Jacobian norm regularisation and conditioning in neural ordinary differential equations

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What to expect

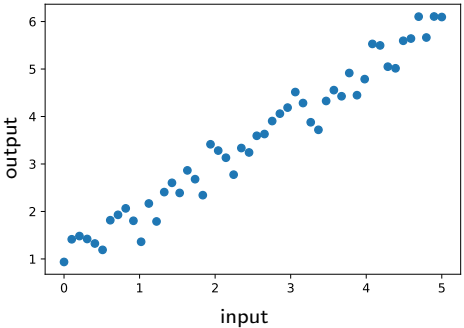
Overview of neural ordinary differential equations (ODEs)

- learnable input-output mapping defined as the solution to an ODE

Neural ODE challenges and Jacobian regularisation

Review selected results

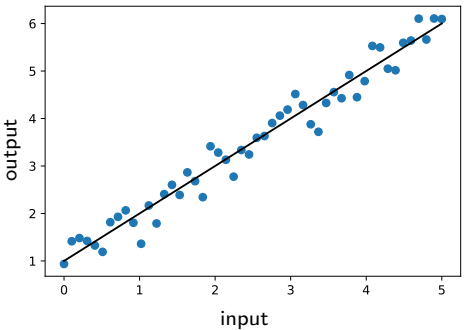
Learnable input-output mapping



1. Choose a function class

$$f(x) = wx + b$$

Learnable input-output mapping

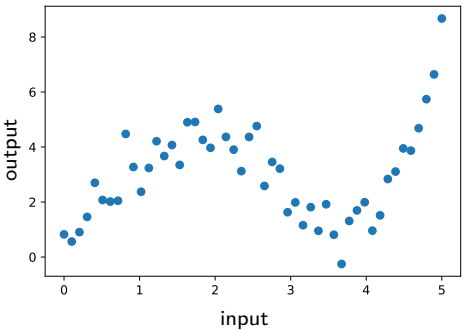


1. Choose a function class
$$f(x) = wx + b$$
2. Determine parameters w and b via gradient based optimisation.
3. Done by defining an objective function (error).

Regularisation adds a penalty to the objective.

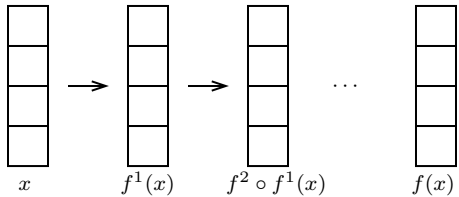
- faster convergence, better generalisation

Learnable input-output mapping: neural networks



1. Choose a function class

$$f(x) = f^n \circ f^{n-1} \circ \cdots \circ f^1(x)$$



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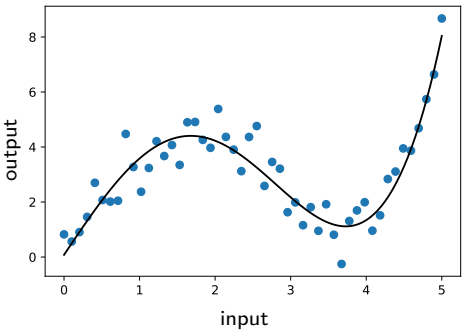

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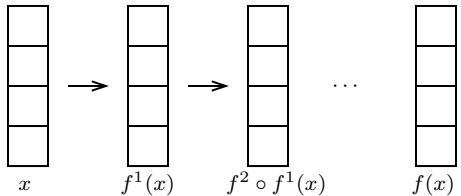
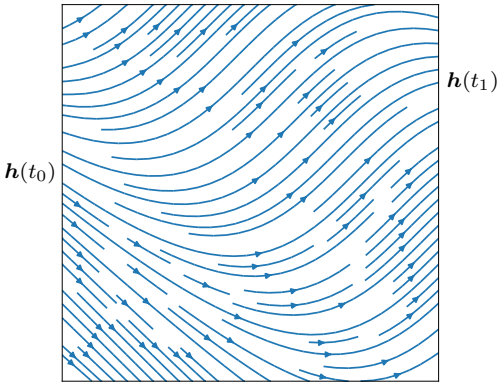


2. Determine parameters via gradient-based optimisation.

Regularisation adds a penalty to the objective.

