Learning continuous-time PDEs from sparse data with graph neural networks

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Abstract

The behavior of many dynamical systems follow complex, yet still unknown partial differential equations (PDEs). While several machine learning methods have been proposed to learn PDEs directly from data, previous methods are limited to discrete-time approximations or make the limiting assumption of the observations arriving at regular grids. We propose a general continuous-time differential model for dynamical systems whose governing equations are parameterized by message passing graph neural networks. The model admits arbitrary space and time discretizations, which removes constraints on the locations of observation points and time intervals between the observations. The model is trained with continuous-time adjoint method enabling efficient neural PDE inference. We demonstrate the model’s ability to work with unstructured grids, arbitrary time steps, and noisy observations. We compare our method with existing approaches on several well-known physical systems that involve first and higher-order PDEs with state-of-the-art predictive performance.

1 Introduction

We consider continuous dynamical systems with a state $u(x, t) \in \mathbb{R}$ that evolves over time $t \in \mathbb{R}^+$ and spatial locations $x \in \Omega \subset \mathbb{R}^D$ of a bounded domain $\Omega$. We assume the system is governed by an unknown partial differential equation (PDE)

$$\dot{u}(x, t) := \frac{du(x, t)}{dt} = F(x, u, \nabla_x u, \nabla^2_x u, \ldots),$$ (1)

where the temporal evolution $\dot{u}$ of the system depends on the current state $u$ and its spatial first and higher-order partial derivatives w.r.t. the coordinates $x$. Such PDE models are the cornerstone of natural sciences, and are widely applicable to modelling of propagative systems, such as behavior of sound waves, fluid dynamics, heat dissipation, weather patterns, disease progression or cellular kinetics [Courant and Hilbert, 2008]. Our objective is to learn the differential $F$ from data.

There is a long history of manually deriving mechanistic PDE equations for specific systems [Cajori, 1928], such as the Navier-Stokes fluid dynamics or the Schrödinger’s quantum equations, and approximating their solution forward in time numerically [Ames, 2014]. These efforts are complemented by data-driven approaches to infer any unknown or latent coefficients in the otherwise known equations [Isakov, 2006, Berg and Nyström, 2017, Santo et al., 2019], or in partially known equations [Freund et al., 2019, Seo and Liu, 2019b, Seo et al., 2020]. A series of methods have studied neural proxies of known PDEs for solution acceleration [Lagaris et al., 1998, Raissi et al., 2017, Weinan and Yu, 2018, Sirignano and Spiliopoulos, 2018] or for uncertainty quantification [Khoo et al., 2017].

Related work. Recently the pioneering work of Long et al. [2017] proposed a fully non-mechanistic method PDE-Net, where the governing PDE equation $F$ (1) is learned from system snapshot observa-
tions as a convolutional neural network (CNN) over the input domain discretised into a spatio-temporal
grid. Further works have extended the approach with residual CNNs [Ruthotto and Haber, 2019],
symbolic neural networks [Long et al., 2019], high-order autoregressive networks [Geneva and
Zabaras, 2020], and feed-forward networks [Xu et al., 2019]. These models are fundamentally
limited to discretizing the input domain with a sample-inefficient grid, while they also do not support
continuous evolution over time, rendering them unable to handle temporally or spatially sparse or
non-uniform observations commonly encountered in realistic applications.

These models are related to the interaction networks where object’s state evolves as a function of its
neighboring objects, which forms dynamic relational graphs instead of grids [Battaglia et al., 2016,
Chang et al., 2016, Sanchez-Gonzalez et al., 2018]. In contrast to the dense solution fields of PDEs,
these models apply message-passing between small number of moving and interacting objects, which
deviates from PDEs that are strictly differential functions.

Contributions. In this paper we propose to learn free-form, continuous-time, a priori fully unknown
PDE model $F(1)$ from sparse data measured on arbitrary timepoints and locations of the coordinate
domain $Ω$ with graph neural networks (GNN). Our contributions are:

- We introduce continuous-time representation and learning of the dynamics of PDE-driven
  systems
- We propose efficient graph representation of the domain structure using the method of lines
  with message passing neural networks
- We achieve state-of-the-art learning performance on realistic PDE systems with irregular
  data, and our model is highly robust to data sparsity
- Efficient and open implementation of all contributions at anonymized url.

