# Robustness with neural ordinary differential equations

Rafael Orive
Work with collaboration A. Álvarez (UAM), D. Fernández (FAU), E. Zuazua (Deusto)
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Universidad Autónoma de Madrid

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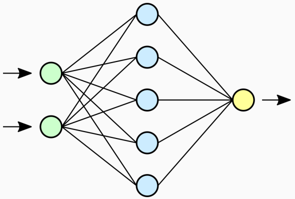
# Supervised Learning setting

- **Setting**: Data $(x, y) \sim \gamma$
- $\gamma$ is (in general) an unknown probability distribution
- **Goal**: Given a sample data $x \in \mathbb{R}^d$ predict $y \in \mathbb{R}^D$
- Choose a model $F$

Feature (input) $x \in \mathbb{R}^d$ $\xrightarrow[F]{\text{Model}}$ Label (output) $F(x) \in \mathbb{R}^D$

Some typical model choices:

- Linear regression
- Neural network
- Neural ODE



# Neural ordinary differential equations

A **neural ODE** (NODE) [Chen, 2018] in its most general form, where $x_0 \in \mathbb{R}^d$ is the **input** (features), $u = [w, b] \in \mathbb{R}^{d_u}$ is the **control** (parameters) and $f$ some **neural network architecture**, is given by

$$\begin{cases} \dot{x}(t) = f(t, x(t), u), \quad t \in (0, T] \\ x(0) = x_0 \end{cases} \tag{1}$$

$$\uparrow\downarrow$$

$$\begin{cases} x^{(t+1)} = x^{(t)} + hf(t, x^{(t)}, u) \\ x^{(0)} = x_0 \end{cases}$$

The **"nonlinear"** in NODEs:

- **Inside**: $f(x, u) = \sigma(w \cdot x + b)$
- **Outside**: $f(x, u) = w\sigma(x) + b$
- **Bottleneck**: $f(x, u) = w_2\sigma(w_1 \cdot x + b)$

**Output:**

$F(x_0) := P \circ \Phi_T(x_0)$

- $\Phi_t(x_0) = x(t; x_0)$ flow map
- $P = Mx + N,\ M, N$ linear

## Optimising the model

- **Loss** function $J(u; x, y)$ as a measure of error between predicted and actual values for each control/parameter $u$.
- **Goal**: Find

$$\min_u \left[\mathbb{E}_{(x,y)\sim\gamma} J(u; x, y)\right]$$

But $\gamma$ is unknown... find instead

$$\min_u \frac{1}{N}\sum_{i=1}^{N} J(u; x_i, y_i)$$

Training data $\{(x_i, y_i)\}_{i=1}^{N} \subseteq \mathbb{R}^d \times \mathbb{R}^D$ $\xrightarrow{\text{Training (optimisation)}}$ "Optimal" parameters (control) $u \in \mathbb{R}^{d_u}$

- **Optimisation** through **Gradient Descent** (GD):

$$u^{k+1} = u^k - \eta \nabla_u J\left[u^k\right]$$

- **Variants** of GD used in practice: SGD, Adam, BFGS, $\cdots$

# Classical training: Discretize $\Longrightarrow$ Optimize

**Idea**: Our solver of the neural ODE is a neural network architecture. Then, we use the the network algorithms.

Remember gradient descent $u^{k+1} = u^k - \delta \nabla_u J\,[u^k]$.

Gradient computation:

1) Discretize $x(t)$

$$x^{(l)} = ODESolver(t, x^{(0)}, \cdots, x^{(l-1)}, u).$$

2) Apply chain rule (backpropagation)

$$\nabla_{u^{(l)}} J = \frac{\partial J}{\partial x^{(L)}} \frac{\partial x^{(L)}}{\partial x^{(L-1)}} \cdots \frac{\partial x^{(l)}}{\partial u^{(l)}}.$$

