XXVI ENMC
ENCONTRO NACIONAL DE MODELAGEM COMPUTACIONAL
XIV ECTM
ENCONTRO DE CIÊNCIA E TECNOLOGIA DE MATERIAIS
2023

ANN-MoC method for inverse transient transport problems in one-dimensional domain

Nelson Garcia Roman
Pedro Costa dos Santos
Pedro Henrique de Almeida Konzen

PPGMAp, IME, UFRGS
Porto Alegre, RS

PPGMAp

Instituto de MATEMÁTICA E ESTATÍSTICA UFRGS

Contents

Introduction: Neutral particle transport

- Engineering and medical applications
- Combustion chambers, glass and ceramic manufacturers
- Nuclear energy production and optic medicine
- Enhance safety protocols and quality control procedures

Introduction: Time dependent Boltzmann equation

- $(t, x) \in (0, t_f] \times [0, 1]$

$$\forall \mu : \; \frac{1}{c}\frac{\partial}{\partial t} I(t, x, \mu) + \mu \frac{\partial I}{\partial x} + \sigma_t I = \sigma_s \Psi(t, x) + q(t, x, \mu),$$

$$\sigma_t = \kappa + \sigma_s$$

- Boundary conditions

$$\forall \mu : \; I(0, x, \mu) = I_0(x, \mu), \; x \in \mathcal{D}$$
$$\forall \mu > 0 : \; I(t, 0, \mu) = I_{\text{in},0}(t, \mu), \; t \in (0, t_f]$$
$$\forall \mu < 0 : \; I(t, 1, \mu) = I_{\text{in},1}(t, \mu), \; t \in (0, t_f]$$

- Average scalar flux

$$\Psi(t, x) := \frac{1}{2} \int_{-1}^{1} I(t, x, \mu) \, d\mu.$$

E. Lewis and W. Miller. 1984. *Computational Methods of Neutron Transport.*

M. Modest. 2013. *Radiative Heat Transfer.*

ANN-MoC method: DOM + TD + SI

- Discrete Ordinates Method + Time Discretization + Source Iteration

$$\forall \mu_j : \ \frac{1}{c}\frac{I_j^{(k+1,l+1)} - I_j^{(k)}}{h_t} + \mu_j \frac{\partial}{\partial x} I_j^{(k+1,l+1)} + \sigma_t I_j^{(k+1,l+1)}(x) \\ = \sigma_s \Psi^{(k+1,l)}(x) + q_j^{(k+1)}(x)$$

$$\forall \mu_j > 0 : \ I_j^{(k+1,l+1)}(0) = I_{j,\text{in},0}^{(k+1,l+1)}$$
$$\forall \mu_j < 0 : \ I_j^{(k+1,l+1)}(1) = I_{j,\text{in},1}^{(k+1,l+1)}$$

- Gaussian quadrature $\{(\mu_j, \omega_j)\}_{j=1}^{n_q}$

$$\Psi^{(k,l)} := \frac{1}{2}\sum_{j=1}^{n_q} I_j^{(k,l)} \omega_j$$

ANN-MoC method: Method of characteristics

- Change of variables: $x(s) = x_0 + s\mu$

$$\frac{d}{ds} I^{(1,l+1)} + \left(\sigma_t + \frac{1}{ch_t}\right) I^{(1,l+1)}(s) = \sigma_s \Psi^{(1,l)}(s) + q_j^{(1)}(s) + \frac{1}{ch_t} I_j^{(0)}(s)$$

- MoC solution form

$$I^{(1,l+1)}(s) = I^{(1,l+1)}(0) e^{-\int_0^s \tilde{\sigma}_t \, ds'} + \int_0^s S^{(l)}(s') e^{-\int_{s'}^s \tilde{\sigma}_t \, ds''} \, ds'$$

where $\tilde{\sigma}_t := \sigma_t + 1/(ch_t)$ and

$$S^{(l)}(s) := \sigma_s \Psi^{(1,l)}(s) + q_j^{(1)}(s) + \frac{1}{ch_t} I_j^{(0)}(s)$$

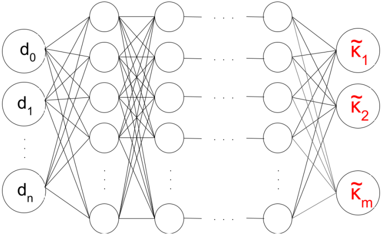
L. Evans. 2010. *Partial Differential Equations.*

ANN-MoC method: ANN scalar flux estimations

- Multilayer perceptron (MLP)

$$\tilde{\kappa} = \mathcal{N}(\boldsymbol{d})$$

$$\{(W^{(l)}, \boldsymbol{b}^{(l)}, \boldsymbol{f}^{(l)})\}_{l=1}^{n_l}$$



- Training set $\{(\boldsymbol{d}^{(s)}, \kappa^{(s)})\}_{s=1}^{n_{\text{train}}}$

$$\min_{\{(W^{(l)}, \boldsymbol{b}^{(l)})\}_{l=1}^{n_l}} \frac{1}{n_s} \sum_{s=1}^{n_s} \left(\tilde{\kappa}^{(s)} - \kappa^{(s)}\right)^2$$

S. Haykin. 2005. *Neural Networks: A Comprehensive Foundation.*

ANN-MoC method: Basic training algorithm

1. Set the MLP architecture.
2. Loop over epochs $e \leftarrow 1, 2, \ldots, n_{\text{epochs}}$:

   2.a. Forward the training set.