Table 1: Comparison of machine-learning based PDE learning methods.

| Model      | Unknown PDE learning | Continuous time | Free-form spatial domain | Free-form initial/boundary conditions | Reference                        |
|------------|----------------------|-----------------|--------------------------|---------------------------------------|-----------------------------------|
| PINN       |                      | ✓               |                          |                                       | Raissi et al. [2017]              |
| AR         |                      |                 | ✓                        |                                       | Geneva and Zabaras [2020]         |
| PDE-net    |                      | ✓               |                          |                                       | Long et al. [2017]                |
| DPM        |                      |                 | ✓                        |                                       | Freund et al. [2019]              |
| DPGN       |                      | ✓               | ✓                        |                                       | Seo and Liu [2019b]               |
| PA-DGN     |                      |                 | ✓                        |                                       | Seo et al. [2020]                 |
| PDE-flows  |                      | ✓               | ✓                        |                                       | this work                         |

2 Methods

In this Section we consider the problem of learning the unknown function $F(1)$ from observations
$(y(t_0),...,y(t_M)) \in \mathbb{R}^{N \times (M+1)}$ of the system’s state $u(t) = (u(x_1,t),...,u(x_N,t))^T$ at $N$
arbitrary spatial locations $(x_1,...,x_N)$ and at $M + 1$ time points $(t_0,...,t_M)$. We introduce
efficient graph convolution neural networks surrogates operating over continuous-time to learn PDEs
from sparse data.

We apply the method of lines (MOL) to numerically solve Equation 1. [Schiesser, 2012]. The
MOL consists of selecting $N$ nodes in $Ω$ and discretizing spatial derivatives in $F$ at these nodes.
We place the nodes to the observation locations $(x_1,...,x_N)$. The discretization leads to $F$ being
approximated by $\hat{F}$ and produces the following system of ordinary differential equations (ODEs)
whose solution asymptotically approximates the solution of Equation (1)

$$\dot{u}(t) = \begin{pmatrix} \dot{u}_1(t) \\ \vdots \\ \dot{u}_N(t) \end{pmatrix} = \begin{pmatrix} \frac{du(x_1,t)}{dt} \\ \vdots \\ \frac{du(x_N,t)}{dt} \end{pmatrix} \approx \begin{pmatrix} \hat{F}(x_1,x_N(1),u_1,u_N(1)) \\ \vdots \\ \hat{F}(x_N,x_N(N),u_N,u_N(N)) \end{pmatrix} \in \mathbb{R}^N. \tag{2}$$
As the discretized $\hat{F}$ inherits its unknown nature from the true PDE function $F$, we approximate $\hat{F}$ by a learnable neural surrogate function.

The system’s state at $x_i$ is defined as $u_i$, while $\mathcal{N}(i)$ is a set of indices of neighboring nodes other than $i$ that are required to evaluate $\hat{F}$ at $x_i$, and $x_{\mathcal{N}(i)}$ with $u_{\mathcal{N}(i)}$ are positions and states of nodes $\mathcal{N}(i)$. This shows that the temporal derivative $\dot{u}_i$ of $u_i$ depends not only on the location and state at the node $i$, but also on locations and states of neighboring nodes, resulting in a locally coupled system of ODEs.

Each ODE in the system follows the solution at a fixed location $x_i$. Numerous ODE solvers have been proposed (such as Euler and Runge-Kutta solvers) to solve the full system

$$\mathbf{u}(t) = \mathbf{u}(0) + \int_0^t \dot{\mathbf{u}}(\tau) d\tau,$$

where $0 \leq \tau \leq t$ is a cumulative intermediate time variable. Solving equation (3) forward in time scales linearly both with respect to the number of nodes $N$ and the number of evaluated time points $M$, while saturating the input space $\Omega$ requires a large number of nodes. In practice, PDEs are often applied for two- and three-dimensional spatial systems where the method is efficient.

