













# EINN: Epidemic Prediction using ML

Mert Saruhan, B.Sc.

December 2, 2023

hs-mittweida.de

# **Agenda**

1 What is EINN?

2 Background

3 EINN Model

4 Results



- EINN is a (Neural Network) machine learning model to predict epidemic dynamics [1]

- EINN is a (Neural Network) machine learning model to predict epidemic dynamics [1]
- Mechanistic models (ODE models e.g SIR/SEIRM) good at trend approximation [1]

- EINN is a (Neural Network) machine learning model to predict epidemic dynamics [1]
- Mechanistic models (ODE models e.g SIR/SEIRM) good at trend approximation [1]
- RNN powered epidemic models good at short and long term epidemic prediction [1]

- EINN is a (Neural Network) machine learning model to predict epidemic dynamics [1]
- Mechanistic models (ODE models e.g SIR/SEIRM) good at trend approximation [1]
- RNN powered epidemic models good at short and long term epidemic prediction [1]
- EINN combines the knowledge of PINN, RNN, and ODE [1]

### Mechanistic epidemic models

- Uses ODE to predict



### Mechanistic epidemic models

- Uses ODE to predict
- Have many models: SIR, SEIR, SEIRM etc.



### Mechanistic epidemic models

- Uses ODE to predict
- Have many models: SIR, SEIR, SEIRM etc.
- Susceptible (S):  $\frac{dS_t}{dt} = -\beta_t \frac{S_t I_t}{N}$



### Mechanistic epidemic models

- Uses ODE to predict
- Have many models: SIR, SEIR, SEIRM etc.
- Susceptible (S):  $\frac{dS_t}{dt} = -\beta_t \frac{S_t I_t}{N}$
- Exposed (E):  $\frac{dE_t}{dt} = \beta_t \frac{S_t I_t}{NI} \alpha_t E_t$



### Mechanistic epidemic models

- Uses ODE to predict
- Have many models: SIR, SEIR, SEIRM etc.
- Susceptible (S):  $\frac{dS_t}{dt} = -\beta_t \frac{S_t I_t}{N}$
- Exposed (E):  $\frac{dE_t}{dt} = \beta_t \frac{S_t I_t}{N} \alpha_t E_t$
- Infected (I):  $\frac{dI_t}{dt} = \alpha_t E_t \gamma_t I_t \mu_t I_t$



### Mechanistic epidemic models

- Uses ODE to predict
- Have many models: SIR, SEIR, SEIRM etc.
- Susceptible (S):  $\frac{dS_t}{dt} = -\beta_t \frac{S_t I_t}{N}$
- Exposed (E):  $\frac{dE_t}{dt} = \beta_t \frac{S_t I_t}{N} \alpha_t E_t$
- Infected (I):  $\frac{dI_t}{dt} = \alpha_t E_t \gamma_t I_t \mu_t I_t$
- Recovered (R):  $\frac{dR_t}{dt} = \gamma_t I_t$



### Mechanistic epidemic models

- Uses ODE to predict
- Have many models: SIR, SEIR, SEIRM etc.
- Susceptible (S):  $\frac{dS_t}{dt} = -\beta_t \frac{S_t I_t}{N}$
- Exposed (E):  $\frac{dE_t}{dt} = \beta_t \frac{S_t I_t}{N} \alpha_t E_t$
- Infected (I):  $\frac{dI_t}{dt} = \alpha_t E_t \gamma_t I_t \mu_t I_t$
- Recovered (R):  $\frac{dR_t}{dt} = \gamma_t I_t$
- Mortality (M):  $\frac{dM_t}{dt} = \mu_t I_t$



#### **RNN**

- RNN is a neural network model
- Uses the previous state as an input to predict the next state
- Used in object detection and NLP

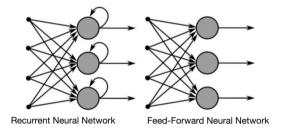


Figure: Example structure of RNN and NN [2]