## Classical training: Optimize $\Longrightarrow$ Discretize

From Pontryagin's Maximum Principle we can directly compute $\nabla_u J$.
Suppose $J$ can be written as

$$J(u; x_0, y) = \int_0^T L(x(t), u)\, dt + \Psi(\Phi_T(x_0), y) \tag{2}$$

**Gradient computation through the adjoint [Massaroli, 2020]**

$$\nabla_u J = \int_0^T \langle p(t), D_u f(t, x(t), u) \rangle \, dt,$$

where $p$ is the solution to

$$\begin{cases} \dot{p}(t) = -D_x f(t, x(t), u)^\intercal p(t) - \nabla_x L(t, x(t), u), \\ p(T) = \nabla_{x(T)} \Psi(x(T), y). \end{cases} \tag{3}$$

Adjoint method IS backpropagation!
Case of time-dependent controls: Gateaux derivative

$$d_u J(u)\eta = \int_0^T \langle p(t), D_u f(u(t), x(t))\eta(t) \rangle \, dt.$$

# Numerical aspects

In the numerical experiments we use **piecewise constant controls**

**Piecewise constant controls**

$$u(t) = u_i, \ t \in [t_i, t_{i+1}]$$

with $t_0 := 0$ y $t_m := T$, then

$$\frac{d}{du_i} J(u) = \int_{t_i}^{t_{i+1}} p(t) D_{u_i} f(x(t), u(t))\, dt \tag{4}$$

where $p$ is the solution to the adjoint equation.

We need to get the gradient for any data:

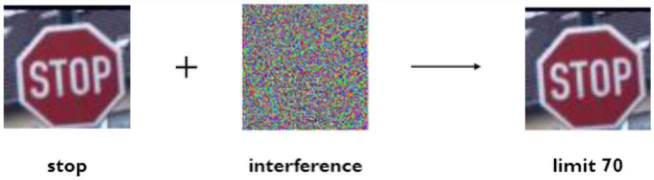
1. Solver the state $x$ in $(0, T]$.
2. Solver the adjoint $p$ in $[0, T)$
3. Integrate (4)

Very **expensive**..., but we get new algorithms with optimize control techniques.

- **Robustness:** the ability to withstand or overcome adverse conditions or rigorous testing.
- Data $(x, y)$ is supposed to follow a probability distribution $\gamma$
- **Classical training** might not give good results for perturbed input data


**Applications** in

- Autonomous driving
- Malware/spam detection
- Malfunctions (aeronautics, medicine)



Input perturbation in classification problems:

- Budget/force $\epsilon > 0$, perturbation $s(\epsilon) \in \mathbb{R}^d$
- Perturbed input $x + s(\epsilon)$

- Random perturbation $s \sim \epsilon \cdot N(0, Id)$
- Adversarial attack $s \in B_\epsilon(0) \subseteq \mathbb{R}^d$

Solution: For a given norm $l$ in $\mathbb{R}^d$, deal with the **robust training** problem

$$\min_u \mathbb{E}_{(x,y)\sim\gamma} \left[ \max_{l(s)\leq\epsilon} J(u; x + s, y) \right]$$

$$\uparrow\downarrow$$

$$\min_u \mathbb{E}_{(x,y)\sim\gamma} \left[ \max_{l(v)\leq 1} J(u; x + \epsilon v, y) \right]$$

1) Solve the inner **maximization** problem

$$H(u; x, y) := \max_{l(v)\leq 1} J(u; x+\epsilon v, y).$$

2) Solve the outer **minimization** problem

$$\min_u \mathbb{E}_{(x,y)\sim\gamma} H(u; x, y).$$

# Inner maximization problem

Taylor expansion of $J$ at $x$ results in

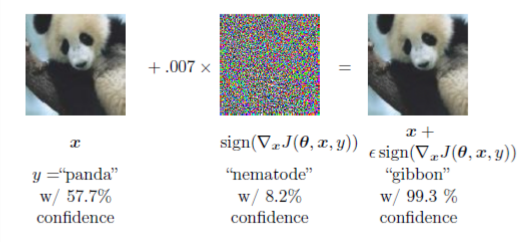
$$\max_{l(v)\leq 1} J(u; x + \epsilon v, y) = J(u; x, y) + \epsilon \max_{l(v)\leq 1} \langle \nabla_x J(u; x, y), v \rangle + O(\epsilon^2)$$

