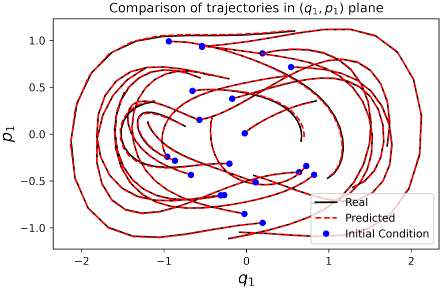
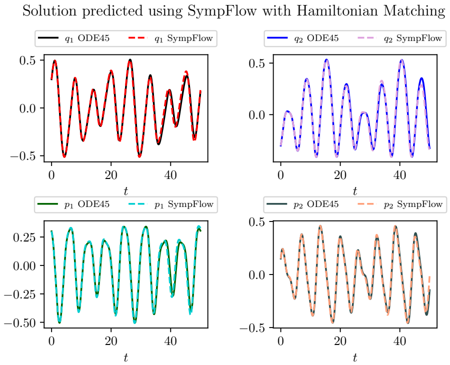
Neural networks and their connections with differential equations





Neural networks

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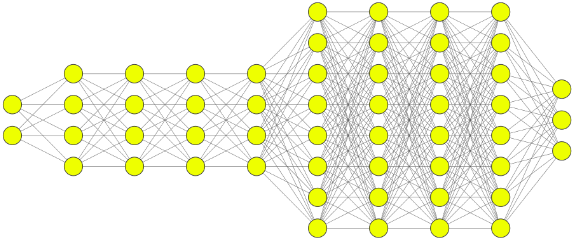

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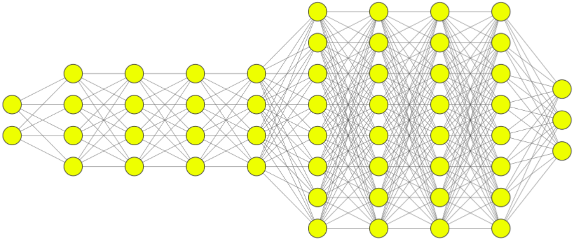

- Mathematically, a neural network is just a **parametric map** $\mathcal{N}_\theta : \mathbb{R}^c \to \mathbb{R}^d$, which is usually defined by composing L functions, called **layers**, as $\mathcal{N}_\theta = F_{\theta_L} \circ ... \circ F_{\theta_1}$, $F_{\theta_i} : \mathbb{R}^{c_i} \to \mathbb{R}^{c_{i+1}}$, $c_1 = c$, $c_{L+1} = d$.

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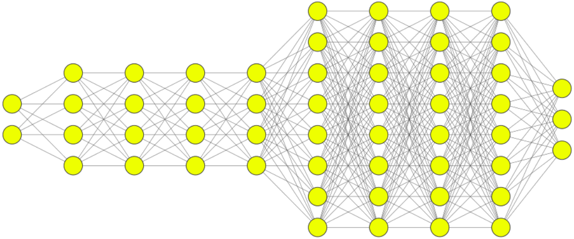

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- The parametrisation strategy behind $\mathcal{N}_\theta$ is defined by the so-called **neural network architecture**.

Examples of layers

- It is common practice to define layers by alternating linear maps, with non-linear functions applied entrywise:

$$F_{\theta_i}(\mathbf{x}) = \Sigma \circ L_i(\mathbf{x}), \;\; \Sigma(\mathbf{x}) := \begin{bmatrix} \sigma(x_1) \\ \vdots \\ \sigma(x_{c_i}) \end{bmatrix}.$$

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- We can also choose $L_i(\mathbf{x}) = k_i * \mathbf{x} + \mathbf{b}_i$, so realise the linear layer by convolution, and get a map that shows up in **convolutional neural networks**

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- One of the simplest loss functions we can work with is the **mean-squared error**. Say that we want to approximate the function $F : \Omega \to \mathbb{R}^d$, $\Omega \subset \mathbb{R}^c$, and we have the dataset $\{(\mathbf{x}_i, \mathbf{y}_i = F(\mathbf{x}_i))\}_{i=1}^N$, $\mathbf{x}_i \in \Omega$, then we can work with the loss function

$$L(\theta) = \frac{1}{N} \sum_{i=1}^{N} \|\mathcal{N}_\theta(\mathbf{x}_i) - \mathbf{y}_i\|_2^2 .$$

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- After minimising the loss function, we hopefully have a good set of parameters θ^* and we can use $\mathcal{N}_{\theta^*}$ to make new predictions, for unseen inputs.

