Estimating scattering potentials in inverse problems with Volterra series and Neural Networks

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Outline

- Motivation
- Preliminaries
  - Linear and nonlinear system identification basics
  - Volterra series
  - Neural Networks
  - Inverse scattering basics
- Estimating scattering potentials with:
  - Volterra model
  - Neural Network

[1] G. Balassa, 'Estimating Scattering Potentials in Inverse Problems with a Non-Causal Volterra Model', Mathematics 10, (2022) 1257.

[2] G. Balassa, 'Estimating scattering potentials in inverse problems with Volterra series and neural networks', Eur. Phys. J. A 58, (2022) 186

Motivation

- System identification techniques → Quantum mechanics.
- Many nonlinear phenomenon → well established methods in engineering (BLA, Volterra, ARX models,...) → not used in QM.
- In particular : low energy scattering
  - The observables (phase shifts,transmission coefficients, ...) depend nonlinearly from the inputs (Energy, angular momenta, …) ← VPA eq. (later)
  - Inversion == determining the potential (real, complex, …) from observables.
    - Usually *ill-conditioned* and/or *ill-defined* problem

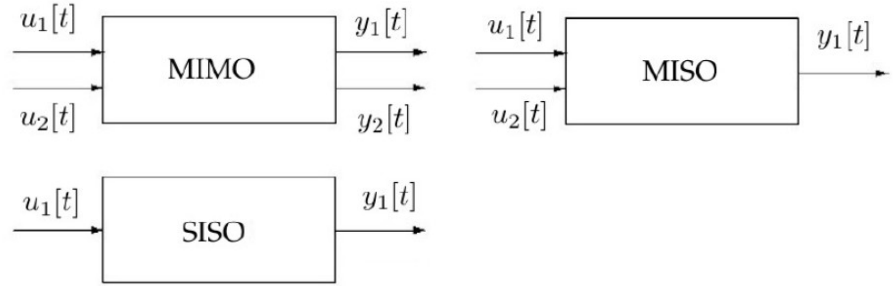
- Existing methods:
  - Fixed energy: *Newton-Sabatier method, Cox-Thompson method*
  - Fixed angular momentum: *Gelfand-Levitan-Marchenko equation*
  - Mixed methods: using energy and angular momenta
- The proposed method:
  - Data-driven
  - Solving the inverse problem by identifying the inverse nonlinear system.
  - Easily extendable
  - … more of this later ….

System identification

- Classification of systems:
  - Number of inputs and outputs: SISO, MISO, MIMO,...
  - Linear or nonlinear
  - Stable or unstable
  - Time variant or time invariant
  - Dynamic or static
  - Causal or non-causal
  - Invertible or non-invertible

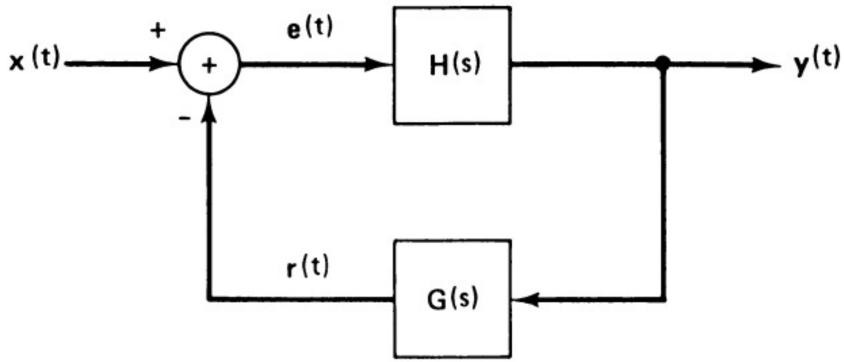
- Linear systems can be well-described by the transfer function 'method'.

$$y(t) = \int_{-\infty}^{\infty} h(\tau)u(t-\tau)d\tau,$$



- In Fourier domain → *Y(s)=H(s)U(s)*
  - Better suited for identification
  - Amplitude (Bode-diagram) and Phase information are both important
- For MIMO, MISO systems → transfer matrix has to be identified
- Stability criteria (only for LTI systems):
  - Nyquist criteria
  - Hurwitz criteria

- The 'closed loop' system → control → achieving optimal working conditions for the LTI systems



$$Q(s) = \frac{Y(s)}{X(s)} = \frac{H(s)}{1 + G(s)H(s)}$$

- **Nonlinear systems:**
  - Something in the dynamics is nonlinear e.g. feedback or the PDE's...
  - Modeling is much harder
  - Stability also problematic

- Modeling nonlinear systems:
  - Best Linear Approximation

    $$g_{BLA}(t) := \arg\min_g \mathcal{E}\left[\left(y - \int_{-\infty}^{\infty} g(\tau)u(t-\tau)d\tau\right)^2\right]$$

    - Weak nonlinearities
    - Linear (transfer function) approximation in the **least squares sense**.
  - Volterra series:
    - Extension of the transfer function method
    - Infinite dimensional convolutional integral representation
  - Neural Networks
    - Dynamic representation with NN constructions
    - MLP, SVM, NARX, C(ellular)NN, C(onv)NN,...

- <u>Volterra series</u>:
  - Extension of the linear model with higher order polynomial terms

$$y(t) = h_0 + \int_{-\infty}^{\infty} h_1(\tau_1)u(t-\tau_1)d\tau_1 + \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} h_2(\tau_1,\tau_2)u(t-\tau_1)u(t-\tau_2)d\tau_1 d\tau_2 + \\ + \cdots + \int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty} h_n(\tau_1,\ldots,\tau_n)u(t-\tau_1)\ldots u(t-\tau_n)d\tau_1\ldots d\tau_n,$$

  - For MIMO systems:
    - Cross-terms are important

$$y(t) = h_0 + \sum_{i=1}^{N} H_1^i\{u_i(t)\} + \sum_{i_1,i_2=1,1}^{N,N} H_2^{i_1,i_2}\{u_{i_1}(t), u_{i_2}(t)\} + \\ \cdots + \sum_{i_1,\ldots i_N=1,\ldots,1}^{N,\ldots,N} H_n^{i_1,\ldots i_N}\{u_{i_1}(t),\ldots u_{i_N}(t)\},$$

