Neural ODEs and Control

March 14, 2023

References

Kidger, Patrick. "On neural differential equations." arXiv preprint arXiv:2202.02435 (2022).

Ruiz-Balet, Domenec, and Enrique Zuazua. "Neural ODE control for classification, approximation and transport." arXiv preprint arXiv:2104.05278 (2021).

$$y(0) = y_0 \qquad \frac{dy}{dt}(t) = f_\theta(t, y(t))$$

- $d = d_1 \times \cdots \times d_k$ and $f_\theta \colon \mathbb{R} \times \mathbb{R}^d \to \mathbb{R}^d$ is (for example) a feedforward neural net
- θ learnable parameters
- existence/uniqueness of solutions?
- solutions are functions $y \colon [0, T] \to \mathbb{R}^d$

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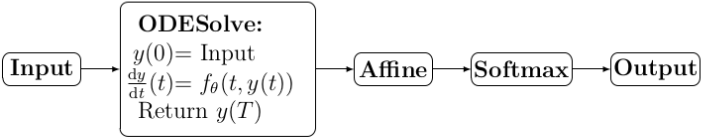

$$\operatorname{softmax}\left(A_\theta\left(y(0) + \int_0^T f_\theta(t, y(t))\, dt\right)\right)$$

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- favorable to maintain interpretability during training

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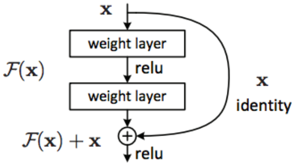
corresponds to the forward equations of *ResNet* blocks



Allows for an interpretation as optimal control problem. Specify the neural ResNet:

$$\theta = \{W(t), A(t), b(t)\}$$

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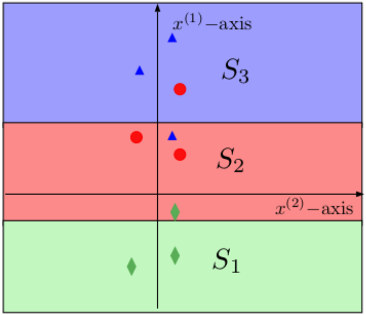
- parameters act as controls $W(t), A(t) \in L^\infty((0,T); R^{d\times d})$, and $b(t) \in L^\infty((0,T); R^d)$
- reformulate classification problem

- split R^d into horizontal strips corresponding to classes $S_1, \ldots, S_m$



- training goal: find controls that steer the training examples into the right strip

Theorem (Zuazua and Ruiz-Balet, 2021)

Let $\{y_i, z_i\}_{i=1}^N \subset \mathbb{R}^d \times \mathbb{R}^d$ *be the dataset to be classified with* $y_i \neq y_j$ *and* $z_i \in S_{m(i)}$.
Then for every $T > 0$ *there exist piecewise constant controls with* $O(N)$ *switches such that*

$$\forall i : \quad y(0) = y_i \implies y(T) \in S_{m(i)}.$$

Sketch of proof

Fully constructive.

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Preparation requires at most N switches, classification at most $3N$.

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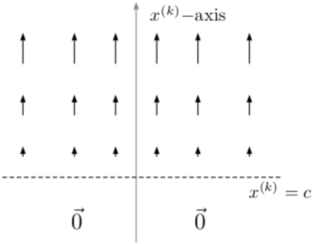
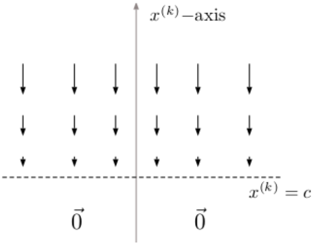
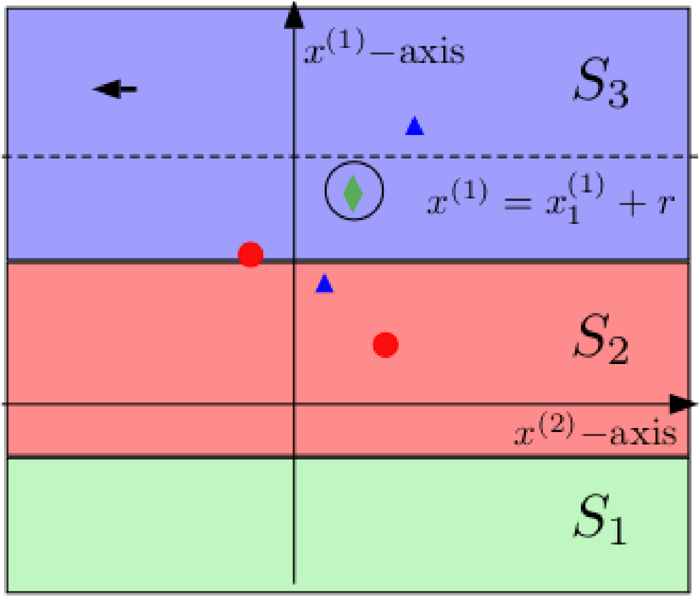
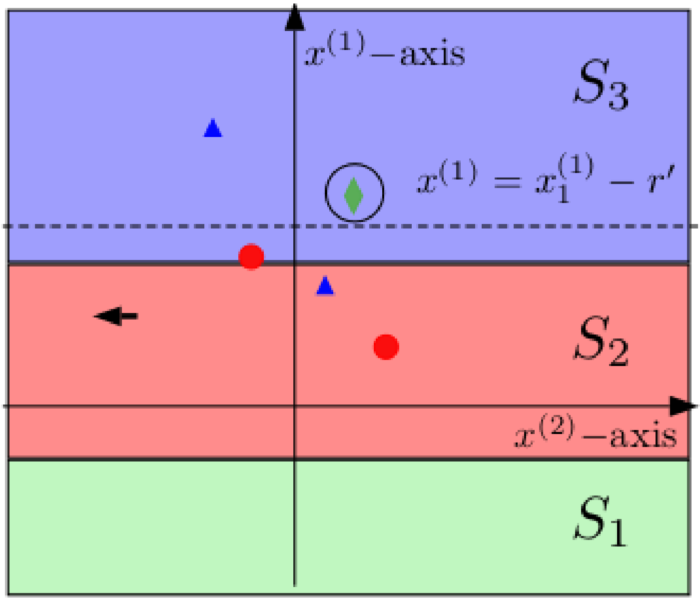
- **expand/contract**: see pictures. decide whether the hyperplane will be repulsive or attractive
- **translate**: flow parallel to the hyperplane