### 2.1 Position-invariant graph neural network differential

After introducing Equation 2, we transition from learning $F$ to learning $\hat{F}$. The value of $\hat{F}$ at a node $i$ must depend only on the nodes $i$ and $\mathcal{N}(i)$. Furthermore, the number of arguments and their order in $\hat{F}$ is not known in advance and might be different for each node. This means that our model $\hat{F}$ must be able to work with an arbitrary number of arguments and must be invariant to permutations of their order. Graph neural networks (GNNs) [Wu et al., 2020] satisfy these requirements. In a more restricted setting, where the number of neighbors and their order is known, (e.g. if the grid is uniform) other types of models such as multilayer perceptrons and convolutional neural networks can be used as well.

We consider a type of GNNs called message passing neural networks (MPNNs) [Gilmer et al., 2017] to represent $\hat{F}$ as

$$\hat{F}_\theta(x_{\mathcal{N}(i)} - x_i, u_i, u_{\mathcal{N}(i)}),$$

where $x_{\mathcal{N}(i)} - x_i = \{x_j - x_i : j \in \mathcal{N}(i)\}$ and $\theta$ denote parameters of the MPNN. This formulation assumes the absence of position-dependent quantities in $\hat{F}$, but models based on this formulation are invariant to translations and rotations of $\Omega$, which makes generalization to systems with different node positions feasible, and prevents overfitting by memorizing position-specific dynamics.

### 2.2 Message passing neural networks

Let a graph $G = (V, E)$ contain nodes $V = \{x_i\}_{i=1}^N$, defined by the measurement positions, and undirected edges $E = \{e_{ij}\}$, and assume each node and edge are associated with a node feature $v_i$ and an edge feature $e_{ij}$, respectively. We use the node neighborhood $\mathcal{N}(i)$ to define edges. Neighbors for each node were selected by applying Delaunay triangulation to the measurement positions. Two nodes were considered to be neighbors if they lie on the same edge of at least one triangle (Figure 1). Delaunay triangulation has such useful properties as maximizing the minimum angle within each triangle in the triangulation and containing the nearest neighbor of each node which helps to obtain a good quality discretization of $\Omega$.

In message passing graph neural networks we propagate a latent state for $K \geq 1$ graph layers, where each layer $k$ consists of first aggregating messages $m^{(k)}_i$ for each node $i$, and then updating the
We evaluate our model’s performance in learning the dynamics of known physical systems. We use an alternative approach, which allows computing the gradient for memory cost, which is required to evaluate the gradient of \( L \). While discrete-time neural PDE models evaluate the system state only at measurement time points, more accurate continuous-time solution for the estimated state generally requires many more evaluations of the system state. We define edge features \( e_{ij} := x_j - x_i \) as location differences. Finally, we use the node states at the last graph layer of the MPNN to evaluate the PDE surrogate

\[
\frac{d\hat{u}(x_i, t)}{dt} = \hat{F}_\theta(x_{N(i)} - x_i, u_i, u_{N(i)}) = h_i^{(K)},
\]

which is used to solve Equation 3 for the estimated states \( \hat{u}(t) = (\hat{u}(x_1, t), \ldots, \hat{u}(x_N, t)) \).

### 2.3 Adjoint method for learning continuous-time MPNN surrogates

Parameters of \( \hat{F}_\theta \) are defined by \( \theta \) which represents parameters of functions \( \phi^{(k)}, \gamma^{(k)} \), \( k = 1, \ldots, K \) in the MPNN. We fit \( \theta \) by minimizing the mean squared error between the observed states \( (y(t_0), \ldots, y(t_M)) \) and the estimated states \( (\hat{u}(t_0), \ldots, \hat{u}(t_M)) \).

\[
\mathcal{L}(\theta) = \int_{t_0}^{t_M} \ell(t, \hat{u}) dt = \int_{t_0}^{t_M} \frac{1}{M+1} \sum_{i=0}^{M} ||\hat{u}(t_i) - y(t_i)||^2 dt + \sum_{i=1}^{M} ||\hat{u}(t_i) - y(t_i)||^2.
\]