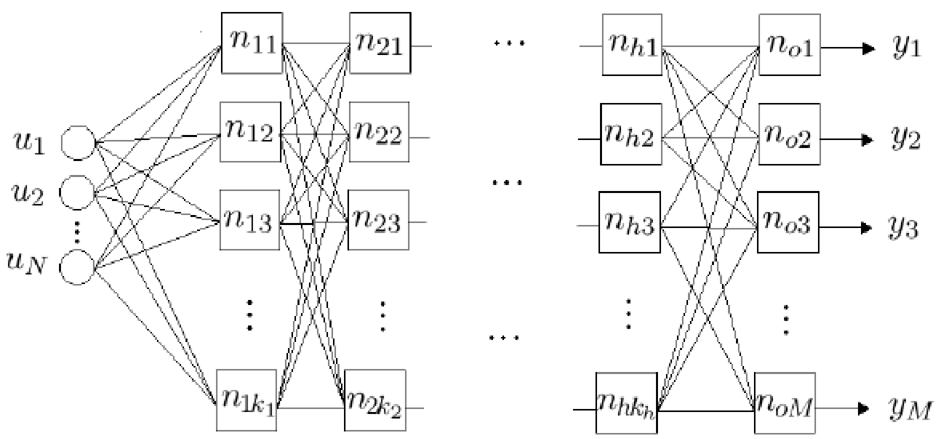
$$H_n^{i_1,\ldots,i_N}\{u_{i_1}(t),\ldots,u_{i_N}(t)\} = \int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty} h_n^{i_1,\ldots,i_N}(\tau_1,\ldots,\tau_n)\times \\ \times u_{i_1}(t-\tau_1)\ldots u_{i_N}(t-\tau_n)d\tau_1\ldots d\tau_n$$

- The Volterra kernels can be identified by multiple methods
  - Frequency domain identification
  - Discretization → finite memory, finitre order + Linear in parameters → linear system of eq's
  - Neural networks + Taylor expansion

- Problems:
  - Too many parameters at higher order
  - Usually ill-conditioned → regularization
  - Monomial basis → correlated coefficients → Wiener series.

Neural Networks

- Interconnected layers with nonlinear and /or linear activation functions.
- Universal approximator.
- Static and dynamic nonlinearities can be modeled.
- Multilayer-Perceptrons (MLP):



$$\underline{y} = \underline{N}^o\left(\underline{b}^o + \underline{\underline{W}}^o \underline{N}^h\left(\underline{b}^h + \underline{\underline{W}}^h \underline{N}^{h-1}\left(\ldots\ \underline{N}^1\left(\underline{b}^1 + \underline{\underline{W}}^1 \underline{u}\right)\right)\right)\right)$$

Inverse scattering basics

- In inverse scattering the characteristics of an object is examined, based on scattering data
- Typical observables:
  - Phase shifts
  - Transmission coefficients
  - Polarization
  - Total and differential cross-sections
- Low-energy elastic scattering can be described by the Schrödinger equation → *electron*+*A*, *N*+*N*, *alpha*+*N*, *A*+*A* … reactions.
- Scattering ~ incoming plane wave + outgoing spherical wave :

$$u_{as} = (e^{i\vec{k}\cdot\vec{x}})_{as} + f(k,\theta,\varphi)\frac{e^{ikr}}{r}.$$

- Cross section: $\boxed{\dfrac{d\sigma}{d\Omega} = |f(k,\theta,\varphi)|^2}$

- For spherical potentials at low energies → partial wave expansion + radial Sch. eq. → **phase shift** can be expressed:

$$f(k,\theta) = \frac{1}{2ik}\sum_{l=0}^{\infty}(2l+1)(e^{2i\delta_l}-1)P_l(\cos\theta)$$

- Generate training data for identification:
  - 1D Lippmann-Schwinger equation

$$\Psi(x) = \phi(x) + \int_{-\infty}^{\infty} dx' G(x,x') V(x) \Psi(x') \qquad G(x,x') = -\frac{i}{2}\frac{e^{ik|x-x'|}}{k}$$

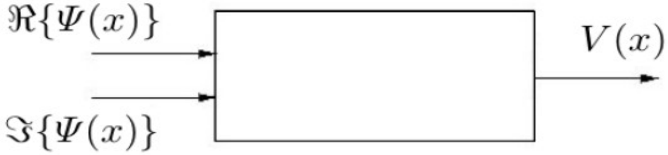
  - 3D Variable Phase Approximation (VPA)

$$\frac{d\delta_l(r)}{dr} = -\frac{U(r)}{k}\Big(j_l(kr)\cdot\cos\delta_l(r) - n_l(kr)\cdot\sin\delta_l(r)\Big)^2,$$

$$\frac{d\delta_0(r)}{dr} = -\frac{U(r)}{k}\sin^2\Big(kr+\delta_0(r)\Big)$$

One-dimensional scattering problem (non-causal Volterra)

- Incoming wave scattered on a bounded potential, giving a scattered wave function.

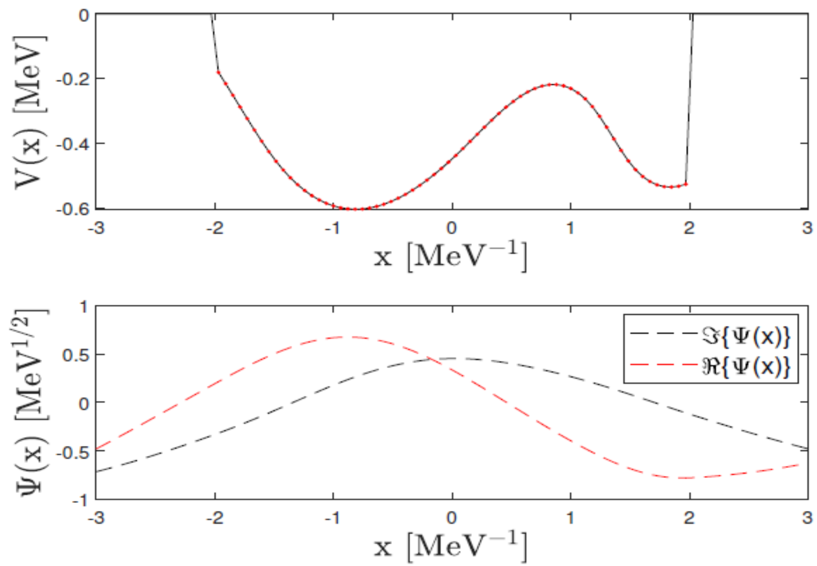


- Inputs: Real and Imaginary parts of the scattered wave-function
-

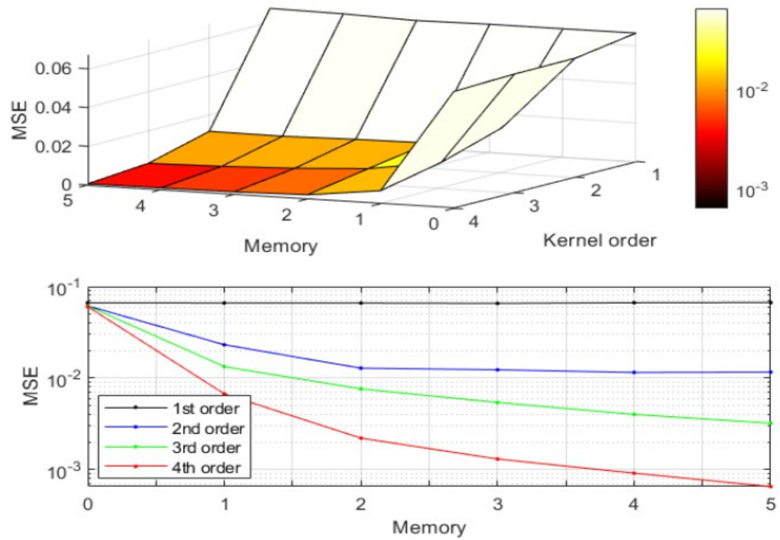
$$\Psi(x) = \phi(x) + \int_{-\infty}^{\infty} dx' G(x,x') V(x) \Psi(x')$$

