Modelling of Highly oscillatory phenomenon by neural networks

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Goal: solve highly oscillatory ODE's, of the form:

$$\begin{cases} \dot{y}^{\varepsilon}(t) & = & f\left(\frac{t}{\varepsilon}, y^{\varepsilon}(t)\right) \\ y^{\varepsilon}(0) & = & y_0 \end{cases} \quad (1)$$

where $\tau \mapsto f(\tau, \cdot)$ is 2π-periodic, by using numerical methods performed by machine learning. ε is a small parameter.

Main tools used:

- Function approximations by neural networks and structure preservation
- Modified field theory for autonomous ODE's
- Averaging theory & Numerical methods for highly oscillatory ODE's

Introduction

Definition (Neural network - MLP)

A ***Multi-Layer Perceptron (MLP)****, is a mapping* $\mathcal{N} : \mathbb{R}^{d_0} \longrightarrow \mathbb{R}^{d_L}$ *given, for all* $x \in \mathbb{R}^{d_0}$*, by:*

$$\mathcal{N}(x) = W_L \cdot \Sigma\left(\cdots W_1 \cdot \Sigma\left(W_0 \cdot x + b_0\right) + b_1 \cdots\right) + b_L \tag{2}$$

where:

- $L+1$ *is the number of* ***layers****.* ***Shallow network:*** $L = 1$*,* ***Deep network:*** $L \geqslant 2$*. Layers* 1 *to* $L-1$ *are named* ***hidden layers****.*
- $b_0 \in \mathbb{R}^{d_0}, b_1 \in \mathbb{R}^{d_1}, \ldots, b_L \in \mathbb{R}^{d_L}$ *are the* ***bias****.*
- $W_0 \in \mathcal{M}_{d_1,d_0}(\mathbb{R}), W_1 \in \mathcal{M}_{d_2,d_1}(\mathbb{R}), \ldots, W_L \in \mathcal{M}_{d_L,d_{L-1}}(\mathbb{R})$ *are the* ***weights****. Lines of* W_i*'s are* ***neurons****.*
- $\Sigma(y_1, \ldots, y_d) = (\sigma(y_1), \ldots, \sigma(y_d))$ *is a componant-wise nonlinear mapping* σ*, e.g.* tanh*, named* ***activation function****.*

Theorem (Universal approximation)

Let $f \in \mathcal{C}^0(\Omega, \mathbb{R}^k)$ where $\Omega \subset \mathbb{R}^d$ is compact. Then, for all $\varepsilon > 0$, there exists $\mathcal{N} : \mathbb{R}^d \longrightarrow \mathbb{R}^k$ a MLP s.t.

$$||f - \mathcal{N}||_{L^\infty(\Omega)} \leqslant \varepsilon \tag{3}$$

Rate of convergence w.r.t. number of weights:

- **Polynomial decay ($L = 1$):** Anastassiou, G. *Quantitative approximations*. Chapman and Hall/CRC, 2000.
- **Polynomial-Exponential decay ($L = 3$):** De Ryck, T., Lanthaler, S., & Mishra, S. (2021). On the approximation of functions by tanh neural networks. Neural Networks, 143, 732-750.

Structure preservation. Example: hamiltonian structure of the neural network. For all $x \in \mathbb{R}^{2d}$

$$\mathcal{N}(x) = J\nabla\mathcal{H}(x) \tag{4}$$

where $\mathcal{H} : \mathbb{R}^{2d} \longrightarrow \mathbb{R}$ is a MLP.

- **Hamiltonian structure (HNN):** David, M., Méhats, F. *Symplectic learning for Hamiltonian neural networks.* arXiv preprint arXiv:2106.11753, 2021.
- **Free-divergence structure (VP-Nets):** Zhu, A., Zhu, B., Zhang, J., Tang, Y., Liu, J. *VPNets: Volume-preserving neural networks for learning source-free dynamics.* arXiv preprint arXiv:2204.13843, 2022.

Autonomous case: f is independant from τ.