- faster convergence, better generalisation

Neural ordinary differential equations



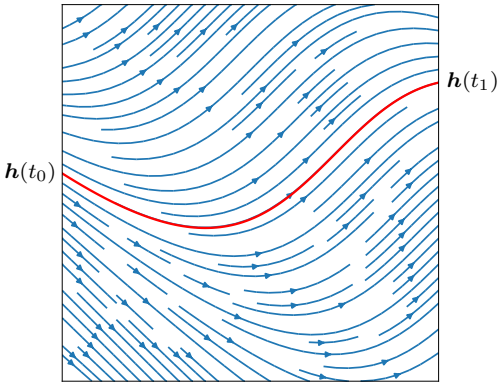
A vector $\boldsymbol{h}(t)$ follows the dynamics f:

$$\frac{d\boldsymbol{h}(t)}{dt} = f(\boldsymbol{h}(t), t)$$

For an input $\boldsymbol{h}(t_0)$ determine output as

$$\boldsymbol{h}(t_1) = \boldsymbol{h}(t_0) + \int_{t_0}^{t_1} f(\boldsymbol{h}(t), t)\, dt$$

Neural ordinary differential equations



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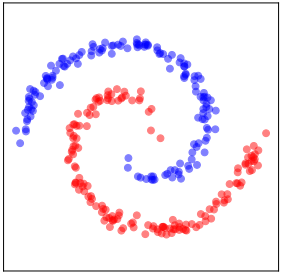
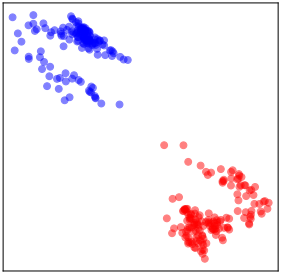
An example: binary classification



input

use a neural network
as the function



output

An example: binary classification

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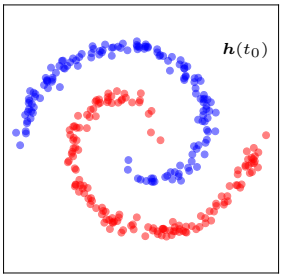

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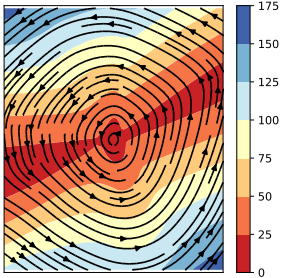
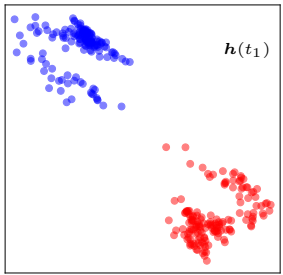




output

More generally useful for

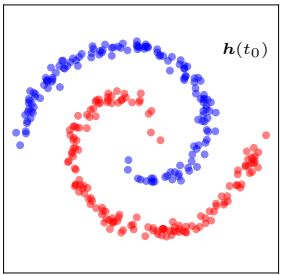
1. Modelling data from continuous-time systems
2. Continuous normalising flows for density estimation

dynamical systems, time-series

An example: binary classification

$$\frac{d\boldsymbol{h}(t)}{dt} = f(\boldsymbol{h}(t), t)$$

$$\boldsymbol{h}(t_0) + \int_{t_0}^{t_1} f(\boldsymbol{h}(t), t)\, dt$$



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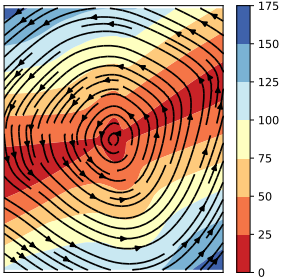
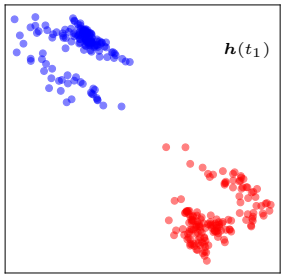




output

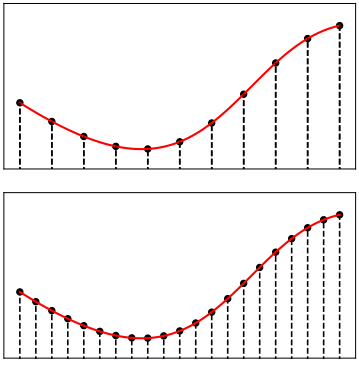
We care about

1. Generalisation and robustness to input perturbations — in high dimensions
2. Computational efficiency

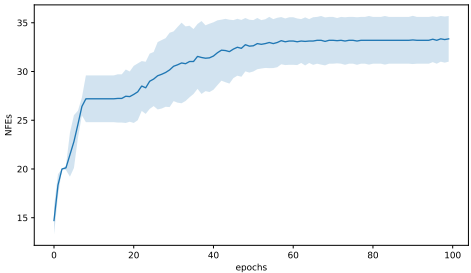
How should we regularise our objective function when training neural ODEs?

The problem: rising number of function evaluations (NFE)

$$\boldsymbol{h}(t_1) = \boldsymbol{h}(t_0) + \int_{t_0}^{t_1} f(\boldsymbol{h}(t), t)\, dt$$



higher accuracy requires higher NFE



NFE rises during training

Comments on conditioning

"poorly conditioned dynamics will lead to difficulties during numerical integration"

Finlay et al. How to train your neural ODE: the world of Jacobian and kinetic regularization, 2020.