While discrete-time neural PDE models evaluate the system state only at measurement time points, more accurate continuous-time solution for the estimated state generally requires many more evaluations of the system state. If an adaptive solver is used to obtain the estimated states, the number of time steps performed by the solver might be significantly larger than \( M \). The amount of memory required to evaluate the gradient of \( \mathcal{L}(\theta) \) by backpropagation scales linearly with the number of solver time steps. This typically makes backpropagation infeasible due to large memory requirements. We use an alternative approach, which allows computing the gradient for memory cost, which is independent from the number of the solver time steps. The approach was presented in [Chen et al. 2018] for neural ODEs and is based on the adjoint method [Pontryagin, 2018]. The adjoint method consists of a single forward ODE pass (3) until state \( \hat{u}(t_M) \) at the final time \( t_M \), and subsequent backward ODE pass solving the gradients. The backward pass is performed by first solving the adjoint equation

\[
\dot{\lambda}(t) = \frac{\partial \ell}{\partial \hat{u}(t)} - \lambda(t)^T \frac{\partial \hat{F}}{\partial \hat{u}(t)},
\]

for the adjoint variables \( \lambda \) from \( t = t_M \) until \( t = 0 \) with \( \lambda(t_M) = 0 \), and then computing

\[
\frac{d\mathcal{L}}{d\theta} = -\int_0^T \lambda(t)^T \frac{\partial \hat{F}}{\partial \theta} dt
\]

to obtain the final gradient.

### 3 Experiments

We evaluate our model’s performance in learning the dynamics of known physical systems. We compare to state-of-the-art competing methods, and begin by performing ablation studies to measure how our model’s performance depends on measurement grid sizes, interval between observations, irregular sampling, amount of data and amount of noise.
3.1 Convection-diffusion ablation studies

The convection-diffusion equation is a partial differential equation that can be used to model a variety of physical phenomena related to the transfer of particles, energy, and other physical quantities inside a physical system. The transfer occurs due to two processes: convection and diffusion. The convection-diffusion equation is defined as

$$\frac{\partial u(x, y, t)}{\partial t} = D \nabla^2 u(x, y, t) - \mathbf{v} \cdot \nabla u(x, y, t),$$

(12)

where $u$ is the concentration of some quantity of interest (full problem specification and setup are in Appendix A.1). Quality of the model’s predictions was evaluated using the relative error between the observed states $y(t_i)$ and the estimated states $\hat{u}(t_i)$:

$$Err = \frac{\|y(t_i) - \hat{u}(t_i)\|}{\|y(t_i)\|}.$$  

(13)

In all following experiments, the training data contains 24 simulations on the time interval $[0, 0.2]$ sec and the test data contains 50 simulations on the time interval $[0, 0.6]$ sec.

**Different grid sizes.** This experiment tests our model’s capability to learn from data with different density of observation points. The time step was set to 0.02 sec resulting in 11 training time points per simulation. The number of observation points $x_i$ (and consequently nodes in the GNN) was set to 3000, 1500 and 750. The resulting grids are shown in the first column of Figure 2b. Relative test errors of the model trained on grids of different sizes are shown in Figure 2a. A comparison of the models’ predictions and the true states of the system for one out of the 50 test cases is shown in Figure 2b. The performance of the model decreases with the number of nodes in the grid. Nonetheless, even with the smallest grid containing 750 nodes, the model is able to learn a reasonably accurate approximation of the system’s dynamics and generalize beyond the training time interval.

**Different measurement time interval.** As will be shown in the following experiments, models with a constant time step are sensitive to the length of the time interval between observations. While showing good performance when the time step is small, such models fail to generalize if the time step is increased. This experiment shows our method’s ability to learn a continuous-time model from data with relatively large time intervals between observations.

Time steps of 0.02, 0.0667 and 0.2 sec, which give 11, 4 and 2 time points respectively, were used. The number of nodes was set to 3000. Relative test errors of the model trained on time grids of different sizes are shown in Figure 3a. A comparison of the models’ predictions and the true states of the system for one of the 50 test cases is shown in Figure 3b. The model is able to recover the continuous-time dynamics of the system even when trained with four time point per simulation. Increasing the frequency of observation does not significantly improve performance. An example of a training simulation with four time points is shown in Figure 4.
Figure 3: a) Relative test errors for different time grids. b) Visualization of the true and learned system dynamics (grids are shown in the first column).

Figure 4: Differences between observations in a train case with 4 time points.