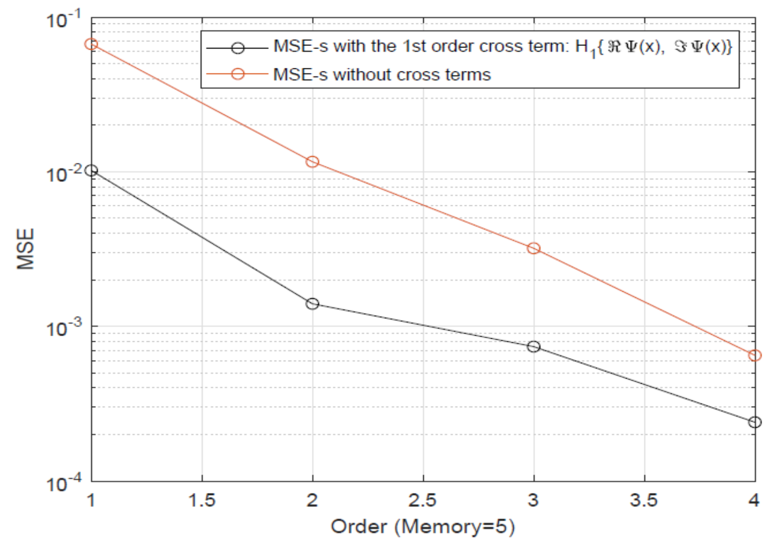
$$G(x,x') = -\frac{i}{2} \frac{e^{ik|x-x'|}}{k}$$

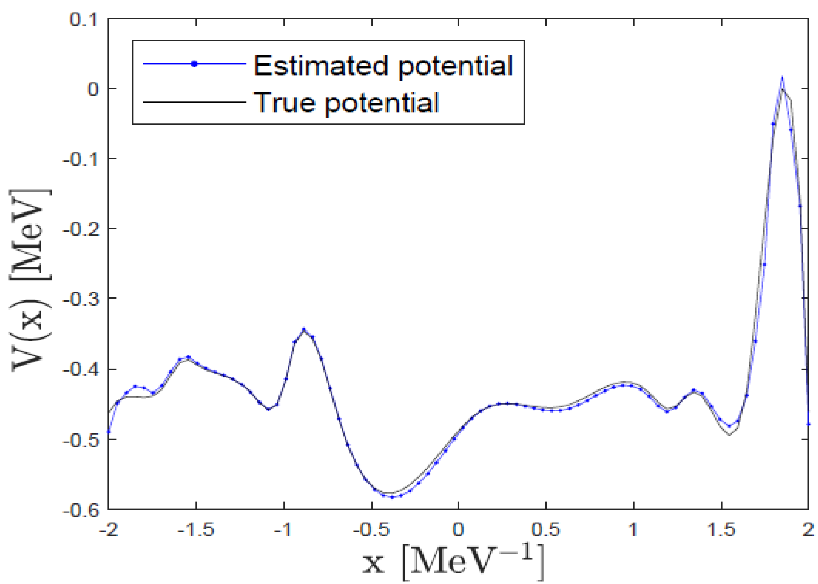
- In the example:
  - $m=1$ MeV, $k=0.5$ MeV
  - $V \in [-2,0]$ MeV
  - $V(x)=0$, if $|x|>2$ MeV^{-1}
  -

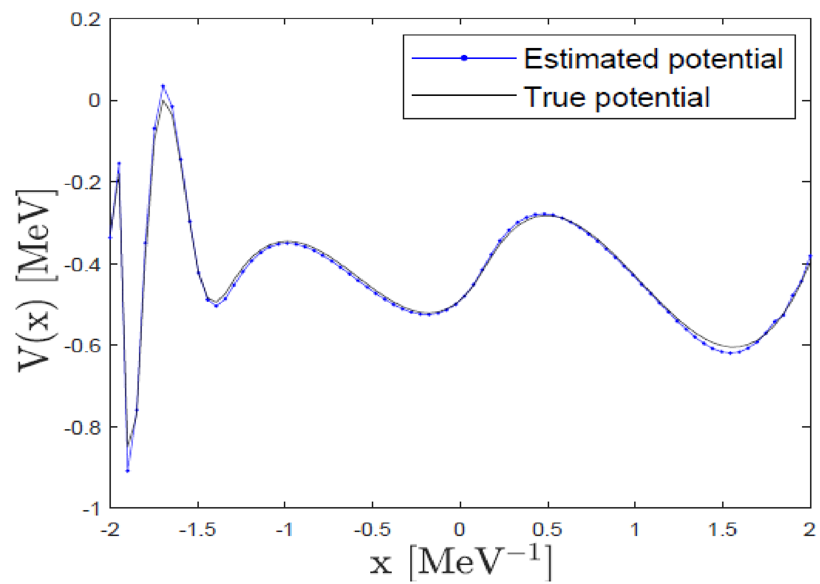


- Identify a non-causal Volterra model
  - 10000 samples, with uniformly distributed random noise as potentials
  - Lippmann-Schwinger eq. → training data


MSE
0.06
0.04
0.02
0
Memory
Kernel order
10^{-2}
10^{-3}
10^{-1}
10^{-2}
10^{-3}
1st order
2nd order
3rd order
4th order
Memory

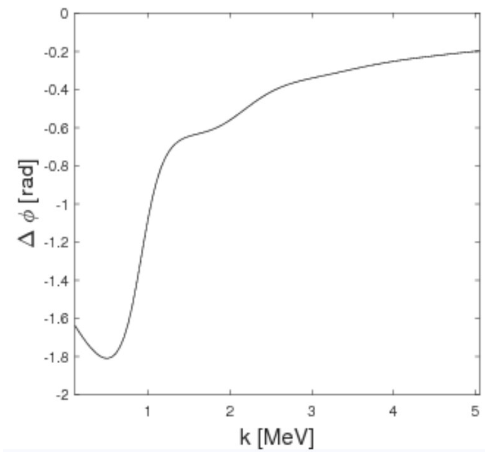

MSE-s with the 1st order cross term: $H_1\{\Re\Psi(x), \Im\Psi(x)\}$
MSE-s without cross terms
MSE
Order (Memory=5)