"flows that need to stretch and squeeze the input space in such a way are likely to lead to ill-posed ODE problems that are numerically expensive to solve"

Dupont et al. Augmented Neural ODEs, 2019.

Jacobian norm regularisation

If $\boldsymbol{h}(t) = \begin{bmatrix} h_1 \\ h_2 \end{bmatrix}$, and $f(\boldsymbol{h}(t), t) = \begin{bmatrix} f_1 \\ f_2 \end{bmatrix}$, then $\boldsymbol{J} = \begin{bmatrix} \frac{\partial f_1}{\partial h_1} & \frac{\partial f_1}{\partial h_2} \\ \frac{\partial f_2}{\partial h_1} & \frac{\partial f_2}{\partial h_2} \end{bmatrix}$

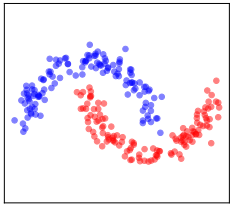
In general: $\boldsymbol{J} = \nabla_{\boldsymbol{h}(t_0)} f(\boldsymbol{h}(t), t)$

$\|\boldsymbol{J}\|_F = \sqrt{\sum_{i=1}^{d} \sum_{j=1}^{d} |\boldsymbol{J}_{i,j}|^2} \ \downarrow$ Frobenius: neural ODE

$\|\boldsymbol{J}\|_2 = \sigma_{\max}(\boldsymbol{J}) \ \downarrow$ spectral: neural network

$\kappa(\boldsymbol{J}) = \frac{\sigma_{\max}(\boldsymbol{J})}{\sigma_{\min}(\boldsymbol{J})} \to 1$ condition number: our work

Jacobian norm regularisation



Binary classification

Intertwining moons dataset

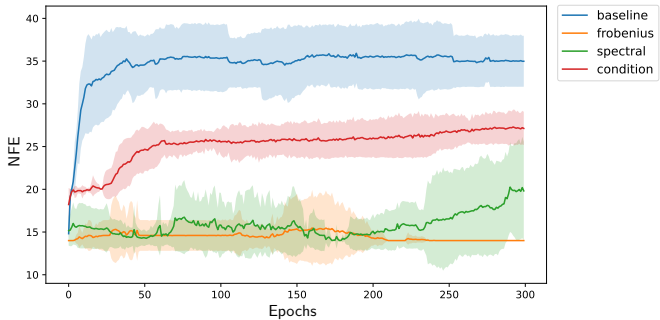
$\|\boldsymbol{J}\|_F = \sqrt{\sum_{i=1}^{d}\sum_{j=1}^{d}|\boldsymbol{J}_{i,j}|^2}\ \downarrow$ Frobenius: neural ODE

$\|\boldsymbol{J}\|_2 = \sigma_{\max}(\boldsymbol{J})\ \downarrow$ spectral: neural network

$\kappa(\boldsymbol{J}) = \dfrac{\sigma_{\max}(\boldsymbol{J})}{\sigma_{\min}(\boldsymbol{J})} \to 1$ condition number: our work

NFE reduction

Frobenius, spectral, and condition number regularisation reduce NFE.



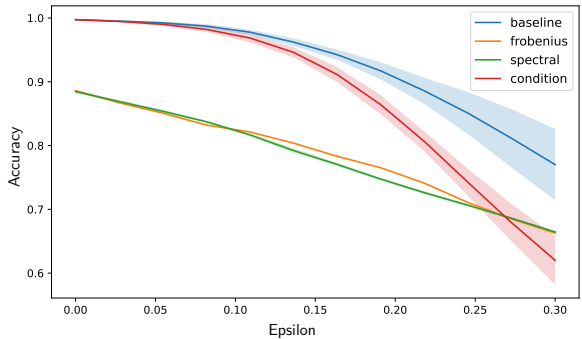
Solid curves and shaded regions indicate mean and standard deviation over 10 runs.

Good! But at what cost?

Performance and robustness

a) Jacobian norm regularisation sacrifices performance for NFE reduction.

b) Robustness to input noise for condition number regularisation.



Jacobian norm regularisation leads to increased distance to decision boundary.

Conclusion

Recall that we want generalisation and a reduced NFE.

1. Jacobian norm regularisation reduces NFE, potentially at a cost to generalisation and robustness. Condition number regularisation seems to help.
2. Jacobian norm regularisation can lead to an increased distance to the decision boundary.

Ongoing work:

1. Efficient condition number estimation.
2. Characterise conditions for rising NFE (stiffness?).
3. Other ways to parameterise the ODE or solution?