Universal approximation theorems

Theorem

Let $\Omega \subset \mathbb{R}^c$ be a compact set and assume $\sigma : \mathbb{R} \to \mathbb{R}$ is not a polynomial. For any continuous function $F : \Omega \to \mathbb{R}$ and for any $\varepsilon > 0$ there is a single-layer neural network

$$\mathcal{N}_\theta(x) := \mathbf{w}^T \sigma(\mathbf{a}\mathbf{x} + \mathbf{b}), \;\; \mathbf{a}, \mathbf{b}, \mathbf{w} \in \mathbb{R}^h,$$

with $h \in \mathbb{N}$ large enough, such that

$$\max_{\mathbf{x} \in \Omega} |F(\mathbf{x}) - \mathcal{N}_\theta(\mathbf{x})| \leq \varepsilon.$$

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This theorem extends to vector-valued functions, and similar results exist also for deeper networks.

Residual Neural Networks (ResNets)

- A particularly interesting network architecture is the one of ResNets. The layers of these networks are of the from

$$F_{\theta_i}(\mathbf{x}) = \mathbf{x} + X_{\theta_i}(\mathbf{x}),$$

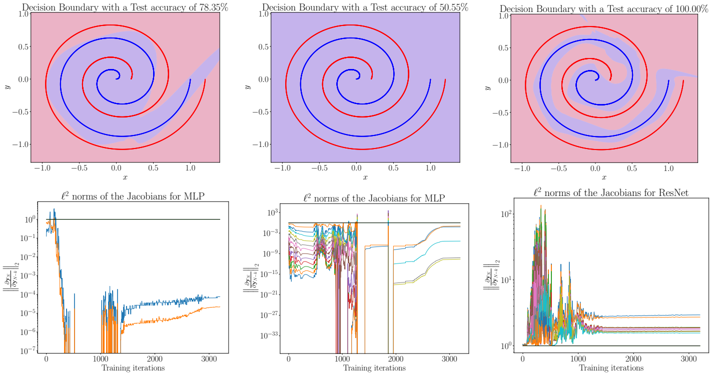
  where an example could be $X_{\theta_i}(\mathbf{x}) = B_i^T \sigma(A_i \mathbf{x} + \mathbf{b}_i)$, $A_i, B_i \in \mathbb{R}^{h \times c_i}$, $\mathbf{b}_i \in \mathbb{R}^h$.
- The reason why they were introduced is because they are much easier to train when the network has a high number of layers.

Why ResNets?

Recall that to minimise the loss function $L(\theta)$ we have to use some numerical method, like gradient descent

$$\theta_{k+1} = \theta_k - \tau \nabla L(\theta_k).$$

If $\|\nabla L(\theta_k)\|_2$ is very large or very small, we will struggle to find a meaningful set of weights.



ResNets as dynamical systems

- Residual Neural Networks (ResNets) are networks of the form $\mathcal{N}_\theta = f_{\theta_L} \circ \ldots \circ f_{\theta_1}$ with

$$f_{\theta_i}(\mathbf{x}) = \mathbf{x} + B_i^\top \sigma\left(A_i \mathbf{x} + \boldsymbol{b}_i\right) \in \mathbb{R}^d, \ \mathbf{x} \in \mathbb{R}^d,$$
$$A_i, B_i \in \mathbb{R}^{h \times d}, \ \boldsymbol{b}_i \in \mathbb{R}^h, \ \theta_i = \left\{A_i, B_i, \boldsymbol{b}_i\right\}.$$

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\end{aligned}
$$

- The layer

$$
f_{\theta_i}(\mathbf{x}) = \mathbf{x} + B_i^\top \sigma\left(A_i \mathbf{x} + \boldsymbol{b}_i\right) = \mathbf{x} + \mathcal{F}_{\theta_i}(\mathbf{x}) \in \mathbb{R}^d
$$

is an explicit Euler step of size 1 for the initial value problem

$$
\begin{cases}
\dot{\mathbf{y}}(t) = B_i^\top \sigma(A_i \mathbf{y}(t) + \boldsymbol{b}_i) = \mathcal{F}_{\theta_i}(\mathbf{y}(t)), \\
\mathbf{y}(0) = \mathbf{x}
\end{cases}
.
$$

- We can define ResNet-like neural networks by choosing a family of parametric functions $\mathcal{S}_\Theta = \left\{\mathcal{F}_\theta : \mathbb{R}^d \to \mathbb{R}^d : \ \theta \in \Theta\right\}$ and a numerical method $\Psi^h_{\mathcal{F}}$, like explicit Euler defined as $\Psi^h_{\mathcal{F}}(\mathbf{x}) = \mathbf{x} + h\mathcal{F}(\mathbf{x})$, and set

$$\mathcal{N}_\theta(\mathbf{x}) = \Psi^{h_L}_{\mathcal{F}_{\theta_L}} \circ \cdots \circ \Psi^{h_1}_{\mathcal{F}_{\theta_1}}(\mathbf{x}), \ \mathcal{F}_{\theta_1}, ..., \mathcal{F}_{\theta_L} \in \mathcal{S}_\Theta.$$

- We could also combine these residual blocks with lifting and projection layers, as for usual neural networks.