Irregular time step. Observations used for training might not be recorded with a constant time step. This might cause trouble for models that are built with this assumption. This experiment tests our model’s ability to learn from data observed at random points in time.

The model is trained on two time grids. The first time grid has a constant time step 0.02 sec. The second grid is the same as the first one but with each time point perturbed by noise $\epsilon \sim \mathcal{N}(0, (0.02)^2)$. This gives a time grid with an irregular time step. The time step for test data was set to 0.01 sec. The number of nodes was set to 3000. Relative test errors of the model trained with constant and irregular time steps are shown in Figure 5. The figure shows that in both cases the model achieves similar performance. This demonstrates the truly continuous-time nature of our model as training and predictions are not restricted to evenly spaced time grids as with most other methods. Note again that none of the previous methods that learn free form (i.e., neural network parameterised) PDEs can be trained with data that is sampled irregularly over time.

Different amount of data. In this experiment, the model is trained on the data containing 1, 5, 10 and 24 simulations on the time interval $[0, 0.2]$ sec with time step 0.01 sec. The test data contains 50 simulations on the time interval $[0, 0.6]$ sec with the same time step. The number of nodes was set to 3000. Relative test errors of the model trained on different numbers of simulations are shown in Figure 6. Performance of the model improves as the amount of training data increases. It should be noted that despite using more data, the relative error does not converge to zero. The most probable reasons for that are insufficient number of nodes in the training data or insufficient model capacity.

Figure 5: Relative test errors for regular and irregular time grids.

Figure 6: Relative test errors for different amounts of training data.
Varying amount of additive noise. While the previous experiments were conducted by assuming noise-free observations of the system’s state, this experiment tests our model’s capability to learn from data with varying amounts of additive noise $\epsilon \sim \mathcal{N}(0, \sigma^2)$. The standard deviation $\sigma$ was set to 0.01, 0.02, and 0.04 while the largest magnitude of the observed states is 1. The time step was set to 0.01 sec. The number of nodes was set to 3000. Noise was added only to the training data.

The relative test errors of the model trained on data with different levels of noise are shown in Figure 7. The results show that the model’s performance decreases as $\sigma$ grows. Nonetheless, even with $\sigma$ set to 0.04, the model is still able to learn a reasonably accurate approximation of the dynamics of the system.

3.2 Benchmark method comparison

The proposed model was compared to two models presented in the literature: PDE-Net [Long et al., 2017] and DPGN [Seo and Liu, 2019a]. PDE-Net is based on a convolutional neural network and employs a constant time-stepping scheme resembling the Euler method. DPGN is based on a graph neural network and implements time-stepping as an evolution map in the latent space.

We used the PDE-Net implementation provided in [Long et al., 2017] except that instead of using the filters values directly, we pass them to an MLP consisting of 2 hidden layers 60 neurons each and hyperbolic tangent activation functions. This helps to improve stability and performance of the model. We use $5 \times 5$ filters without moment constraints. The number of $\delta t$-blocks was set to the number of time steps in the training data. The maximum PDE order was set to 4. Our implementation of DPGN followed that from [Seo and Liu, 2019a] with latent diffusivity $\alpha = 0.001$. The number of parameters in all models was close to 20k.

The training data contains 24 simulations on the time interval $[0, 0.2]$ sec with the following time steps: 0.01, 0.02 and 0.04 sec. The test data contains 50 simulations on the time interval $[0, 0.6]$ sec with the same time steps. The data was generated on a $50 \times 50$ regular grid as PDE-net cannot be applied to arbitrary spatial grids. The performance of the models was evaluated using the relative error averaged over time. Mean relative test errors of the models are shown in Figure 8. The figure shows that performance of the discrete-time models is strongly dependent on the time step while performance of the continuous-time model remains at the same level. At the smallest time step, PDE-Net, which is a CNN-based model, outperforms other models which are based on message passing neural networks. This might indicate that MPNNs is not an optimal choice for representing $\hat{F}_\theta$ for this particular PDE system, or that the MPNN surrogate model that we have chosen could be further improved by e.g. increasing its capacity. Yet again, our MPNN model is applicable to arbitrary space discretizations, whereas CNNs-based models are limited to regular grids.