Definition (Modified field w.r.t. a numerical method)

Let consider a one step numerical method $\Phi_h(\cdot)$. The ***modified vector field w.r.t.*** Φ_h, *denoted $\tilde{f}_h$, is defined by the relation:*

$$\varphi^f_{nh}(y_0) = \left(\Phi_h^{\tilde{f}_h}\right)^n (y_0) \tag{5}$$

Example: Forward Euler scheme, linear ODE: $\dot{y}(t) = ay(t)$, $f(y) = ay$.

$$y(nh) = e^{anh} y_0 = \left(1 + h \cdot \frac{e^{ha} - 1}{h}\right)^n y_0 \tag{6}$$

thus $\tilde{f}_h(y) = \left(\frac{e^{ha}-1}{h}\right) y$

Proposition (Property of the modified field)

- ***Perturbation w.r.t.*** h: *If* Φ *is of order* p*, then* $\tilde{f}_h(y) = f(y) + h^p R(y,h)$

Backward error analysis: Hairer, E., Lubich, C., Wanner, G. *Geometric Numerical integration: structure-preserving algorithms for ordinary differential equations.* Springer, 2006.

Theorem (Solution of highly oscillatory ODE)

For all $t \in \mathbb{R}$:

$$y^\varepsilon(t) \quad = \quad \phi^\varepsilon_{\frac{t}{\varepsilon}}\left(\varphi_t^{F^\varepsilon}(y_0)\right) \tag{7}$$

where:

- F^ε *is called* ***averaged field****. Structure:* $F^\varepsilon(y) = \langle f\rangle(y) + \varepsilon F_1(y) + \varepsilon^2 F_2(y) + \cdots$, *where* $\langle f\rangle$ *is the average field w.r.t. time variable:*

$$\langle f\rangle(y) \quad := \quad \frac{1}{2\pi}\int_0^{2\pi} f(\tau, y)\mathrm{d}\tau \tag{8}$$

- $\phi^\varepsilon_\tau(y) = y + \varepsilon \cdot G^\varepsilon(\tau, y)$ *(Near to identity mapping) and is* 2π*-periodic w.r.t.* τ.

Theorem (P. Chartier, M. Lemou, F. Méhats, G. Vilmart - 2020)

There exists a numerical method of order r, named ***uniformly accurate method****,* $\Phi_h(\cdot)$*, s.t.*

$$\underset{0 \leqslant n \leqslant N}{Max} \left|(\Phi_h)^n (y_0) - y^{\varepsilon}(nh)\right| \leqslant Ch^r \tag{9}$$

where $h = \frac{T}{N}$ *and the constant* C *is independant from* ε*.*

Uniformy accurate methods: Chartier, P., Lemou, M., Méhats, F., & Vilmart, G. (2020). *A new class of uniformly accurate numerical schemes for highly oscillatory evolution equations.* Foundations of Computational Mathematics, 20, 1-33.

Example: Forward Euler - Micro-Macro method

We solve with Forward Euler the system:

$$\begin{cases} \dot{v}(t) & = & F^{[1]}(v(t)) \\ \dot{w}(t) & = & f\left(\frac{t}{\varepsilon}, \Phi^{[1]}_{\frac{t}{\varepsilon}}(v(t)) + w(t)\right) - \left(\frac{1}{\varepsilon}\partial_\tau \Phi^{[1]}_{\frac{t}{\varepsilon}} + \partial_y \Phi^{[1]}_{\frac{t}{\varepsilon}} F^{[1]}\right)(v(t)) \end{cases}$$

where $F^{[1]} = F^\varepsilon + \mathcal{O}(\varepsilon^2)$ and $\Phi^{[1]} = \Phi^\varepsilon + \mathcal{O}(\varepsilon^2)$ are computable with explicit formulas. This is a UA-method of order 1. We get:

$$y^\varepsilon(t) = \Phi^{[1]}(v(t)) + w(t) \tag{10}$$

Autonomous ODE's

- **Autonomous ODE:**

$$\begin{cases} \dot{y}(t) & = & f\left(y(t)\right) \\ y(0) & = & y_0 \end{cases} \tag{11}$$

- **Numerical method:** $\Phi_h(\cdot)$, assumed to be of order p.
- **Goal:** Approximate the modified field $\tilde{f}_h$ by a neural network $f_\theta(\cdot, h)$ in order to get approximated solution $y_n^* = \left(\Phi_h^{f_\theta(\cdot,h)}\right)^n (y_0)$ very close to the exact solution $y(nh)$.