Neural networks for dynamical systems discovery

- Apart from using dynamical systems and numerical analysis to study neural networks, we can also use neural networks to solve and discover differential equations.

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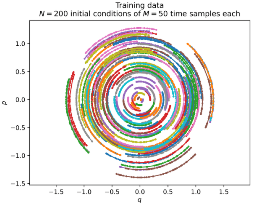
- Apart from using dynamical systems and numerical analysis to study neural networks, we can also use neural networks to solve and discover differential equations.
- The task of dynamical systems discovery can be summarised as follows:



$$\Longrightarrow \begin{bmatrix} \dot{q} \\ \dot{p} \end{bmatrix} = \begin{bmatrix} p \\ -q \end{bmatrix}.$$

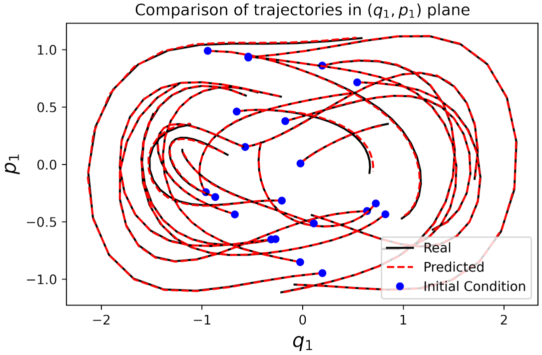
- To train the overall model $\mathcal{N}_\theta$ we can minimise the loss function

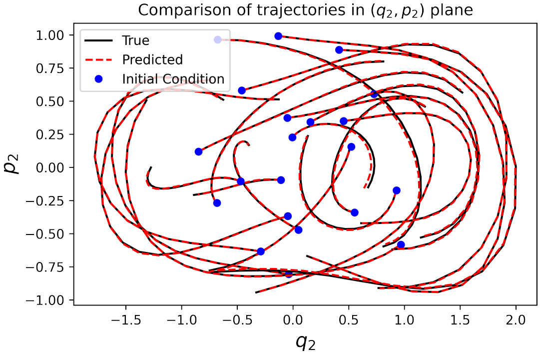
$$\mathcal{L}(\theta) = \frac{1}{NM} \sum_{n=1}^{N} \sum_{m=1}^{M} \left\| \left(\Psi^h_{\mathcal{N}_\theta} \right)^m (\mathbf{x}_0^n) - \mathbf{y}_m^n \right\|_2^2,$$

where $\mathbf{x}_0^n \in \Omega \subset \mathbb{R}^{2n}$, and $\mathbf{y}_m^n \approx \phi^{m\,h}(\mathbf{x}_0^n)$.

Example with Hamiltonian system

$$H(q,p) = \frac{1}{2}\begin{bmatrix} p_1 & p_2 \end{bmatrix}^T \begin{bmatrix} 5 & -1 \\ -1 & 5 \end{bmatrix} \begin{bmatrix} p_1 \\ p_2 \end{bmatrix} + \frac{q_1^4 + q_2^4}{4} + \frac{q_1^2 + q_2^2}{2}.$$





Neural networks solving differential equations

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- We can define a network $\mathcal{N}_\theta : \mathbb{R} \times \mathbb{R}^d \to \mathbb{R}^d$. We can also enforce the initial condition, so that $\mathcal{N}_\theta(0, \mathbf{x}_0) = \mathbf{x}_0$ for every $\mathbf{x}_0 \in \mathbb{R}^d$. This can be done for example by defining
$$\mathcal{N}_\theta(t, \mathbf{x}) = \mathbf{x} + \widetilde{\mathcal{N}}_\theta(t, \mathbf{x}) - \widetilde{\mathcal{N}}_\theta(0, \mathbf{x}),$$
for an arbitrary network $\widetilde{\mathcal{N}}_\theta : \mathbb{R} \times \mathbb{R}^d \to \mathbb{R}^d$.

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for an arbitrary network $\widetilde{\mathcal{N}}_\theta : \mathbb{R} \times \mathbb{R}^d \to \mathbb{R}^d$.
- To train $\mathcal{N}_\theta$ we can minimise the loss function
$$\mathcal{L}(\theta) = \frac{1}{N_r} \sum_{i=1}^{N_r} \left\| \frac{d}{dt} \mathcal{N}_\theta\left(t, \mathbf{x}_0^i\right)\Big|_{t=t_i} - \mathcal{F}\left(\mathcal{N}_\theta\left(t_i, \mathbf{x}_0^i\right)\right) \right\|_2^2$$
at sufficiently many collocation points $t_i \in [0, T]$ and $\mathbf{x}_0^i \in \mathbb{R}^d$.

Example: Hénon–Heiles

Equations of motion

$$\dot{x} = p_x, \;\; \dot{y} = p_y, \;\; \dot{p}_x = -x - 2xy, \;\; \dot{p}_y = -y - (x^2 - y^2).$$