#### **RNN**

- RNN is a neural network model
- Uses the previous state as an input to predict the next state
- Used in object detection and NLP

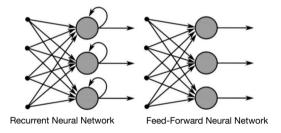


Figure: Example structure of RNN and NN [2]

#### **RNN**

- RNN is a neural network model
- Uses the previous state as an input to predict the next state
- Used in object detection and NLP

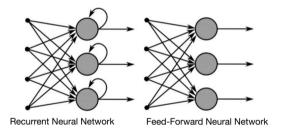


Figure: Example structure of RNN and NN [2]

#### **PINN**

- Uses physics laws to predict the next state
- Uses PDE (partial differential equation) and ODE (ordinary differential equation) as a loss estimator
- L<sub>data</sub>: loss from data fitting
- L<sub>physics</sub>: loss from physics laws

e.g. 
$$\vec{a} = -\mu \|\vec{v}\| \vec{v} - \vec{g}, \vec{v} = \frac{df}{dt}, \vec{a} = \frac{d^2f}{dt^2}$$

$$\mathsf{L}_{\mathsf{physics}} = \tfrac{1}{N} \sum_{i=0}^{N-1} \left( -\mu \| \tfrac{df_i}{dt_i} \| \tfrac{df_i}{dt_i} - \vec{g} - \left( \tfrac{d^2 f_i}{dt_i^2} \right) \right)^2$$

•  $L_{total} = L_{data} + L_{physics}$ 



#### **PINN**

- Uses physics laws to predict the next state
- Uses PDE (partial differential equation) and ODE (ordinary differential equation) as a loss estimator
- L<sub>data</sub>: loss from data fitting
- L<sub>physics</sub>: loss from physics laws

e.g. 
$$\vec{a} = -\mu \|\vec{v}\|\vec{v} - \vec{g}$$
,  $\vec{v} = \frac{df}{dt}$ ,  $\vec{a} = \frac{d^2f}{dt^2}$ 

$$\mathsf{L}_{\mathsf{physics}} = \frac{1}{N} \sum_{i=0}^{N-1} \left( -\mu \| \frac{df_i}{dt_i} \| \frac{df_i}{dt_i} - \vec{g} - \left( \frac{d^2 f_i}{dt_i^2} \right) \right)^2$$

•  $L_{total} = L_{data} + L_{physics}$ 



#### **PINN**

- Uses physics laws to predict the next state
- Uses PDE (partial differential equation) and ODE (ordinary differential equation) as a loss estimator
- L<sub>data</sub>: loss from data fitting
- L<sub>physics</sub>: loss from physics laws

e.g. 
$$\vec{a} = -\mu ||\vec{v}||\vec{v} - \vec{g}$$
,  $\vec{v} = \frac{df}{dt}$ ,  $\vec{a} = \frac{d^2f}{dt^2}$ 

$$\mathsf{L}_{\mathsf{physics}} = \frac{1}{N} \sum_{i=0}^{N-1} \left( -\mu \| \frac{df_i}{dt_i} \| \frac{df_i}{dt_i} - \vec{g} - \left( \frac{d^2 f_i}{dt_i^2} \right) \right)^2$$

•  $L_{total} = L_{data} + L_{physics}$ 



#### **PINN**

- Uses physics laws to predict the next state
- Uses PDE (partial differential equation) and ODE (ordinary differential equation) as a loss estimator
- L<sub>data</sub>: loss from data fitting
- L<sub>physics</sub>: loss from physics laws

e.g. 
$$\vec{a} = -\mu \|\vec{v}\| \vec{v} - \vec{g}$$
,  $\vec{v} = \frac{df}{dt}$ ,  $\vec{a} = \frac{d^2f}{dt^2}$ 

$$\mathsf{L}_{\mathsf{physics}} = \frac{1}{N} \sum_{i=0}^{N-1} \left( -\mu \| \frac{df_i}{dt_i} \| \frac{df_i}{dt_i} - \vec{g} - \left( \frac{d^2 f_i}{dt_i^2} \right) \right)^2$$