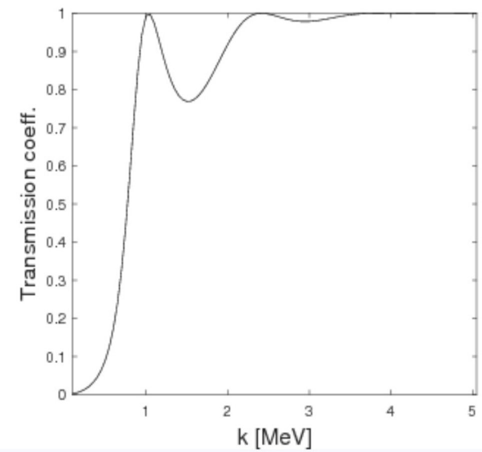

Estimated potential
True potential
V(x) [MeV]
x [MeV^{-1}]

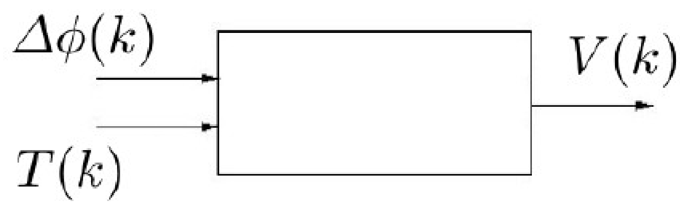

Estimated potential
True potential
V(x) [MeV]
x [MeV^{-1}]

Scattering problem in Fourier space (non-causal Volterra)

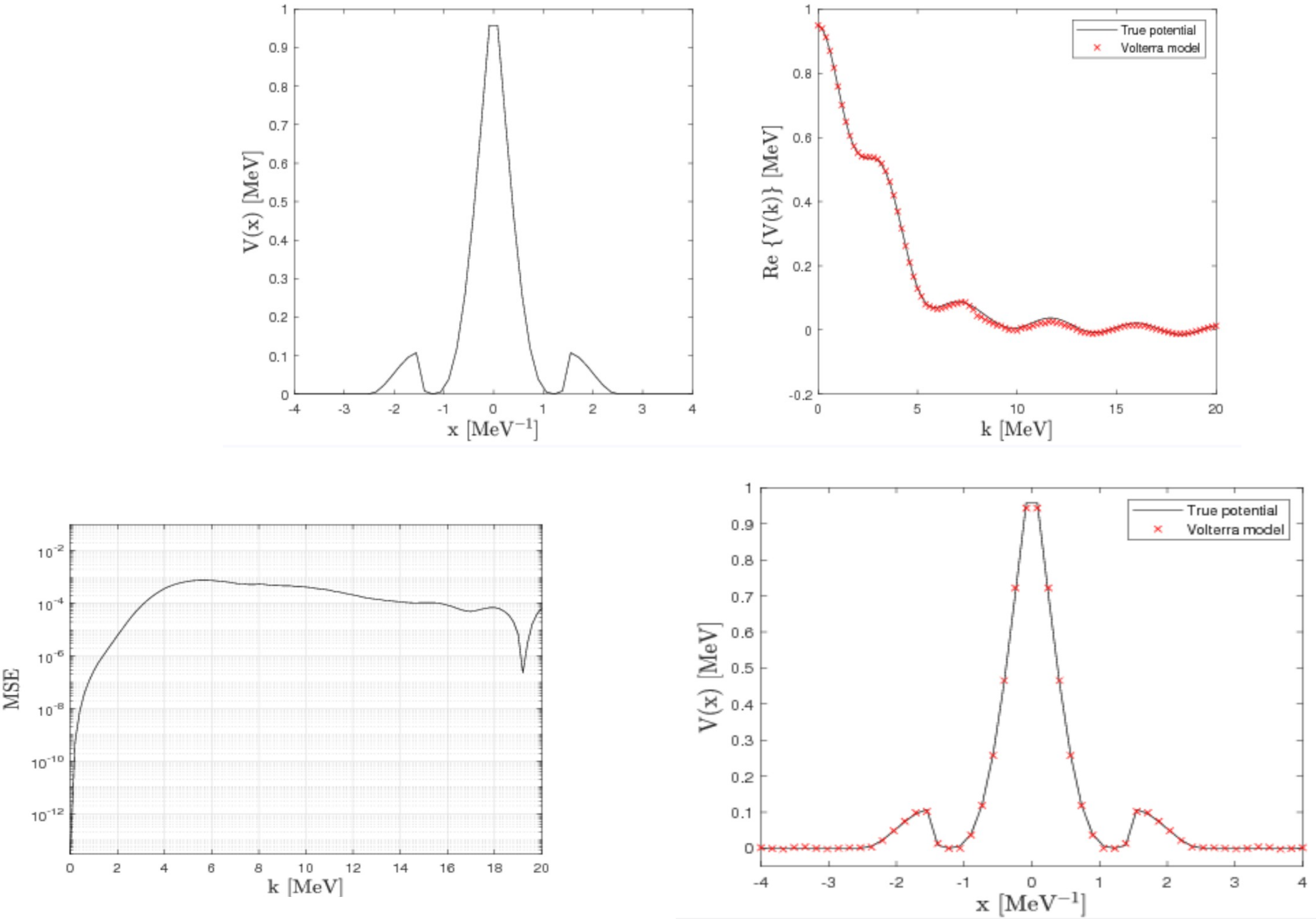
- Observables: **phase shifts** and **transmission coefficients**
- Identify a non-causal MISO Volterra system with:
  - **Inputs**: Phase shifts & Transmission coefficients
  - **Output**: Fourier transform of x ∈ *[-4,4]* MeV^{-1}, *N=50*), with *k* ∈ *[0,20]* MeV, *Δk =0.2* MeV
- Only symmetric potentials → Fourier transform is real
- One **2nd order non-causal** Volterra system for every *k, with **1st order cross-terms**, and **M=35** memories (+/-35Δk).*