- **Structure of f_θ:**

$$f_\theta(y,h) \quad = \quad f(y) + h^p R_\theta(y,h)$$

- **Data creation:** Computation of exact solutions $y_1^{(k)} = \varphi^f_{h^{(k)}}(y_0^{(k)})$ with accurate and expensive integrator, where, for all $0 \leqslant k \leqslant K-1$, $y_0^{(k)} \in \Omega \subset \mathbb{R}^d$, $h^{(k)} \in [h_-, h_+]$ are randomly selected.
- **Training of the neural network:** Optimization of **MSE Loss**:

$$Loss_{Train} \quad = \quad \frac{1}{K_0}\sum_{k=0}^{K_0-1}\frac{1}{{h^{(k)}}^{2p+2}}\Bigg|\underbrace{\Phi_{h^{(k)}}^{f_\theta(\cdot,h^{(k)})}\left(y_0^{(k)}\right)}_{=\hat{y_1}^{(k)}} - y_1^{(k)}\Bigg|^2$$

- **Good training:** $Loss_{Train}$ has the same decay pattern than:

$$Loss_{Test} \quad = \quad \frac{1}{K-K_0}\sum_{k=K_0}^{K-1}\frac{1}{{h^{(k)}}^{2p+2}}\left|\hat{y_1}^{(k)} - y_1^{(k)}\right|^2$$

- **Numerical integration:** $f_\theta(\cdot, h)$ is an accurate approximation of $\tilde{f}_h$, thus we get a small numerical error:

$$e_n^* = \left(\Phi_h^{f_\theta(\cdot,h)}\right)^n (y_0) - \varphi_{nh}^f(y_0) \tag{12}$$

Denoting the **learning error** by

$$\delta := \underset{(y,h)\in\Omega\times[h_-,h_+]}{\mathrm{Max}} \frac{\left|\tilde{f}_h(y,h) - f_\theta(y,h)\right|}{h^p} \tag{13}$$

Theorem (M.B., P.Chartier, M.Lemou, F.Méhats - 2023[1])

Assuming that

- *For any pair smooth vector fields f_1 and f_2, we have*

$$\forall 0 \leq h \leq h_+, \quad \left|\left|\Phi_h^{f_1} - \Phi_h^{f_2}\right|\right|_{L^\infty(\Omega)} \leqslant Ch\,||f_1 - f_2||_{L^\infty(\Omega)} \quad (14)$$

for some positive constant C, independent of f_1 and f_2;

- *For any smooth vector field f, there exists a constant $L > 0$ such that $\forall 0 \leq h \leq h_+, \forall (y_1, y_2) \in \Omega^2$:*

$$\left|\Phi_h^f(y_1) - \Phi_h^f(y_2)\right| \leqslant (1 + Lh)\,|y_1 - y_2|. \quad (15)$$

Then there exist two constants $\tilde{C}, \tilde{L} > 0$ such that:

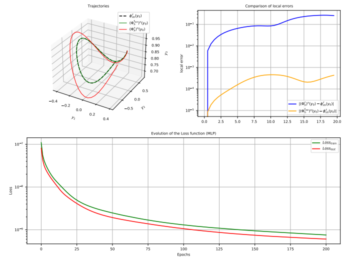
$$\underset{0 \leqslant n \leqslant N}{Max} |e_n^*| \leqslant \frac{C\delta h^p}{\tilde{L}} \left(e^{\tilde{L}T} - 1\right) \quad (16)$$

[1] B., M., Chartier, P., Lemou, M., & Méhats, F. (2023). *Machine Learning Methods for Autonomous Ordinary Differential Equations*. arXiv preprint arXiv:2304.09036.

$$\begin{cases} \dot{y_1} = -\frac{1}{6} y_2 y_3 \\ \dot{y_2} = \frac{2}{3} y_1 y_3 \\ \dot{y_3} = -\frac{1}{2} y_1 y_2 \end{cases},$$

Parameters	
# Math Parameters:	
Interval where time steps are selected:	$[h_-, h_+] = [0.5, 2.5]$
Time for ODE simulation:	$T = 20$
Time step for ODE simulation:	$h = 0.5$
# AI Parameters:	
Domain where data are selected:	$\Omega = \left\{x \in [-2,2]^2 : 0.98 \leqslant \lvert x \rvert \leqslant 1.02\right\}$
Number of data:	$K = 100\,000\,000$
Proportion of data for training:	80% - $K_0 = 80\,000\,000$
Number of terms in the perturbation (MLP's):	$N_t = 1$
Hidden layers per MLP:	2
Neurons on each hidden layer:	250
Epochs:	200