•  $L_{total} = L_{data} + L_{physics}$ 



#### **PINN**

- Uses physics laws to predict the next state
- Uses PDE (partial differential equation) and ODE (ordinary differential equation) as a loss estimator
- L<sub>data</sub>: loss from data fitting
- L<sub>physics</sub>: loss from physics laws

e.g. 
$$\vec{a} = -\mu \|\vec{v}\| \vec{v} - \vec{g}$$
,  $\vec{v} = \frac{df}{dt}$ ,  $\vec{a} = \frac{d^2f}{dt^2}$ 

$$\mathsf{L}_{\mathsf{physics}} = \frac{1}{N} \sum_{i=0}^{N-1} \left( -\mu \| \frac{df_i}{dt_i} \| \frac{df_i}{dt_i} - \vec{g} - \left( \frac{d^2 f_i}{dt_i^2} \right) \right)^2$$

•  $L_{total} = L_{data} + L_{physics}$ 



### **PINN for Systems Biology**

- Recent works with PINN for Systems Biology [3, 4]: better PINN for SIR mechanics
- Uses time t as input for Neural Network N(t) and rate of change in ODE systems f<sub>ODE</sub>(t)
- Uses  $(\frac{dN(t)}{dt} f_{ODE}(t))$  as a loss

#### **PINN for Systems Biology**

- Recent works with PINN for Systems Biology [3, 4]: better PINN for SIR mechanics
- Uses time t as input for Neural Network N(t) and rate of change in ODE systems  $f_{ODE}(t)$

#### **PINN for Systems Biology**

- Recent works with PINN for Systems Biology [3, 4]: better PINN for SIR mechanics
- Uses time t as input for Neural Network N(t) and rate of change in ODE systems  $f_{\rm ODE}(t)$
- Uses  $(\frac{dN(t)}{dt} f_{ODE}(t))$  as a loss

### **Model summary**

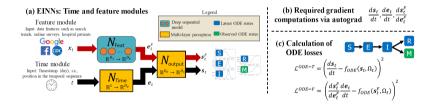
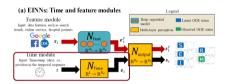


Figure: EINN Model. (a) The training model. (b) Needed gradients to train the model using autograd. (c) ODE losses of feature module and time module. Taken from: [1]



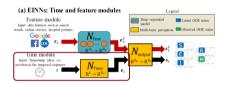
#### Source model (Time module)



- Source model is a PINN for Systems Biology



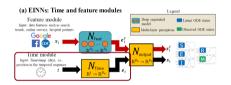
#### Source model (Time module)



- Source model is a PINN for Systems Biology
- Input: time



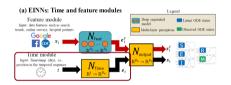
#### Source model (Time module)



- Source model is a PINN for Systems Biology
- Input: time
- Output: embedding of the epidemic ODE states ( $e_t$ )



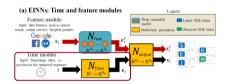
#### Source model (Time module)



- Source model is a PINN for Systems Biology
- Input: time
- Output: embedding of the epidemic ODE states ( $e_t$ )



#### Source model (Time module)



- Source model is a PINN for Systems Biology
- Input: time
- Output: embedding of the epidemic ODE states (e<sub>t</sub>)
- Model freezes when  $e_t \approx e_t^F$



#### Time module losses

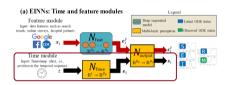
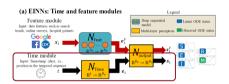


Figure: Cropped model summary showing the training summary. Cropped from: [1]

 ODE loss for time module  $(L^{ODE-T})$  [11:

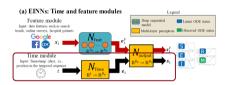
$$\frac{1}{N+1} \sum_{t=t_0}^{t_N} \left[ \frac{ds_t}{dt} - f_{\text{ODE}}(s_t, \Omega_t) \right]^2$$
 $s_t$ : predicted ODE states at time t using time module path

#### Time module losses



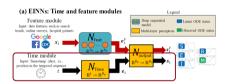
- In the ODE states, Mortality (M) is observed and other states are latent [5]

#### Time module losses



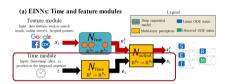
- In the ODE states, Mortality (M) is observed and other states are latent [5]
- $L^{\text{Data-T}}$  [1]:  $\frac{1}{N+1} \sum_{t=t_0}^{t_N} \left[ \hat{M}_t M_t \right]^2$ M: mortality,  $\hat{M}_t$ : predicted mortality using time module path

#### Time module losses



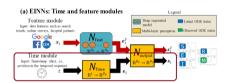
- Adding monoticity loss (loss from latent states) to make learning less challenging using domain knowledge

#### Time module losses



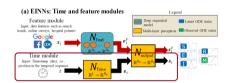
- Adding monoticity loss (loss from latent states) to make learning less challenging using domain knowledge
- $L^{\text{Mono}} = \frac{1}{N+1} \left( \sum_{t=t_0}^{t_N} \frac{dS_t}{dt} \text{ReLU} \left( \frac{dS_t}{dt} \right) + \right)$  $\sum_{t=t_0}^{t_N} -1 \frac{dR_t}{dt} \text{ReLU}(-\frac{dR_t}{dt})$

#### Time module losses



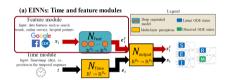
- Adding parameter to loss to track parameter change with time

#### Time module losses



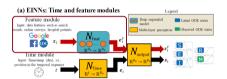
- Adding parameter to loss to track parameter change with time
- $L^{\mathsf{Param}} = \frac{1}{N+1} \sum_{t=t_0}^{t_N} \left[ \Omega_{t+1} \Omega_t \right]^2$

### **Target model (Feature module)**



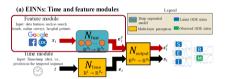
- Target model is an RNN model

### **Target model (Feature module)**



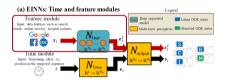
- Target model is an RNN model
- Input  $(x_t)$ : Features relevant to the problem

### **Target model (Feature module)**



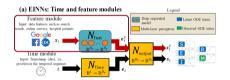
- Target model is an RNN model
- Input  $(x_t)$ : Features relevant to the problem
- Output: embedding of the epidemic ODE states  $(e_t^F)$

### **Target model (Feature module)**



- Target model is an RNN model
- Input  $(x_t)$ : Features relevant to the problem
- Output: embedding of the epidemic ODE states  $(e_t^F)$
- Model freezes when  $e_t \approx e_t^F$

#### **Target model (Feature module)**



- Target model is an RNN model
- Input  $(x_t)$ : Features relevant to the problem
- Output: embedding of the epidemic ODE states  $(e_t^F)$
- Model freezes when  $e_t \approx e_t^F$
- Loss ( $L^{\text{Emb}}$ ):  $\frac{1}{N+1} \sum_{t=t_0}^{t_N} [e_t e_t^F]^2$

### **Target module losses**

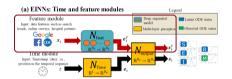


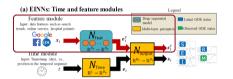
Figure: Cropped model summary showing the training summary. Cropped from: [1]

•  $e_t \approx e_t^F$  required for gradient trick for ODF loss from feature module

$$ullet$$
  $e_tpprox e_t^F \Rightarrow rac{ds_t^r}{dt} = rac{ds_t^r}{de_t^F}rac{de_t^r}{dt} pprox rac{ds_t^r}{de_t^F}rac{de_t}{dt}$ 

$$\frac{1}{N+1} \sum_{t=t_0}^{t_N} \left[ \frac{ds_t^F}{de_t^F} \frac{de_t}{dt} - f_{\text{ODE}}(s_t^F, \Omega_t) \right]$$