**Modified robust training problem**

$$\min_u \mathbb{E}_{(x,y)\sim\gamma} \left[ J(u; x, y) + \epsilon \max_{l(v)\leq 1} \langle \nabla_x J(u; x, y), v \rangle \right]$$

$\ell^\infty$ norm (Fast Gradient Sign Method [Goodfellow, 2014]):

- $\|\nabla_x J(u; x, y)\|_1 = \max_{\|v\|_\infty \leq 1} \langle \nabla_x J(u; x, y), v \rangle$
- $v = sign(\nabla_x J(u; x, y))$ maximizes $\langle \nabla_x J(u; x, y), v \rangle$



# Linear sensitivity of loss

From Pontryagin's Maximum Principle we can directly compute $\nabla_{x_0} J$.

**Linear sensitivity - initial data**

For $u \in L^2((0,T), \mathbb{R}^{d_u})$, $y \in \mathbb{R}^d$ fixed, linear sensitivity of $x_0 \to J(u; x_0, y)$ in the direction $v \in \mathbb{R}^d$ is

$$\nabla_{x_0} J(x_0) v := \lim_{\epsilon \to 0} \frac{J(u; x_0 + \epsilon v) - J(x_0)}{\epsilon} = p(0) \cdot v$$

where $p(t)$ is the solution to the adjoint equation.

$$\begin{cases} \dot{p}(t) = -D_x f(x(t), u(t))^\intercal p(t) - \nabla_x L(t, x(t), u), \quad t \in [0, T) \\ p(T) = D_{\Phi_T(x_0)} J(u; x_0, y) \end{cases}$$

**New penalty term**

$$\epsilon \max_{l(v) \leq 1} \langle \nabla_x J(u; x, y), v \rangle = \epsilon \max_{l(v) \leq 1} \langle p(0), v \rangle$$

# New loss function

### Augmented loss function

Let the control $u \in L^2((0,T);\mathbb{R}^{d_u})$ be fixed and let $x(t)$ y $p(t)$ be the solutions of the state and adjoint equation respectively. For fixed $\epsilon > 0$ the augmented loss function

$$J_l[u;x_0;\epsilon] := J[u;x_0] + \epsilon \max_{l(v)\leq 1} \langle p(0), v\rangle$$

approximates the minimization problem with linear precision in $\epsilon$.

If $l$ is the norm $\ell^r$ for $r \in [1,\infty]$, the augmented loss function can be written as

$$J_r[u;x_0;\epsilon] := J[u;x_0] + \epsilon \|p(0)\|_{r'}$$

where $r$ and $r'$ are Hölder conjugates, i.e. $1/r + 1/r' = 1$.

Proof is based on Hölder inequality.

### Gradient of quadratic penalty term

Control $u$ be fixed and the quadratic penalty term

$$S[u] := \|p_u(0)\|_2^2$$

where $p_u$ is the adjoint with control $u$. Then,

$$\begin{aligned} d_u S(u)\eta := & -\int_0^T q(t)\cdot D_{xx} f(x(t),u(t))^\intercal[\delta_\eta x(t), p(t)] \\ & -\int_0^T q(t)\cdot D_{ux} f(x(t),u(t))^\intercal[\eta(t), p(t)]\, dt \end{aligned}$$

$q$ is the perturbation with respect the penalty term

$$\begin{cases} \dot{q}(t) = D_x f(x(t),u(t))q(t), & t\in(0,T] \\ q(0) = -p_u(0) \end{cases} \tag{5}$$

$\delta_\eta x$ is the sentivity with respect the controls

$$\begin{cases} \dot{\delta_\eta} x(t) = D_x f(x(t),u(t))\delta_\eta x + D_u f(x(t),u(t))\eta(t), & t\in(0,T] \\ \delta_\eta x(0) = 0. \end{cases} \tag{6}$$