Computational time for training: 1 Day 21 h 59 min 51 s



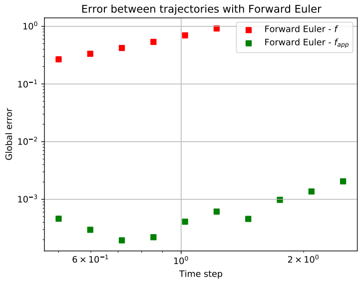


Figure: Left: Comparison between $Loss$ decays (green: $Loss_{Train}$, red: $Loss_{Test}$), trajectories (dashed dark: exact flow, red: numerical flow with f, green: numerical flow with $f_\theta(\cdot, h)$) and local error (blue: exact flow and numerical flow with f, yellow: exact and numerical flow with $f_\theta(\cdot, h)$). Right: Integration errors (green: integration with f, red: integration with $f_\theta(\cdot, h)$).

Highly oscillatory ODE's

- **Goal:** Find an approximation of the solution of

$$\begin{cases} \dot{y}^\varepsilon(t) & = & f\left(\frac{t}{\varepsilon}, y^\varepsilon(t)\right) \\ y^\varepsilon(0) & = & y_0 \end{cases} \tag{17}$$

- **General strategy:** Use the Micro-Macro UA-method

$$\begin{cases} \dot{v}(t) & = & F^{[1]}(v(t)) \\ \dot{w}(t) & = & f\left(\frac{t}{\varepsilon}, \Phi^{[1]}_{\frac{t}{\varepsilon}}(v(t)) + w(t)\right) - \left(\frac{1}{\varepsilon}\partial_\tau \Phi^{[1]}_{\frac{t}{\varepsilon}} + \partial_y \Phi^{[1]}_{\frac{t}{\varepsilon}} F^{[1]}\right)(v(t)) \end{cases}$$

$$y^\varepsilon(t) \quad = \quad \Phi^{[1]}(v(t)) + w(t)$$

and transform this system into an autonomous system in order to use the strategy used for autonomous ODE's.

- **Transformation to autonomous system:**
  Let denote $W(t) = (v(t), w(t))$. We denote the Micro-Macro system:

$$\dot{W}(t) = G^{\varepsilon}\left(\frac{t}{\varepsilon}, W(t)\right) \tag{18}$$

  If we denote $X(t) = \left(\frac{t}{\varepsilon}, W(t)\right)$, we have this system:

$$\dot{X}(t) = \mathcal{G}^{\varepsilon}(X(t)) \tag{19}$$

  where $\mathcal{G}^{\varepsilon}(\tau, W) = \left(\frac{1}{\varepsilon}, G^{\varepsilon}(\tau, W)\right)$. This is an autonomous system.
- **"Modified field" (Forward Euler):** We get:

$$W(t_0 + h) = W(t_0) + h \cdot \tilde{G}_h^{\varepsilon}\left(\frac{t_0}{\varepsilon}, W(t_0)\right) \tag{20}$$

- **Data creation:** Computation of exact solutions $W_1^{(k)} = \varphi^{G^{\varepsilon^{(k)}}}_{t_0^{(k)},h^{(k)}}(W_0^{(k)})$ where $t_0^{(k)} \in [0, 2\pi]$ with accurate and expensive integrator, where $W_0^{(k)}$ is randomly selected in the compact set $\Omega \subset \mathbb{R}^{2d}$, $h^{(k)}$ and $\varepsilon^{(k)}$ are randomly selected in $[h_-, h_+]$ and $[\varepsilon_-, \varepsilon_+]$, for all $0 \leqslant k \leqslant K-1$.
- **Neural network structure:**

$$G_\theta(\tau, W, \varepsilon, h) \quad = \quad G^\varepsilon(\tau, W) + hR_\theta(\cos(\tau), \sin(\tau), W, \varepsilon, h) \qquad (21)$$