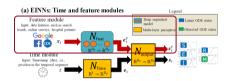
### **Target module losses**



- $e_t \approx e_t^F$  required for gradient trick for ODE loss from feature module
- $e_t \approx e_t^F \Rightarrow \frac{ds_t^F}{dt} = \frac{ds_t^F}{de_t^F} \frac{de_t^F}{dt} \approx \frac{ds_t^F}{de_t^F} \frac{de_t}{dt}$
- Loss ODE from feature module (L<sup>ODE-F</sup>) [1]:

$$\frac{1}{N+1}\sum_{t=t_0}^{t_N}\left[\frac{ds_t^F}{de_t^F}\frac{de_t}{dt}-f_{\mathsf{ODE}}(s_t^F,\Omega_t)\right]^{\frac{1}{N}}$$

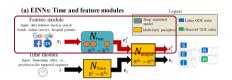
### **Target module losses**



- $e_t \approx e_t^F$  required for gradient trick for ODF loss from feature module
- $e_t \approx e_t^F \Rightarrow \frac{ds_t^F}{dt} = \frac{ds_t^F}{de_t^F} \frac{de_t^F}{dt} \approx \frac{ds_t^F}{de_t^F} \frac{de_t}{dt}$
- Loss ODE from feature module  $(L^{ODE-F})$  [1]:

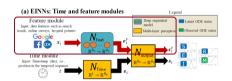
$$\frac{1}{N+1}\sum_{t=t_0}^{t_N}\left[\frac{ds_t^F}{de_t^F}\frac{de_t}{dt}-f_{\mathsf{ODE}}(s_t^F,\Omega_t)\right]^2$$

### **Target module losses**



- $\hat{M}_{t}^{F}$ : predicted mortality using feature module path

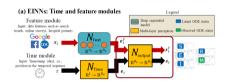
### **Target module losses**



- $\hat{M}_{t}^{F}$ : predicted mortality using feature module path
- Loss from data ( $L^{Data-F}$ ):

$$\frac{1}{N+1}\sum_{t=t_0}^{t_N}\left[\hat{M}_t^F-M_t\right]^2$$

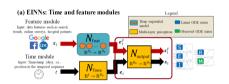
### **Target module losses**



- N<sub>output</sub> feed-forward Neural Network
- Alligning findings from both paths

• 
$$L^{\text{Output}} = \frac{1}{N+1} \sum_{t=t_0}^{t_N} \left[ s_t - s_t^F \right]$$

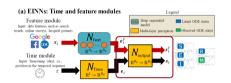
### **Target module losses**



- N<sub>output</sub> feed-forward Neural Network
- Alligning findings from both paths

• 
$$L^{\text{Output}} = \frac{1}{N+1} \sum_{t=t_0}^{t_N} \left[ s_t - s_t^F \right]$$

### **Target module losses**



- N<sub>output</sub> feed-forward Neural Network
- Alligning findings from both paths

• 
$$L^{\text{Output}} = \frac{1}{N+1} \sum_{t=t_0}^{t_N} \left[ s_t - s_t^F \right]^2$$

- Generation: The NN learns directly from ODE generated data [1, 6, 7]
- Regularization: The NN predicts states and parameters of an ODE and learns from the parameters [1, 8, 9]
- Ensembling: Combines predictions of RNN and SEIRM/SIR outputs in one NN for a final prediction [1, 10, 11]
- EINNs-NoGradMatching: skipping  $e_t \approx e_t^F$  part [1]

