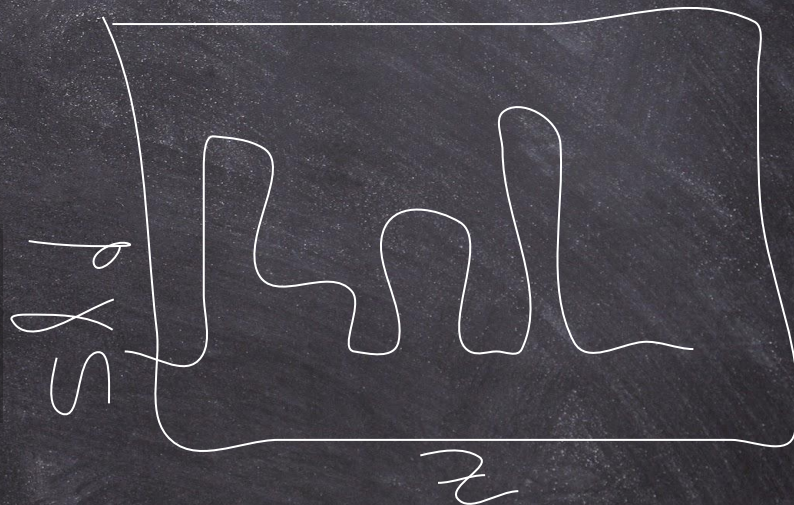
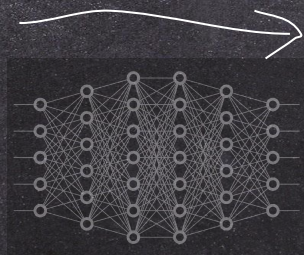
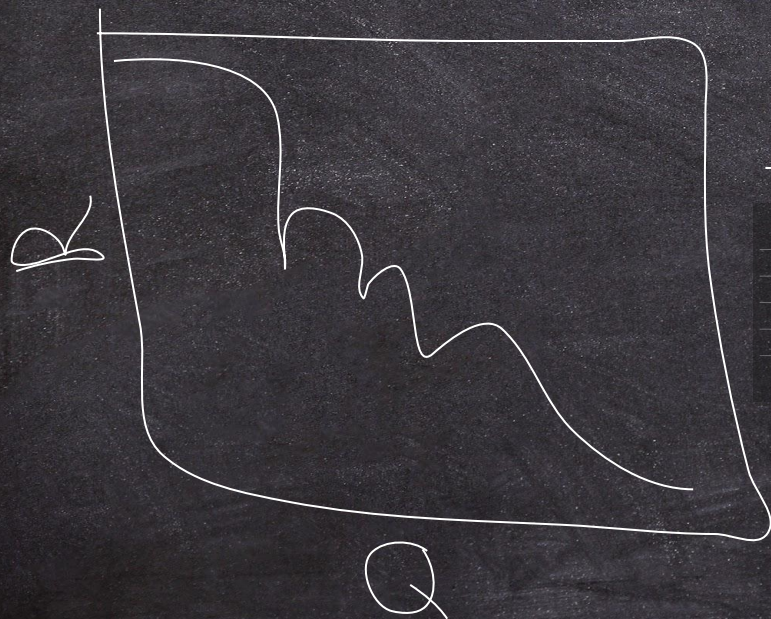