# Numerical aspects

In the numerical experiments we use **piecewise constant controls** $u(t) = u_i,\ t \in [t_i, t_{i+1}]$

**Gradient penalty term**

$$\frac{d}{du_i}[S(u)]\eta(t) := -\int_{t_i}^{T} q(t) \cdot D_{xx} f(x(t), u(t))^\intercal [\delta_\eta x(t), p(t)] dt \\ - \int_{t_i}^{t_{i+1}} q(t) \cdot D_{u_i x} f(x(t), u(t))^\intercal [\eta(t), p(t)]\, dt$$

where $p$ is the solution to the adjoint equation (3).

We need to get the gradient for any data:

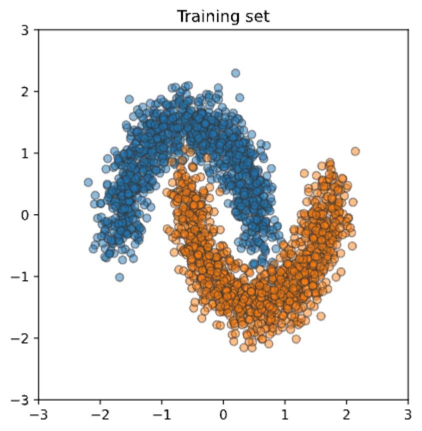
1. Solver the state $x$ in $(0, T]$.
2. Solver the adjoint $p$ in $[0, T)$
3. Solver $q$ and $\delta_\eta x$ in $(0, T]$
4. Integrate (4) and penalty term

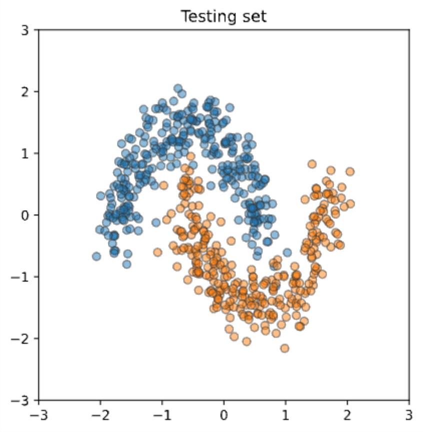
Very **expensive**..., but we get new algorithms with optimize control techniques.

## Numerical experiments

- In the numerical experiments we use piecewise constant controls consisting of 10 pieces (stacked NODEs)
- Normal perturbed data
- Dormand-Prince-Shampine solvers
- Adams, BFGS optimizers solvers
- Modified neural ODE architecture of Wohrer, Massaroli
- Expensive but not too much