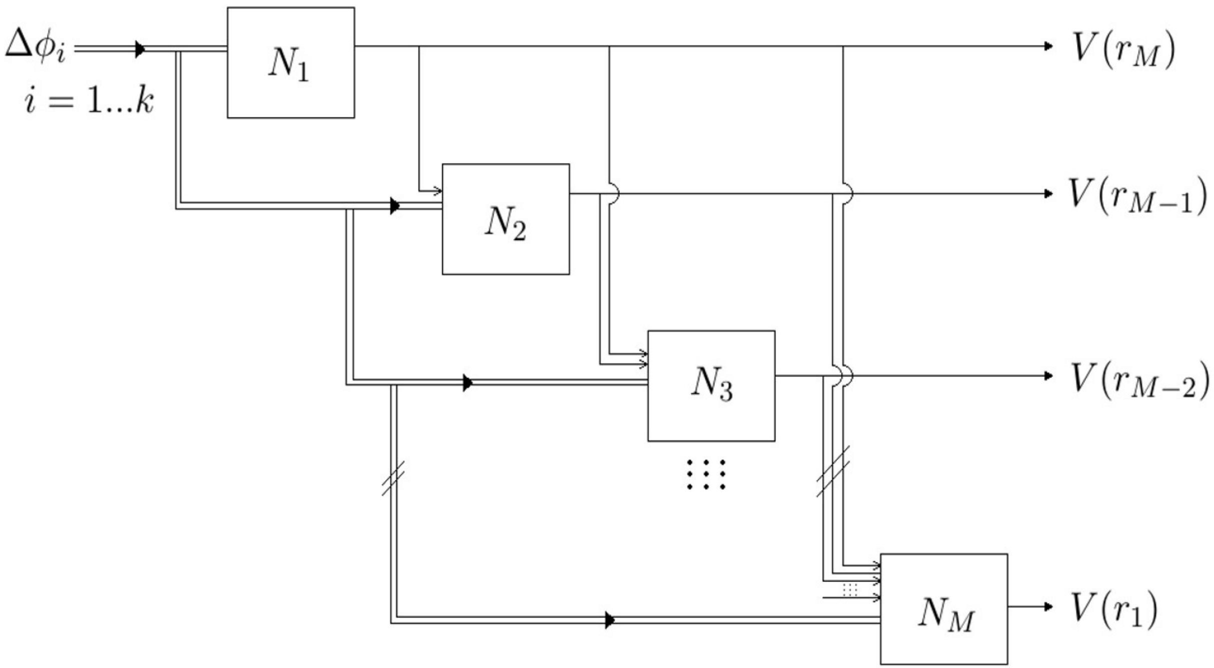


$$V(k_i) = h_0 + H_1^{\Delta\phi}\left[\Delta\phi[k]\right] + H_1^{T}\left[T[k]\right] + $$
$$+ H_2^{\Delta\phi,T}\left[\Delta\phi[k], T[k]\right],$$


V(x) [MeV]
x [MeV^{-1}]
Re {V(k)} [MeV]
k [MeV]
True potential
Volterra model
MSE
k [MeV]
V(x) [MeV]
x [MeV^{-1}]
True potential
Volterra model

NEURAL NETWORK MODEL

- Radially symmetric potentials, and fixed angular momenta
- Method:
  - The last point $V(r_M)$ is estimated only from the phase shift information.
  - $V(r_{M-1})$ is then estimated from the phase shift and the estimated $V(r_M)$, and so on...
  - In each block a multilayer-perceptron (or a Volterra model) is identified.



$$V(r_M) = N_1(\Delta\phi_1, \Delta\phi_2, \ldots, \Delta\phi_k),$$

$$V(r_{M-1}) = N_2(\Delta\phi_1, \Delta\phi_2, \ldots, \Delta\phi_k, V(r_M)),$$

$$\vdots$$

$$V(r_1) = N_M(\Delta\phi_1 \ldots, \Delta\phi_k, V(r_M), \ldots, V(r_2)),$$

Model parameters (EXAMPLE 1):

- m=1 GeV, r ∈ [0,6] fm, V(r) ∈ [-10,0] MeV.
- 20 inversion points
- Input: $\Delta\phi(T_{lab})$, with *T_{lab}=[1,6,11,...,99] MeV*
- Training/validation/error (10000/2000/1000)
- Network complexity:

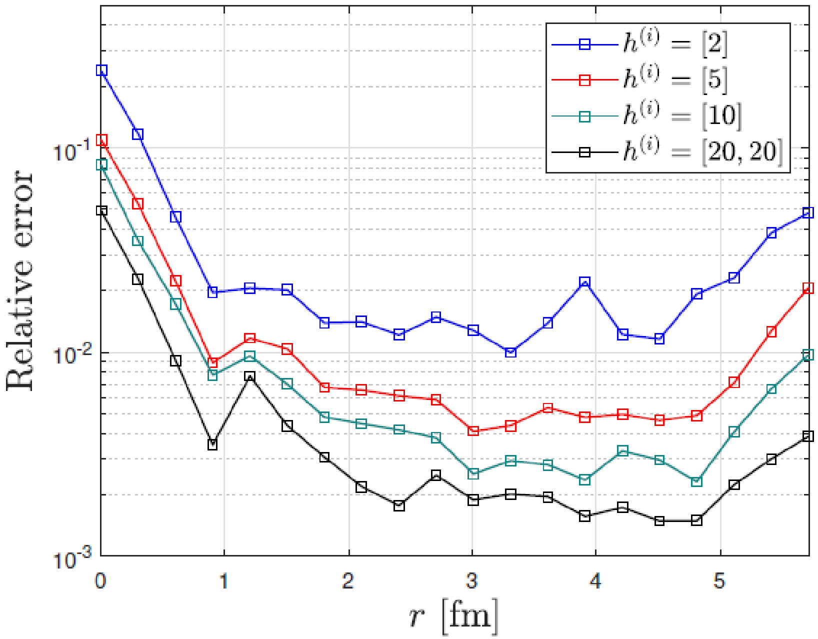


Fig. 8. Relative errors in the inversion points for four different MLP's.