3.3 Other dynamical systems

The model was tested on two more dynamical systems in order to evaluate its ability to work with a wider range of problems. We selected the heat equation and the Burgers’ equations for that purpose. The heat equation is one of the simplest PDEs while the Burgers’ equations are more complex than the convection-diffusion equation due to the presence of nonlinear convective terms. The increase in the problems’ difficulty allows to trace the change in the model’s performance as we move from simpler to more complex dynamics while keeping the number of model parameters fixed.
Heat equation. The heat equation describes the behavior of diffusive systems. The equation is defined as $\frac{\partial u}{\partial t} = D\nabla^2 u$, where $u$ is the temperature field (full problem specification and setup are in Appendix A.2). Figure 9a shows relative test errors of the model, and Figure 9b demonstrates the real and predicted evolution of the system for one of the test cases. The heat equation describes simpler dynamics than the convection diffusion equation which allowed the model to achieve slightly smaller test errors.

Burgers’ equations. The Burgers’ equations is a system of two coupled PDEs with nonlinear convection terms. It describes the behavior of dissipative systems with nonlinear propagation effects. The equations are defined in a vector form as $\frac{\partial \mathbf{u}(x, y, t)}{\partial t} = D\nabla^2 \mathbf{u}(x, y, t) - \mathbf{u}(x, y, t) \cdot \nabla \mathbf{u}(x, y, t)$, where $\mathbf{u}$ is the velocity vector field (full problem specification and setup are in Appendix A.3). For visualization and error measurement purposes, the velocity vector field is converted to a scalar field defined by the velocity magnitude at each node. Figure 10a shows relative test errors of the model, and Figure 10b demonstrates the real and predicted evolution of the system for one of the test cases. The Burgers’ equations describe more complex dynamics than the previous two cases which is reflected in higher relative test errors. Nonetheless, visual comparison of the true and predicted states shows that the model was able to achieve sufficient accuracy at approximating the unknown dynamics.

4 Conclusion

We present a continuous-time model of dynamical systems whose behavior is governed by PDEs. The model accurately recovers the system’s dynamics even when observation points are sparse and the data is recorded at irregular time intervals. Comparison with discrete-time models reveals the advantage of continuous-time models for datasets with larger time intervals between observations, which is typical for real-world applications where measurements can be either tedious or costly, or both. Discretization of the coordinate domain with the method of lines provides a general modeling framework in which arbitrary surrogate functions can be used for approximating $\hat{F}$. The continuous-time nature of the model enables the use of various time integrators ranging from the Euler method to highly accurate adaptive methods. This allows to optimize the choice of the surrogate function and time integration scheme depending on the structure of the data.
Broader Impact

In this work we introduce learning of PDE systems from irregularly measured data. This is a major step in extending the applicability of neural PDE learning. Spatially or temporally irregularly measured datasets are common in climate studies, life sciences and large-scale fluid dynamics. Our contributions represent a major step towards learning realistic real-world dynamical systems. While ethical considerations are not immediate, this work will have positive effects on our understanding of natural sciences through data.

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A Problem specification and setup

A.1 Convection-diffusion ablation studies

The convection-diffusion equation is a partial differential equation that can be used to model a variety of physical phenomena related to the transfer of particles, energy, and other physical quantities inside a physical system. The transfer occurs due to two processes: convection and diffusion.

Training and testing data was obtained by solving the following initial-boundary value problem on $\Omega = [0, 2\pi] \times [0, 2\pi]$ with periodic boundary conditions:

$$\frac{\partial u(x, y, t)}{\partial t} = D \nabla^2 u(x, y, t) - \nu \cdot \nabla u(x, y, t), \quad (x, y) \in \Omega, \ t \geq 0,$$

$$u(x, 0, t) = u(x, 2\pi, t), \quad x \in [0, 2\pi], \ t \geq 0,$$

$$u(0, y, t) = u(2\pi, y, t), \quad y \in [0, 2\pi], \ t \geq 0,$$

$$u(x, y, 0) = u_0(x, y), \quad (x, y) \in \Omega,$$

where the diffusion coefficient $D$ was set to 0.25 and the velocity field $\nu$ was set to $(5.0, 2.0)^T$. The initial conditions $u_0(x, y)$ were generated as follows:

$$\hat{u}_0(x, y) = \sum_{k,l=-N}^{N} \lambda_{kl} \cos (kx + ly) + \gamma_{kl} \sin (kx + ly)$$

$$u_0(x, y) = \frac{\hat{u}_0(x, y) - \min \hat{u}_0(x, y)}{\max \hat{u}_0(x, y) - \min \hat{u}_0(x, y)},$$

where $N = 4$ and $\lambda_{kl}, \gamma_{kl} \sim N(0, 1)$. The generated data contains $N_s$ simulations. Each simulation contains values of $u(x, y, t)$ at time points $(t_1, \ldots, t_{M})$ and locations $(x_1, \ldots, x_N)$, where $x_n = (x_n, y_n)$. Numerical solutions that represent the true dynamics were obtained using the backward Euler solver with the time step of 0.0002 seconds on a computational grid with 4100 nodes. Training and testing data used in the following experiments is downsampled from these solutions. Quality of the model’s predictions was evaluated using the relative error between the observed states $y(t_i)$ and the estimated states $\hat{u}(t_i)$:

$$Err = \frac{\|y(t_i) - \hat{u}(t_i)\|}{\|y(t_i)\|}.$$ 

The model used for all following experiments contains a single graph layer. The mean was selected as the aggregation function. Functions $\phi^{(1)}(u_i, \cdot)$ and $\gamma^{(1)}(u_i, u_j - u_i, x_j - x_i)$ were represented by multilayer perceptrons with 3 hidden layers and hyperbolic tangent activation functions. Input/output sizes for $\phi^{(1)}$ and $\gamma^{(1)}$ were set to $4/40$ and $41/1$ respectively. The number of hidden neurons was set to 60. This gives approximately 20k trainable parameters.

We followed the implementation of the adjoint method and ODE solvers from torchdiffeq Python package [Chen et al., 2018]. In all following experiments, adaptive-order implicit Adams solver was used with rtol and atol set to $1.0 \cdot 10^{-7}$. Rprop [Riedmiller and Braun, 1992] optimizer was used with learning rate set to $1.0 \cdot 10^{-6}$ and batch size set to 24.

A.2 Heat equation experiment

Training and testing data was obtained by solving the following initial-boundary value problem on $\Omega = (0, 1) \times (0, 1)$ with Dirichlet boundary conditions:

$$\frac{\partial u(x, y, t)}{\partial t} = D \nabla^2 u(x, y, t), \quad (x, y) \in \Omega, \ t \geq 0,$$

$$u(x, y, t) = u_0(x, y), \quad (x, y) \in \partial \Omega, \ t \geq 0,$$

$$u(x, y, 0) = u_0(x, y), \quad (x, y) \in \Omega,$$
where \( \partial \Omega \) denotes the boundaries of \( \Omega \) and diffusion coefficient \( D \) was set to 0.2. The initial conditions \( u_0(x, y) \) were generated as follows:

\[
\bar{u}_0(x, y) = \sum_{k,l=-N}^{N} \lambda_{kl} \cos (kx + ly) + \gamma_{kl} \sin (kx + ly) \\
u_0(x, y) = \frac{\bar{u}_0(x, y) - \min \bar{u}_0(x, y)}{\max \bar{u}_0(x, y) - \min \bar{u}_0(x, y)},
\]

where \( N = 10 \) and \( \lambda_{kl}, \gamma_{kl} \sim \mathcal{N}(0, 1) \). The generated data contains \( N \) simulations. Each simulation contains values of \( u(x, y, t) \) at time points \( \{t_1, \ldots, t_M\} \) and locations \( \{(x_1, \ldots, x_N)\} \), where \( x_n = (x_n, y_n) \). Numerical solutions that represent the true dynamics were obtained using the backward Euler solver with the time step of 0.0001 seconds on a computational grid with 4100 nodes. Training and testing data used in the experiments with the heat equation is downsamples from these solutions.