- **Training of the neural network:** Optimization of:

$$Loss_{Train} \quad = \quad \frac{1}{K_0} \sum_{k=0}^{K_0-1} \frac{1}{{h^{(k)}}^4} \left| \hat{W_1}^{(k)} - W_1^{(k)} \right|^2$$

where $\hat{W_1}^{(k)} = W_0^{(k} + hG_\theta\left(\frac{t_0^{(k)}}{\varepsilon^{(k)}}, W_0^{(k)}, \varepsilon^{(k)}, h^{(k)}\right)$

- **Good training:** $Loss_{Train}$ has the same decay pattern than:

$$Loss_{Test} \quad = \quad \frac{1}{K-K_0} \sum_{k=K_0}^{K-1} \frac{1}{{h^{(k)}}^4} \left| \hat{W_1}^{(k)} - W_1^{(k)} \right|^2$$

We get an approximated solution of the ODE:
Denoting the **learning error** by

$$\delta \quad := \quad \underset{(\tau,W,\varepsilon,h)\in[0,2\pi]\times\Omega\times[\varepsilon_-,\varepsilon_+]\times[h_-,h_+]}{\mathrm{Max}} \frac{\left|G_\theta(\tau,W,\varepsilon,h) - \tilde{G_h^\varepsilon}(\tau,W)\right|}{h}$$

If we denote $(W_n^*)_{0\leqslant n\leqslant N}$ the sequence given by $W_0^* = W(0)$ and, for all $n \in \mathbb{N}$:

$$W_{n+1}^* \quad = \quad W_n^* + h \cdot G_\theta\left(\frac{nh}{\varepsilon}, W_n^*, \varepsilon, h\right) \tag{22}$$

we get the flollowing proposition:

Proposition

For $T > 0$, there exist constants $C, L > 0$ s.t. for all $n \in [\![0, N]\!]$:

$$\underset{0\leqslant n\leqslant N}{Max} |W_n^* - W(nh)| \quad \leqslant \quad \frac{e^{LT}-1}{L} C\delta h \tag{23}$$

$$\dot{y}^{\varepsilon}(t) = y^{\varepsilon}(t)\left(1 - y^{\varepsilon}(t)\right) + \sin\left(\frac{t}{\varepsilon}\right) \tag{24}$$

Parameters	
# Math Parameters:	
Interval where time steps h are selected:	$[h-, h_+] = [0.001, 0.1]$
Interval where small parameters ε are selected:	$[\varepsilon_-, \varepsilon_+] = [0.01, 1]$
Time for ODE simulation:	$T = 1$
Time step for ODE simulation:	$h = 0.1$
Small parameter for ODE simulation:	$\varepsilon = 0.1$
# AI Parameters:	
Domain where data are selected:	$\Omega = [0, 2] \times [-2, 2]$
Number of data:	$K = 10\,000$
Proportion of data for training:	80% - $K_0 = 8\,000$
Hidden layers per MLP:	2
Neurons on each hidden layer:	200
Epochs:	2000

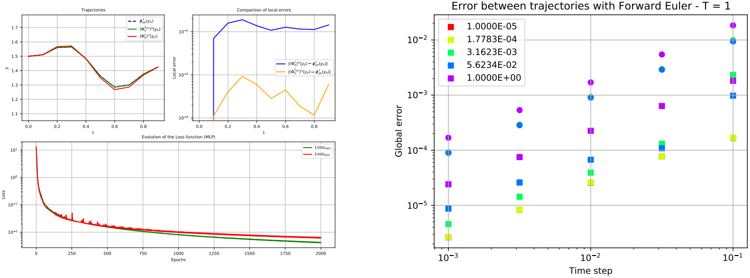


Figure: Left: Comparison between *Loss* decays (green: $Loss_{Train}$, red: $Loss_{Test}$), trajectories (dashed dark: exact flow, red: numerical flow with f, green: numerical flow with $G_\theta(\cdot, h)$) and local error (blue: exact flow and numerical flow with f, yellow: exact and numerical flow with $G_\theta(\cdot, h)$). Right: Integration errors (circles: integration with G, squares: integration with $G_\theta(\cdot, h)$). Integration with Machine Learning is very powerful for small values of ε.

- Improve results for highly oscillatory ODE's with Micro-Macro scheme.
- Use other Neural Network structure.

Thanks for your attention !