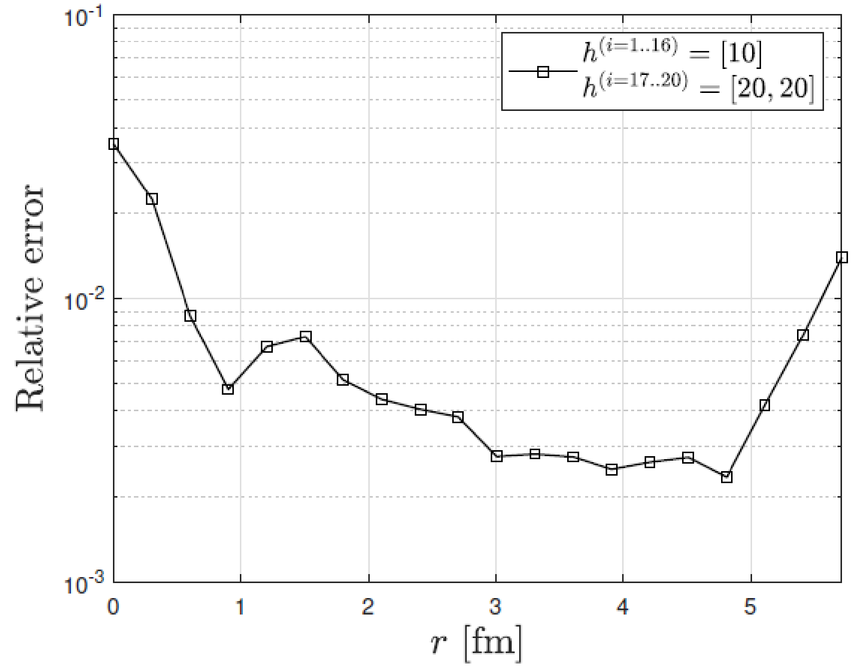
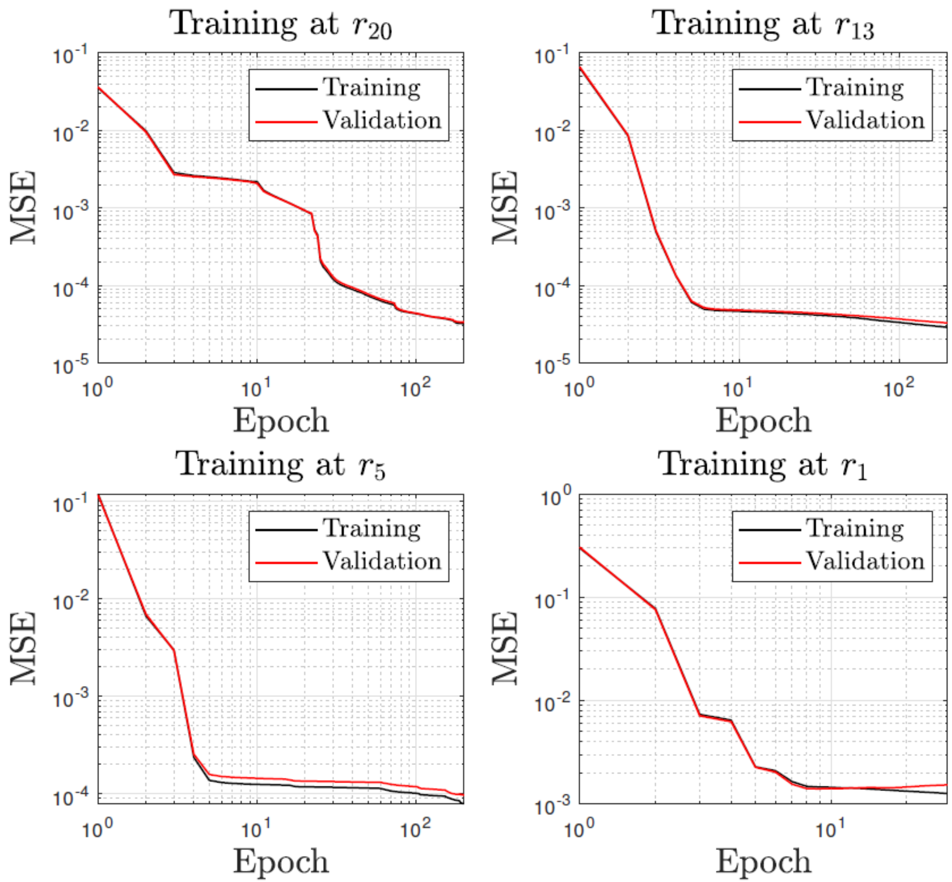


Fig. 9. Relative errors in the inversion points for the identified MLP. The $h^{(i)}$ notation refers to the number of neurons used in the hidden layers in the i'th inversion point, where i corresponds to the distance r_{20-i+1}.

- Simple well-defined problem in the operating range
- Nonlinear dynamics
- Accuracy shows the typical behaviour for MLP's



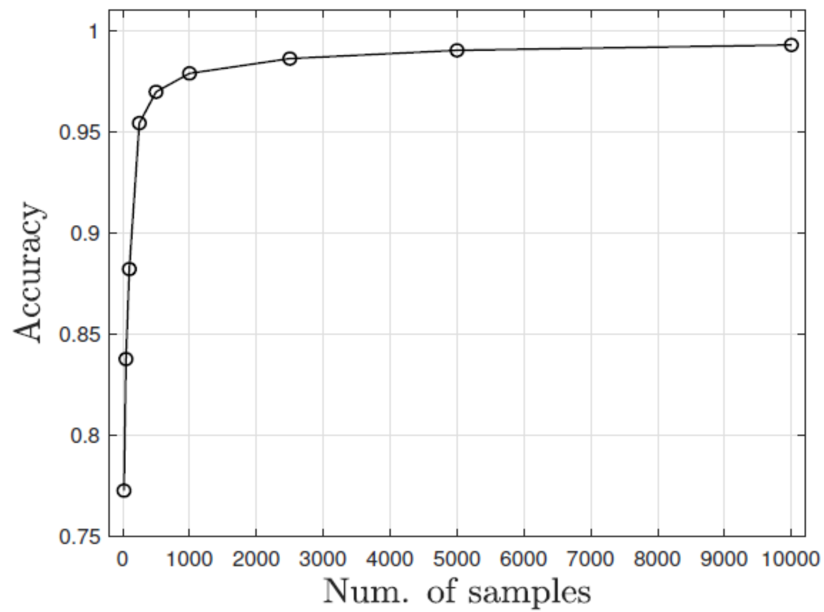


Fig. 11. Model accuracy dependence on the number of training samples.

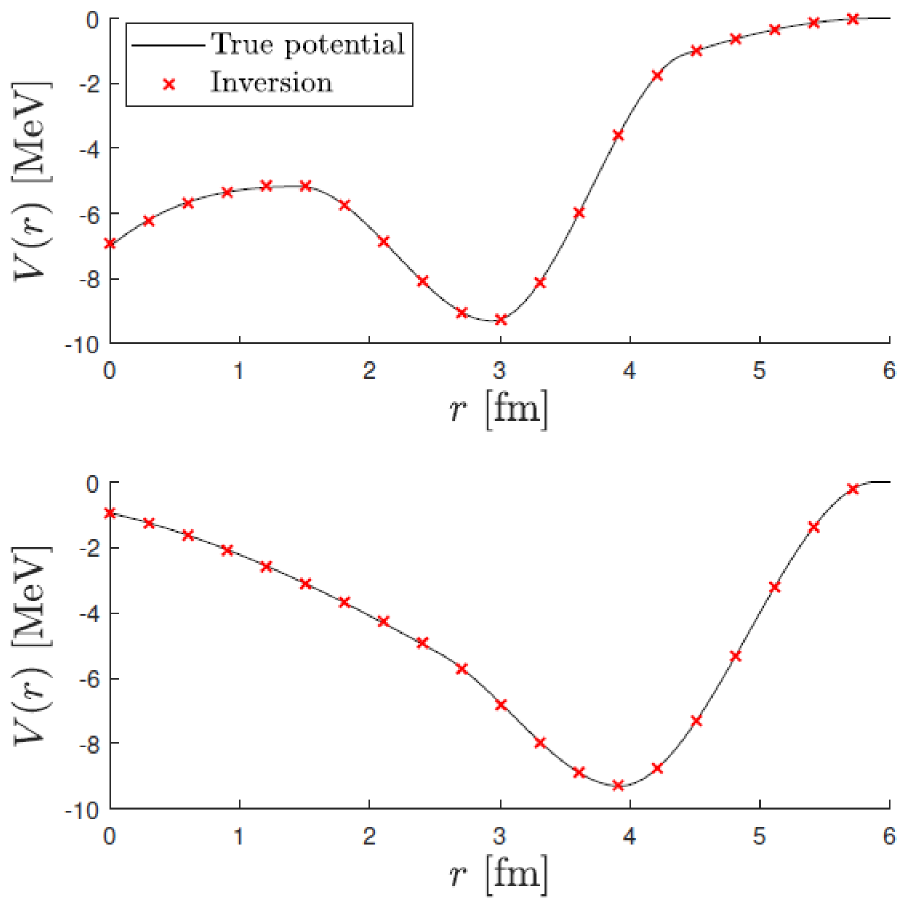


Fig. 12. Validation of the model for two randomly generated potentials. The red markers represent the values at the inversion points, while the black lines are the true potentials.

