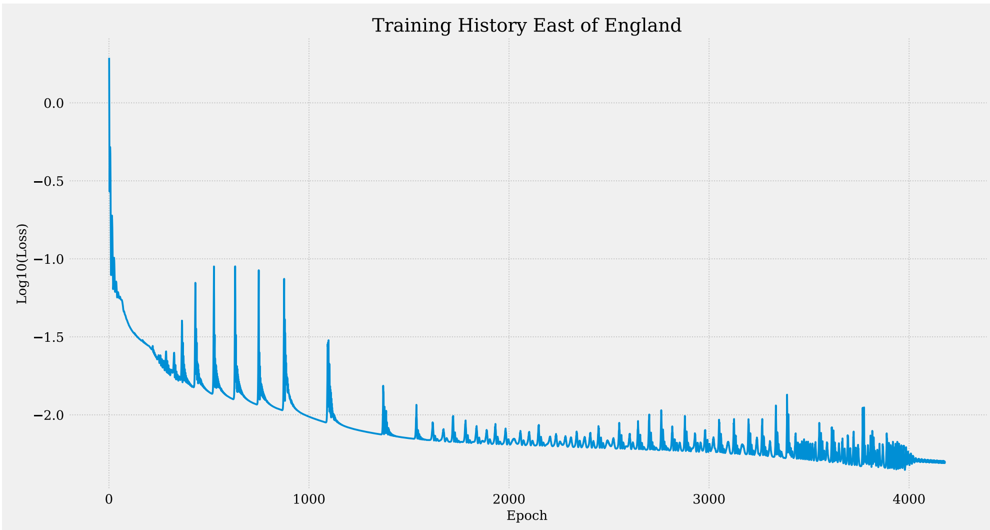

Figure 8: Training history of the PINN model for the East of England region.

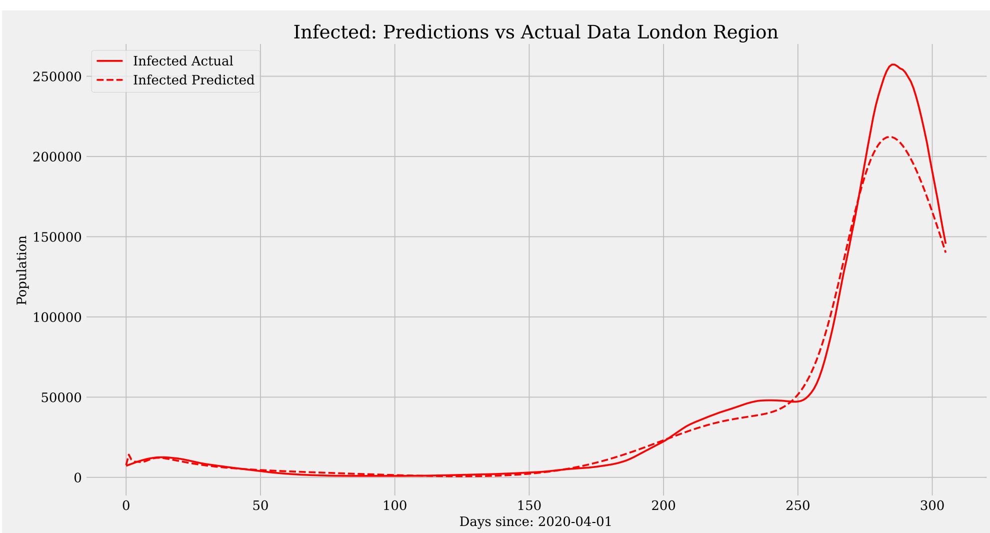

Figure 9: Predicted number of infectious individuals in the London region.

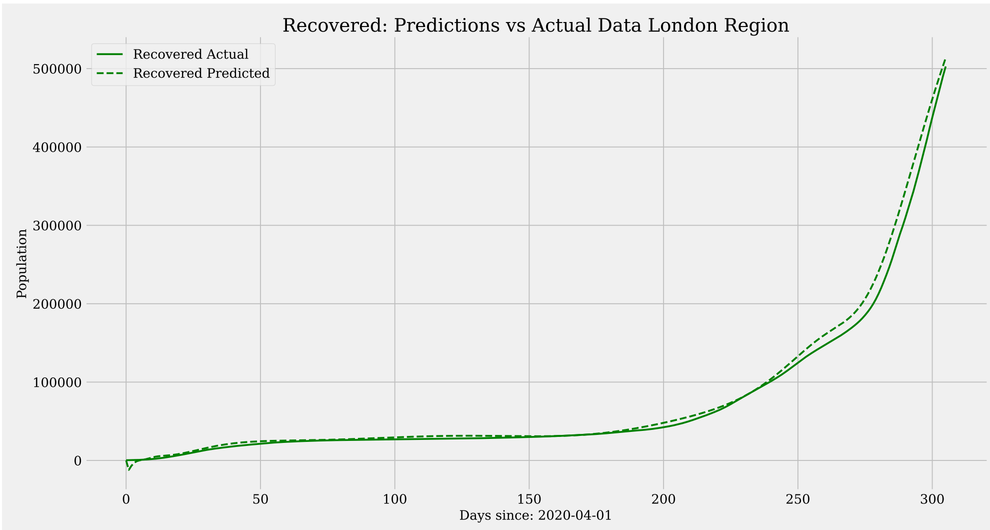

Figure 10: Predicted number of recovered individuals in the London region.

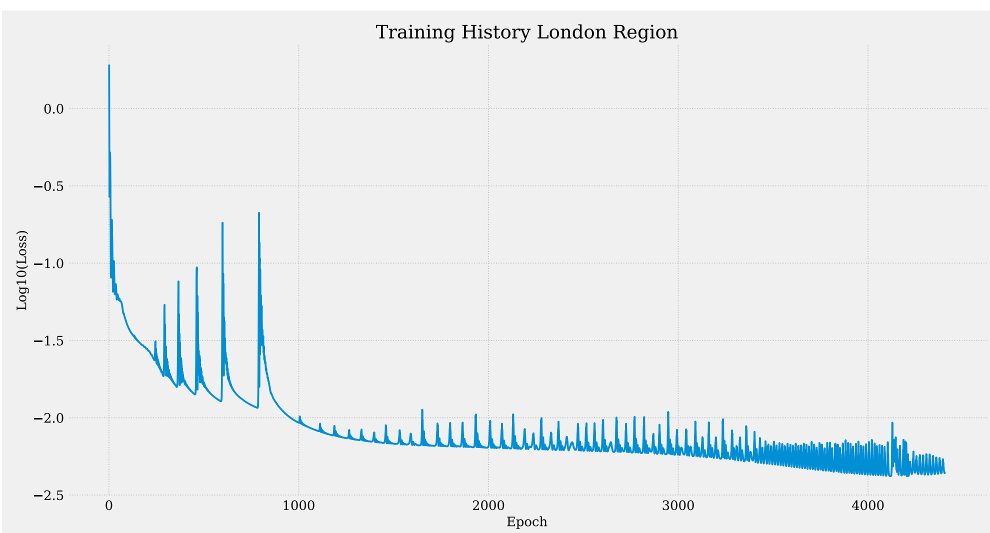

Figure 11: Training history of the PINN model for the London region.