Model	Short-term (1-4 wks)			Long-term (5-8 wks)			Trend correlation
	NR1	NR2	ND	NR1	NR2	ND	PC
Task 1: C	OVID-19	Forecasti	ing (US N	iational +	47 states	)	
RNN (GRU+Atten)	1.09	0.50	0.86	1.19	0.53	0.96	0.08
Mechanistic model (SEIRM)	2.35	1.13	1.36	7.14	2.99	3.11	0.53
GENERATION	0.79	0.35	0.60	0.93	0.40	0.74	-0.01
REGULARIZATION	1.05	0.48	0.81	1.19	0.53	0.97	0.09
Ensembling	0.91	0.41	0.68	0.93	0.40	0.69	-0.01
EINNs (ours)	0.54	0.24	0.38	0.85	0.37	0.66	0.46
PINN (time module standalone)	0.84	0.38	0.64	0.93	0.40	0.72	0.24
EINNs-NoGradMatching	0.64	0.29	0.49	0.98	0.43	0.79	0.03
Task	2: Influe	nza Forec	asting (1	HHS re	gions)		
RNN (GRU+Atten)	0.72	0.38	0.67	1.19	0.51	1.14	-0.03
Mechanistic model (SIRS)	0.72	0.38	0.51	1.16	0.55	0.81	0.71
GENERATION	0.76	0.4	0.71	1.21	0.52	1.15	-0.14
REGULARIZATION	1.19	0.64	1.00	1.22	0.54	0.9	-0.45
Ensembling	0.89	0.47	0.77	0.83	0.35	0.73	-0.69
EINNs (ours)	0.53	0.27	0.37	1.01	0.42	0.73	0.68
PINN (time module standalone)	0.55	0.29	0.44	1.13	0.48	1.02	-0.47
EINNs-NoGradMatching	0.53	0.27	0.38	1.02	0.42	0.76	0.50

Figure: Short-term, Long-term, and Trend results. NR: Normalized RMSE (Lower is better), ND: Normal Deviation (Lower is better) PC: Pearson Correlation (Higher is better). Image taken from: [1]



- Better short and long term prediction than RNN and Mechanistic model (SEIRM)
- Better trend correlation than RNN and sligtly less trend correlation than Mechanistic model (SEIRM)

# Bibliography I

- A. Rodríguez, I. Cui, N. Ramakrishnan, B. Adhikari, and B. A. Prakash, [1] *Einns: Epidemiologically-informed neural networks*, 2023. DOI: 10.48550/arXiv.2202.10446.arXiv: 2202.10446 [cs.LG].
- A guide to recurrent neural networks: Understanding rnn and lstm networks, [2] https://builtin.com/data-science/recurrent-neural-networksand-lstm. Accessed: 2023-11-26.
- A. Yazdani and et al., Systems biology informed deep learning for inferring [3] parameters and hidden dynamics. PLOS Comp. Bio., 2020.
- [4] G. Karniadakis and et al., *Physics-informed machine learning*, 2021.



# **Bibliography II**

- J. T. Wu and et al., Nowcasting and forecasting the potential domestic and [5] international spread of the 2019-ncov outbreak originating in wuhan, china: A modelling study, 2020.
- L. Wang and et al., Defsi: Deep learning based epidemic forecasting with [6] synthetic information, 2019.
- Sanchez-Gonzalez and et al., Learning to simulate complex physics with [7] graph networks, 2020.
- I. Gao and et al., Stan: Spatio-temporal attention network for pandemic [8] prediction using real-world evidence, 2021.



## **Bibliography III**

- N. Gaw and et al., Integration of machine learning and mechanistic models [9] accurately predicts variation in cell density of glioblastoma using multiparametric mri, 2019.
- [10] A. Adiga and et al., All models are useful: Bayesian ensembling for robust high resolution covid-19 forecasting, 2021.
- [11] T. K. Yamana and et al., *Individual versus superensemble forecasts of* seasonal influenza outbreaks in the united states, 2017.



# Thank You

- Mert Saruhan, B.Sc.

Mathematics for Network and Data Science (MA20w1-M)

Hochschule Mittweida
University of Applied Sciences
Technikumplatz 17 | 09648 Mittweida

hs-mittweida.de