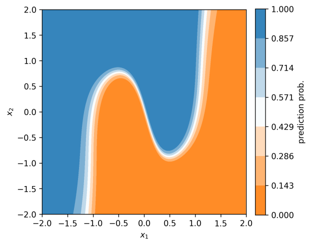
# Experiments



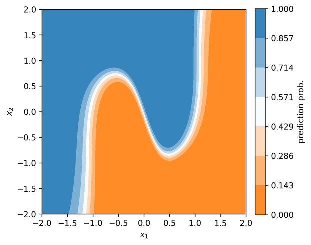



# Experiments

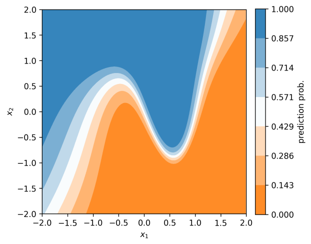
$\epsilon = 0$



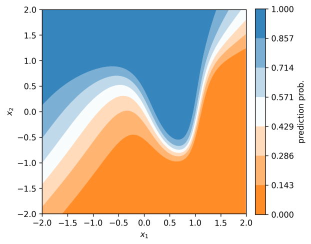

$\epsilon = 0.1$




$\epsilon = 0.2$




$\epsilon = 0.3$

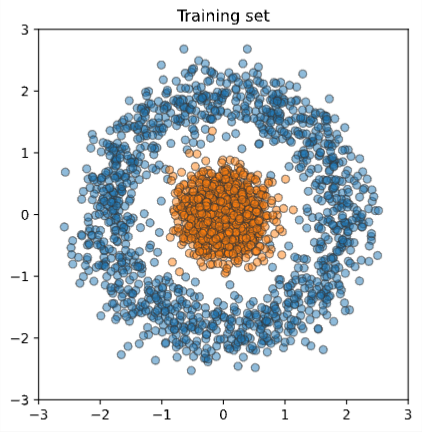


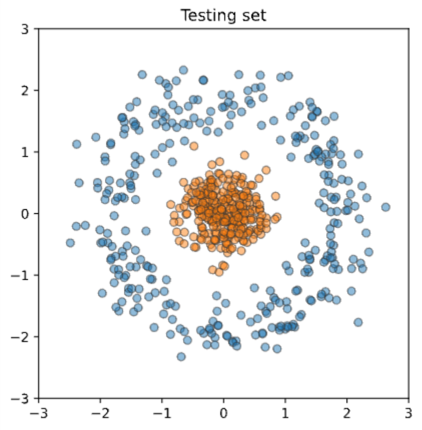
## Experiments

- We perform robust trainings with differents values $\epsilon$ given to penalty term
- We compare the performance in perturbed testing set

| Evaluation set | Classical training | 0.1-robust | 0.2-robust | 0.3-robust |
|---|---|---|---|---|
| Test | 0.042488 | 0.041761 | 0.075317 | 0.092077 |
| 0.1-FGSM-attack test | 0.064908 | 0.063728 | 0.085838 | 0.207678 |
| 0.1-perturbed test | 0.046271 | 0.041761 | 0.080335 | 0.182127 |
| 0.2-perturbed test | 0.075131 | 0.087367 | 0.080335 | 0.190990 |
| 0.3-perturbed test | 0.0105135 | 0.0102906 | 0.092077 | 0.199580 |

# Experiments



# Experiments

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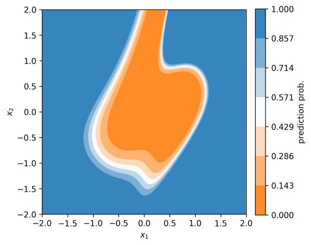
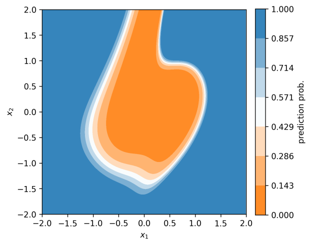
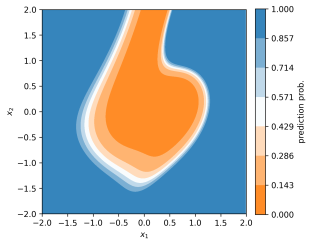


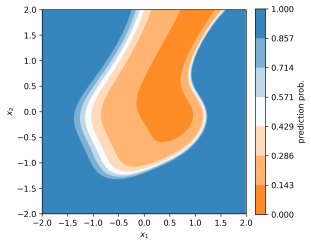

$\epsilon = 0.1$




$\epsilon = 0.2$




$\epsilon = 0.3$



**Conclusions:**

- Adversarial attacks are a threat to Machine Learning models
- NODEs let us treat problems about neural networks from a continuous point of view
- Generalize gradient computation of the penalty term to a more general norm
- **Main takeaway:** memory efficient methods for computing gradient of loss function

**Conclusions:**

- Adversarial attacks are a threat to Machine Learning models
- NODEs let us treat problems about neural networks from a continuous point of view
- Generalize gradient computation of the penalty term to a more general norm
- **Main takeaway:** memory efficient methods for computing gradient of loss function

**Future directions:**

- More simulations (with adversarial attacks).
- Choice of $\epsilon > 0$ for robust training
- Consider other types of perturbation
- Enable robust training only in some part of the training process and then switch to classical training
- Implementation with Bayesian techniques

**Thank you for your attention!**