The main application : NN $^3S_1$ phase shifts

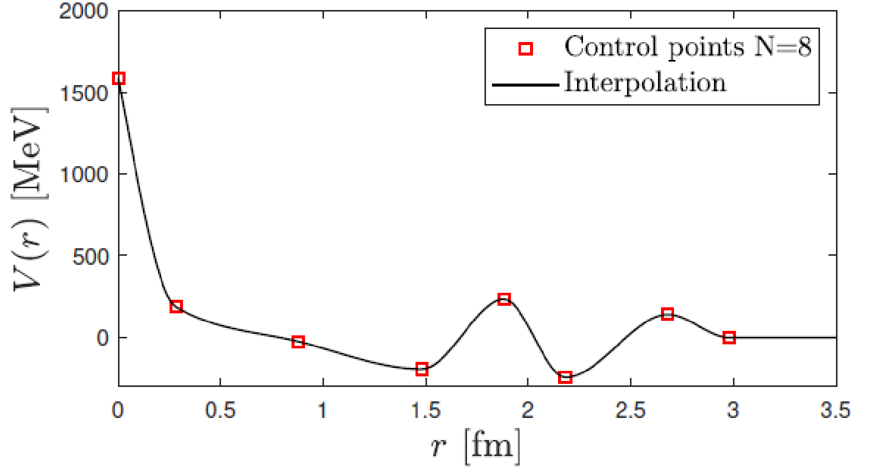
- *neutron+proton* scattering
- Preliminary knowledge → define the operating range
  - 1 bound state (the deuteron) → 180° phase shift 'jump'
  - Typical nuclear force
    - Attractive at 'large' distance (few fm)
    - Strongly repulsive core (below r~0.5 fm)
      - Coulomb
      - nonperturbative QCD
    - Vanishing potential at r~5-6 fm
- The operating range is set to be:
  - *V(r) goes to zero at r~3-4 fm*
  - *V(r) bounded in the whole range (no infinities at zero)*
  - *V(r)* $\in$ *[-500,500] MeV at r>0.5 fm*
  - *V(r)* $\in$ *[-500,20000] MeV at r<0.5 fm*
  - *No restriction to the number of bound states*

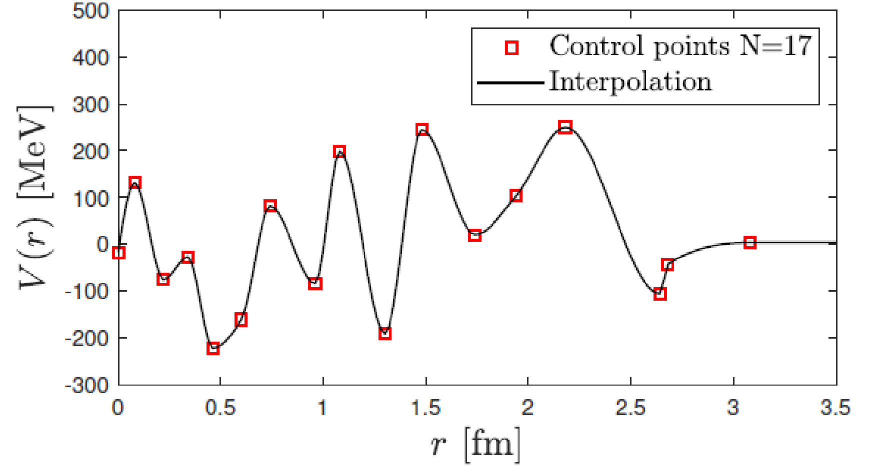
- Generating training data → want to generate random potentials in the desired operating range

- Method:

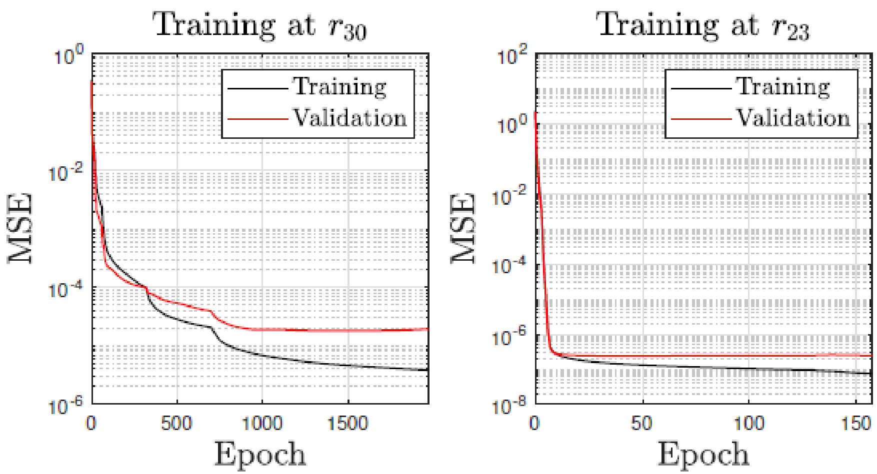
  1. Generate 3 random numbers →
     - number of control points
     - Place of control points
     - Values of control points

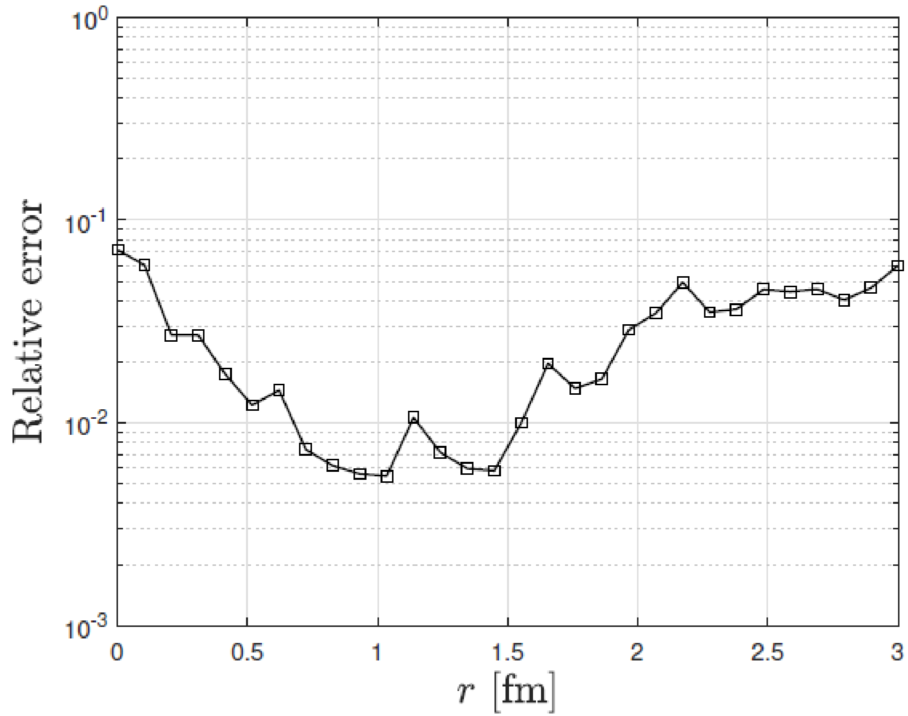
  3. Use Picewise cubic hermitian interpolating polynomials (PCHIP) to interpolate between the control points.