The model used for all experiments with the heat equation contains a single graph layer. The model used for all experiments with the heat equation contains a single graph layer. The initial conditions \( u_0(x, y) \) for each component were generated as follows:

\[
\bar{u}_0(x, y) = \sum_{k,l=-N}^{N} \lambda_{kl} \cos (kx + ly) + \gamma_{kl} \sin (kx + ly) \\
u_0(x, y) = 6 \times \left( \frac{\bar{u}_0(x, y) - \min \bar{u}_0(x, y)}{\max \bar{u}_0(x, y) - \min \bar{u}_0(x, y)} - 0.5 \right),
\]

where \( N = 2 \) and \( \lambda_{kl}, \gamma_{kl} \sim \mathcal{N}(0, 1) \). The generated data contains \( N \) simulations. Each simulation contains values of \( u(x, y, t) \) at time points \( \{t_1, \ldots, t_M\} \) and locations \( \{(x_1, \ldots, x_N)\} \), where \( x_n = (x_n, y_n) \). Numerical solutions that represent the true dynamics were obtained using the backward Euler solver with the time step of 0.0016 seconds on a computational grid with 5446 nodes. Training and testing data used in the experiments with the heat equation is downsamples from these solutions.

The model used for all experiments with the Burgers’ equations contains a single graph layer. The model used for all experiments with the heat equation contains a single graph layer. The mean was selected as the aggregation function. Functions \( \phi^{(1)} \) and \( \gamma^{(1)} \) were represented by multilayer perceptrons with 3 hidden layers and hyperbolic tangent activation functions. Input/output sizes for \( \phi^{(1)} \) and \( \gamma^{(1)} \) were set to 4/40 and 41/1 respectively. The number of hidden neurons was set to 60. This gives approximately 20k trainable parameters.

A.3 Burgers’ equations experiment

Training and testing data was obtained by solving the following initial-boundary value problem on \( \Omega = [0, 2\pi] \times [0, 2\pi] \) with periodic boundary conditions:

\[
\begin{align*}
\frac{\partial u(x, y, t)}{\partial t} & = D \nabla^2 u(x, y, t) - u(x, y, t) \cdot \nabla u(x, y, t), & (x, y) \in \Omega, \ t \geq 0, \\
u(x, 0, t) & = u(x, 2\pi, t), & t \geq 0, \\
u(0, y, t) & = u(2\pi, y, t), & t \geq 0, \\
u(x, y, 0) & = u_0(x, y), & (x, y) \in \Omega, \ t = 0,
\end{align*}
\]

where the diffusion coefficient \( D \) was set to 0.15. The unknown function is now vector-valued. Therefore, the initial conditions \( u_0(x, y) \) for each component were generated as follows:

\[
\bar{u}_0(x, y) = \sum_{k,l=-N}^{N} \lambda_{kl} \cos (kx + ly) + \gamma_{kl} \sin (kx + ly) \\
u_0(x, y) = 6 \times \left( \frac{\bar{u}_0(x, y) - \min \bar{u}_0(x, y)}{\max \bar{u}_0(x, y) - \min \bar{u}_0(x, y)} - 0.5 \right),
\]

where \( N = 2 \) and \( \lambda_{kl}, \gamma_{kl} \sim \mathcal{N}(0, 1) \). The generated data contains \( N \) simulations. Each simulation contains values of \( u(x, y, t) \) at time points \( \{t_1, \ldots, t_M\} \) and locations \( \{(x_1, \ldots, x_N)\} \), where \( x_n = (x_n, y_n) \). Numerical solutions that represent the true dynamics were obtained using the backward Euler solver with the time step of 0.0016 seconds on a computational grid with 5446 nodes. Training and testing data used in the experiments with the heat equation is downsamples from these solutions.
We followed the implementation of the adjoint method and ODE solvers from torchdiffeq Python package [Chen et al., 2018]. In all following experiments, adaptive-order implicit Adams solver was used with rtol and atol set to $1.0 \cdot 10^{-7}$. Rprop [Riedmiller and Braun, 1992] optimizer was used with learning rate set to $1.0 \cdot 10^{-6}$ and batch size set to 24.

In the experiment, the training data contains 24 simulations on the time interval $[0, 0.8]$ sec with time step $0.04$ sec resulting in 21 time point. The test data contains 50 simulations on the time interval $[0, 2.4]$ sec with the same time step. The number of observation points $x_i$ was set to 5000.