$x^{(1)}-$axis
S_3
$x^{(1)}=x_1^{(1)}+r$
S_2
$x^{(2)}-$axis
S_1



$x^{(1)}$−axis
S_3
$x^{(1)} = x_1^{(1)} - r'$
S_2
$x^{(2)}$−axis
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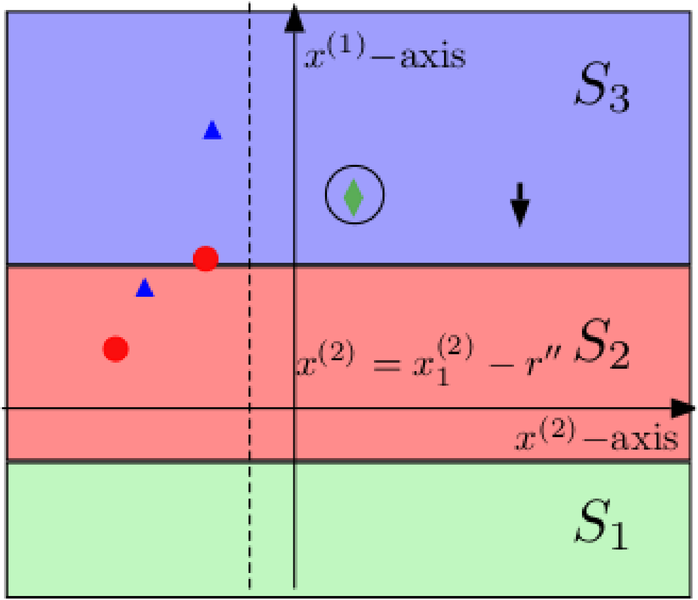
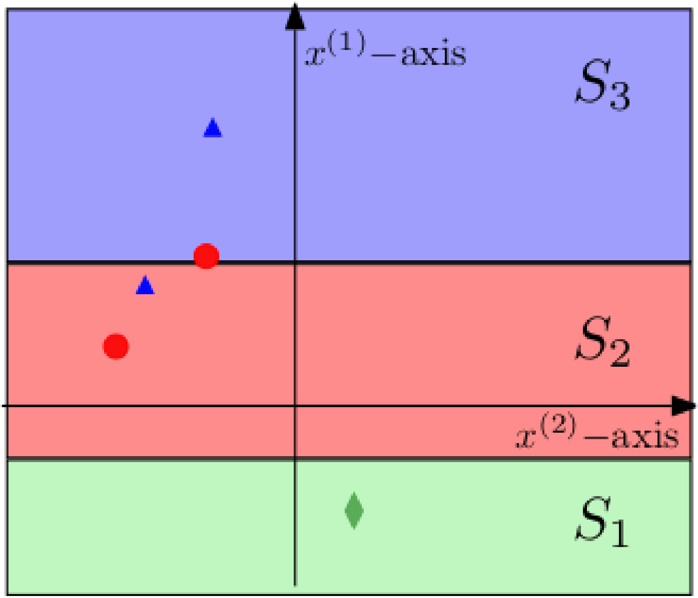


$x^{(1)}$−axis
S_3
$x^{(2)} = x_1^{(2)} - r''$
S_2
$x^{(2)}$−axis
S_1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- in the continuous-depth interpretation: dynamically adding layers during training
- regularization = fewer moves with lower amplitude? generalization bounds?