# TOWARDS REFLECTIVITY PROFILE INVERSION THROUGH ARTIFICIAL NEURAL NETWORKS

-- MLZ USERS MEETING 2020, 10.12.2020 --

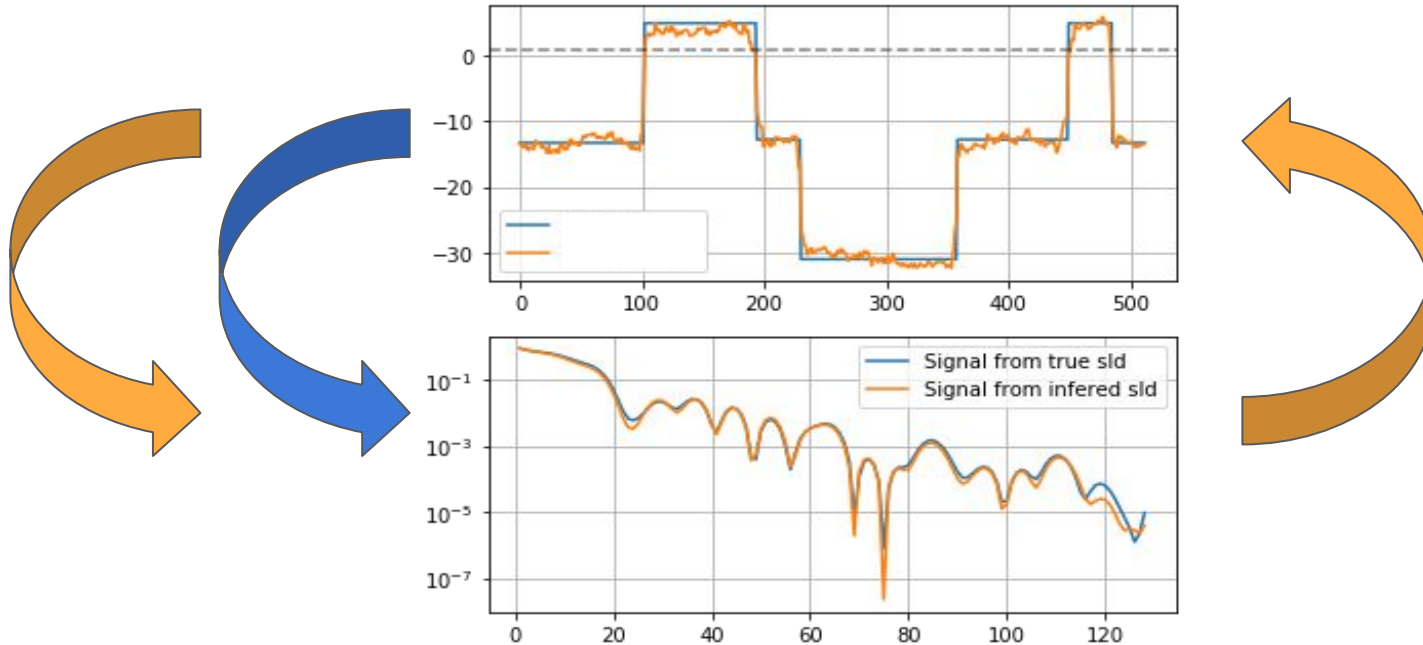
MLZ  
Heinz Maier-Leibnitz Zentrum



JUAN MANUEL CARMONA LOAIZA,  
j.carmona.loaiza@fz-juelich.de

# Traditional Fitting

- Simulate Reflectometry Curve from a “**layer model**” SLD profile (e.g. with BornAgain)
- Change the SLD profile, informed by the mismatch between experiment and data
- Simulate a new Reflectometry Curve from the modified SLD profile

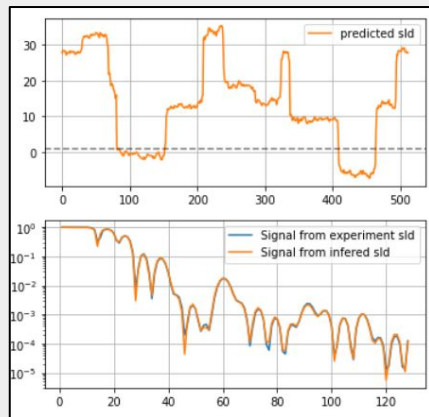


# Batch Fitting - Prototype Idea of Overall Workflow - “One Click Fitting”

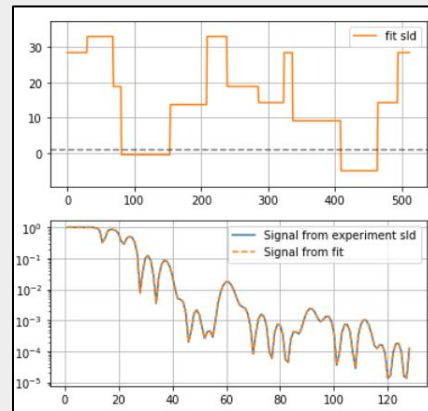
Load reflectometry file(s)

#	q_z	R(q_z)	sigma q_z	sigma R(q_z)
4.1184e-02	6.9507e-02	2.0592e-04	7.0940e-02	
4.2012e-02	1.3261e-01	2.1006e-04	6.0862e-02	
4.2432e-02	7.9832e-02	2.1216e-04	4.1090e-02	
4.2856e-02	1.4300e-02	2.1428e-04	1.4521e-02	
4.3285e-02	1.1842e-02	2.1642e-04	1.2015e-02	
4.3718e-02	2.9100e-02	2.1859e-04	1.7072e-02	
4.4155e-02	8.1983e-02	2.2077e-04	2.6714e-02	
4.4596e-02	5.3027e-02	2.2298e-04	2.0641e-02	
4.5042e-02	2.3183e-02	2.2521e-04	1.1773e-02	
4.5493e-02	1.9686e-02	2.2746e-04	1.0271e-02	
4.5948e-02	5.3344e-02	2.2974e-04	1.6593e-02	
4.6407e-02	8.6670e-03	2.3204e-04	6.4497e-03	
4.6871e-02	3.6320e-02	2.3436e-04	1.1884e-02	
4.7340e-02	5.2602e-02	2.3670e-04	1.3861e-02	
4.7813e-02	4.0785e-02	2.3907e-04	1.1788e-02	