$$\tilde{\boldsymbol{\kappa}}_{\text{train}} \leftarrow \mathcal{N}\left(\boldsymbol{d}_{\text{train}}\right)$$

   2.b. Compute the loss function.

$$\mathcal{L} \leftarrow \frac{1}{n_{\text{train}}} \sum_{s=1}^{n_{\text{train}}} \left| \tilde{\kappa}_{\text{train}}^{(s)} - \kappa_{\text{train}}^{(s)} \right|^2$$

   2.c. Backward the loss function to compute the gradients.

$$\frac{\partial \mathcal{L}}{\partial \boldsymbol{b}^{(l)}}, \ \frac{\partial \mathcal{L}}{\partial W^{(l)}}, \ l = 1, 2, \ldots, n_l$$

   2.d. Perform a gradient-based optimizer step.

$$W^{(l)} \leftarrow W^{(l)} - l_r \frac{\partial \mathcal{L}}{\partial W^{(l)}}$$

$$\boldsymbol{b}^{(l)} \leftarrow \boldsymbol{b}^{(l)} - l_r \frac{\partial \mathcal{L}}{\partial \boldsymbol{b}^{(l)}}$$

   2.e. Check the stopping criterion.

Direct solver test

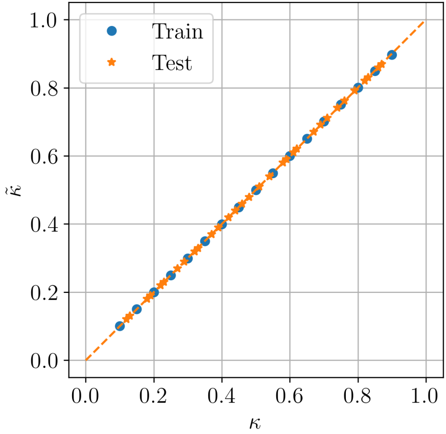
- Manufactured solution: $\hat{I}(t,x,\mu) := e^{-\sigma_t|x-t|^2}$
- Source equation:
  $q(t,x,\mu) = [2\sigma_t(1-\mu)(x-t)+\kappa]\, e^{-\sigma_t|x-t|^2}$
- Parameters: $h_t = 0.01$, $n_x = n_q = 100$
- Stopping criterion: $\texttt{tol} = 1.49 \times 10^{-8}$

Table: Comparison between the direct solver approximations and the exact solution at $t_f = 1.0$.

κ	$\Psi(0.0)$	$\Psi(0.5)$	$\Psi(1.0)$	ε_{rel}
0.9	$3.667e-1$	$7.748e-1$	$9.974e-1$	$4.5e-3$
0.5	$3.664e-1$	$7.740e-1$	$9.971e-1$	$5.3e-3$
0.1	$3.660e-1$	$7.730e-1$	$9.968e-1$	$6.4e-3$
exact	$3.679e-1$	$7.788e-1$	$1.000e+0$	

Results - Problem 1: Homogeneous medium

- Absorption coefficient: $0.1 < \kappa < 0.9$
- MLP architecture: 2 - 25 - 25 - 25 - 1
- Training set with 17 samples
- Test set with 32 samples
- $d_0 = (\Psi(t_{d,3}, 0))$, $d_1 = (\Psi(t_{d,3}, 1))$



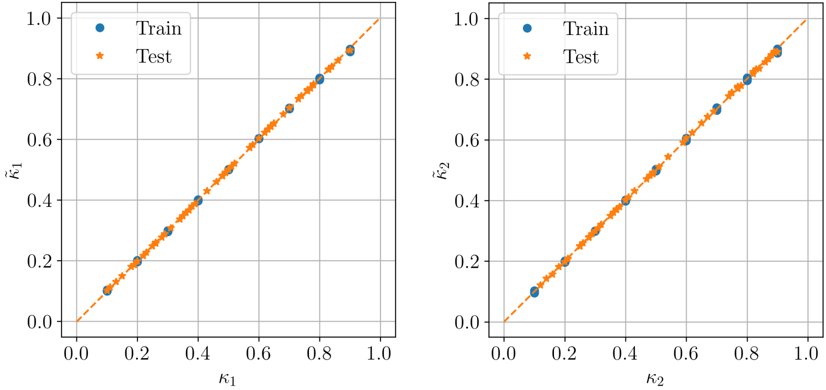
$R^2_{train} = 0.99998$

$R^2_{test} = 0.99999$

Results - Problem 2: Heterogeneous medium

- Absorption coefficient: $0.1 < \kappa_1, \kappa_2 < 0.9$
- MLP architecture: 4 - 25 - 25 - 25 - 25 - 2
- Training set with 81 samples
- Test set with 64 samples
- $d_0 = (\Psi(t_{d,2}, 0), \Psi(t_{d,3}, 0))$, $d_1 = (\Psi(t_{d,2}, 1), \Psi(t_{d,3}, 1))$

$$R^2_{train} = R^2_{test} = 0.9999$$



Final considerations

- ANN-MoC method for inverse transport problems
  MoC method with ANN that estimates κ
- High accuracy on the estimation of κ in both problems
- The accuracy of the inverse model highly depends on the accuracy of the direct solutions
- Further work
  - Development of more accurate direct solver
  - Enhance the computational performance
  - More realistic problems

Thanks for your attention!

Research group

Site UFRGS

professor.ufrgs.br/pedro

PPGMAp

Instituto de MATEMÁTICA E ESTATÍSTICA UFRGS