- **Model structure:**
  - 30 inversion points in r ∈ *[0,3] fm*
  - *Tlab= [1 5 10 15 20 25 50 75 100 125 150 175 200 225 250 275 300] MeV*
  - 10000 training and 2000 validation samples





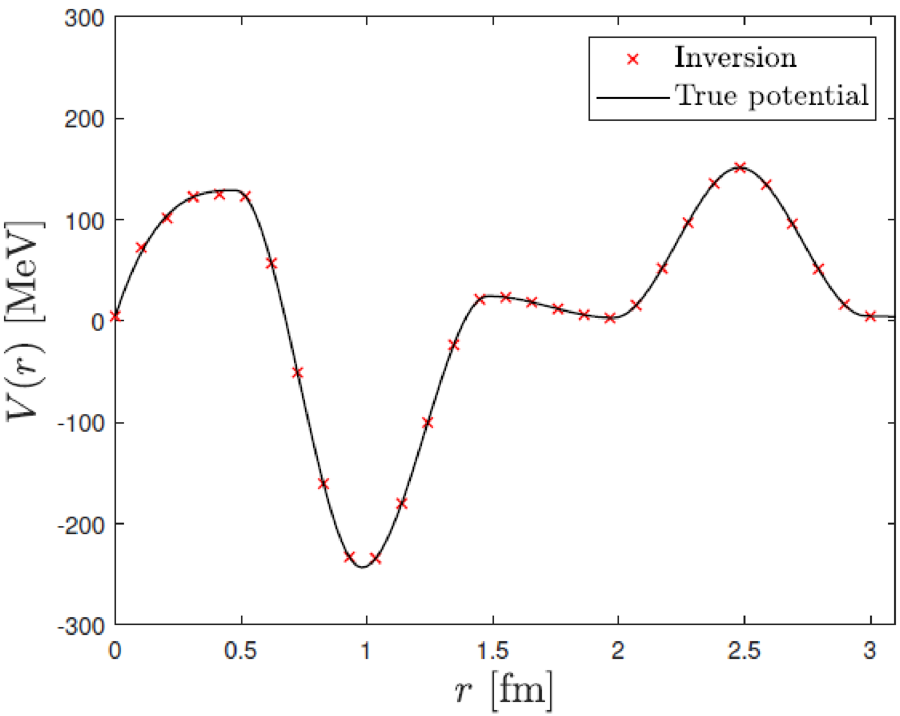


Fig. 16. Validation of the model for a randomly generated test potential.

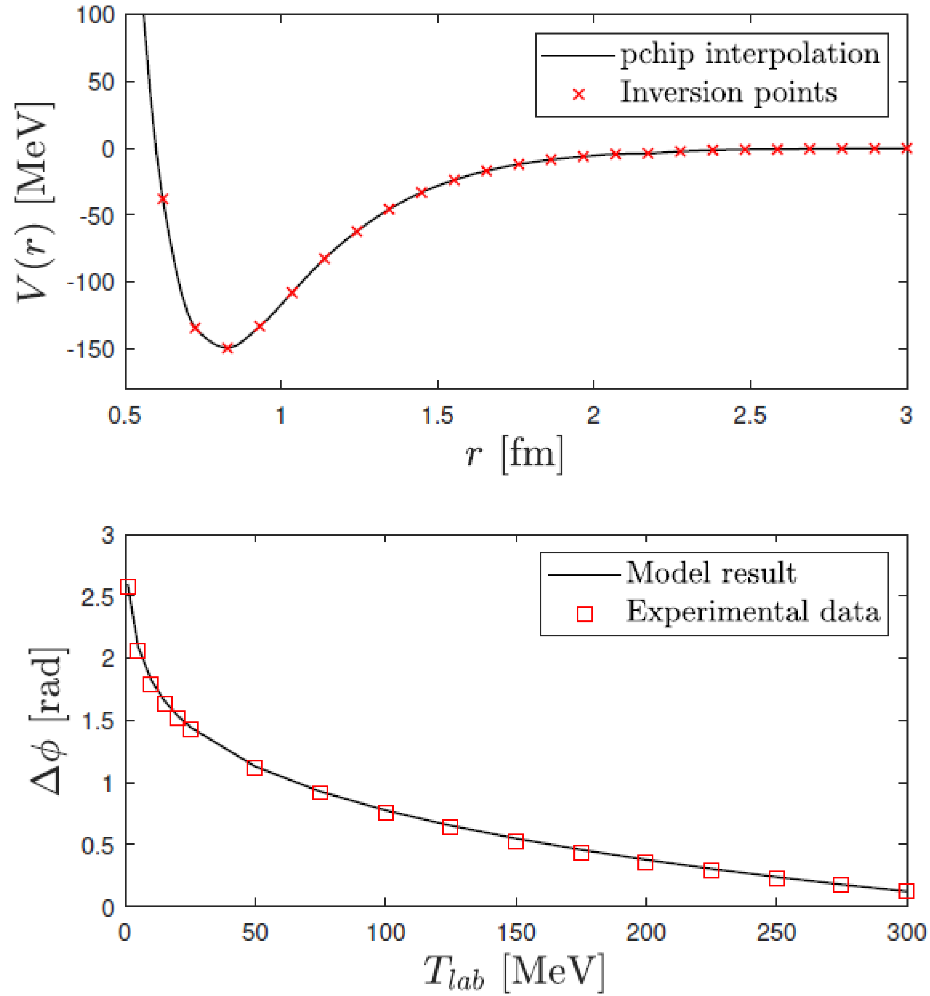


Fig. 17. Estimated $^3S_1$ NN potential, obtained from the neural network inversion model. The upper panel shows the calculated values at the inversion points, and also the PCHIP interpolation between the inversion points, while the lower panel shows the calculated and measured phase shifts.

Summary

- The inverse scattering problem is usually hard to solve, but very important in nuclear physics.
- Nonlinear system identification techniques can be used to obtain good estimates to the scattering potentials.
- Two models were proposed:
  - Volterra series
  - Neural networks
- The low-energy *neutron+proton* interaction potential is estimated by the Neural Network inversion method → comparable results between the measured and the calculated phase shifts.
- The method can be easily extended to describe other systems/problems as well.