Show reflectometry profile together with a first guess fit



Improve the fit either by hand or by traditional minimizers



Output file

Number of layers: 13

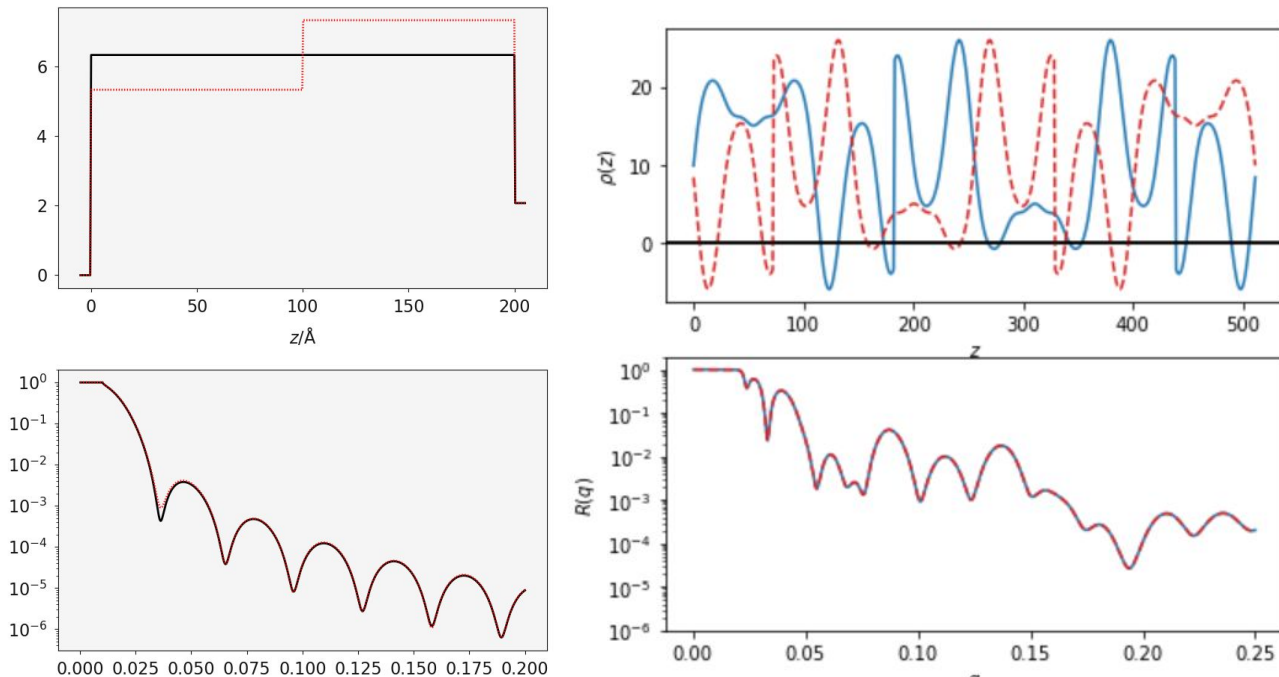
Layer1:  
SLD: 28  
Thickness: 20  
Roughness: 1  
Layer2:  
SLD: 32  
Thickness: 20  
Roughness: 2

[...]

Layer13:  
SLD: 28  
Thickness: 10  
Roughness: 3

Overall fit error: [Chi^2, RQ^4, ... ?]

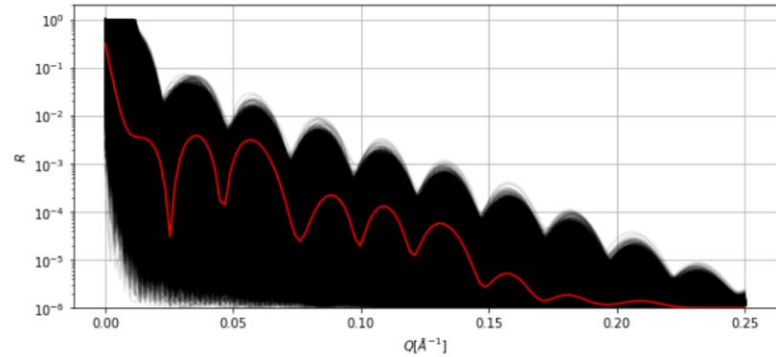
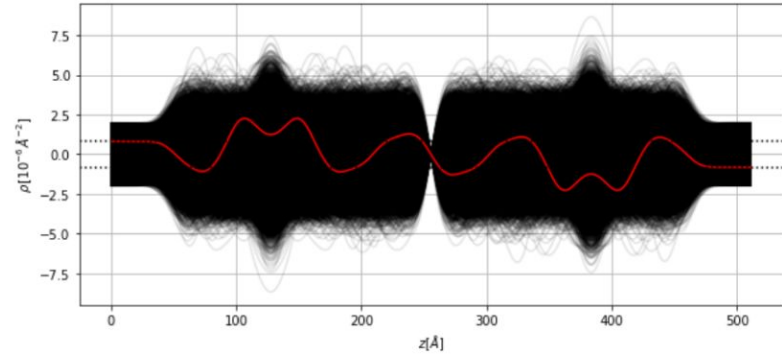
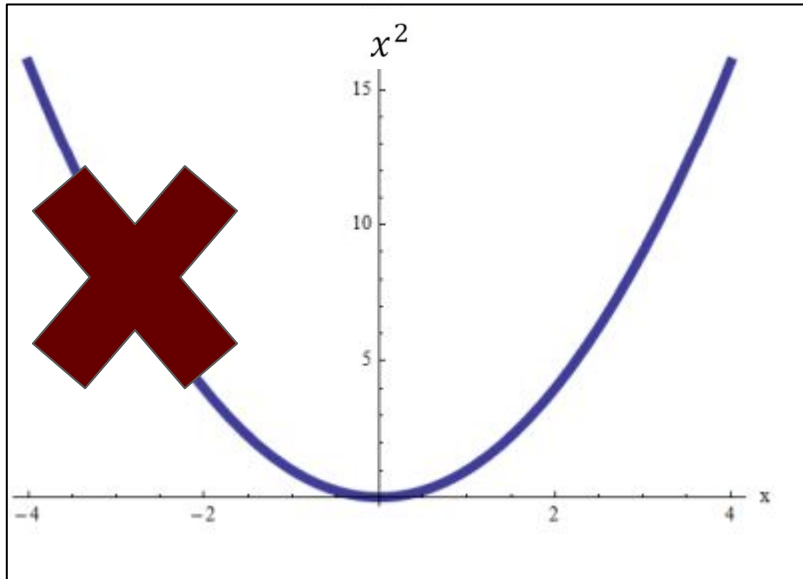
# The phase problem



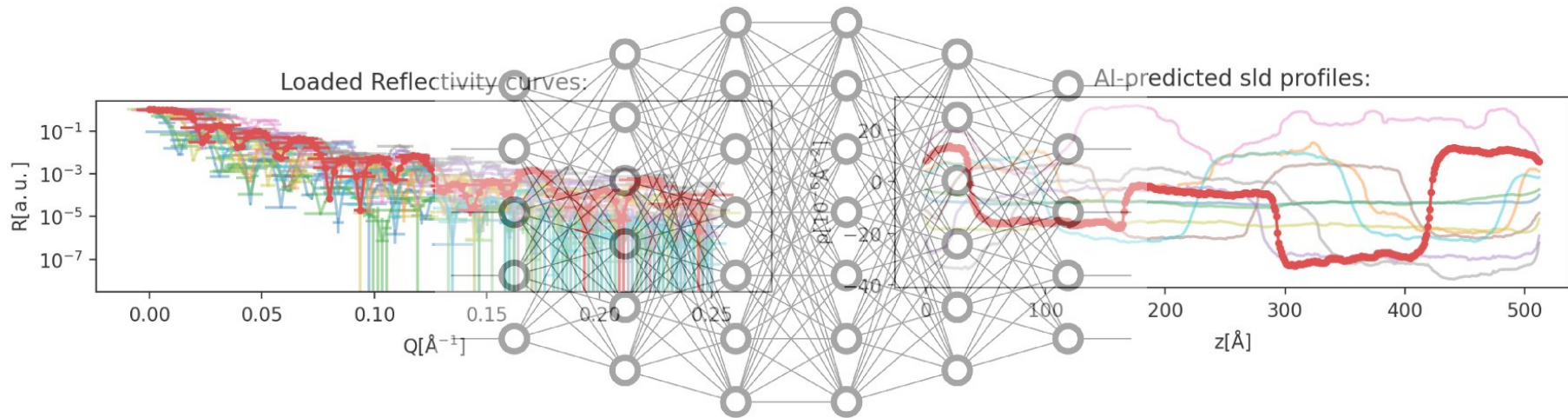
$$r(Q) = \frac{4\pi}{iQ} \int_0^L \psi(k_{0z}, z) \rho(z) e^{ik_{0z} z} dz$$

# Phase problem Workaround: Take a *branch*

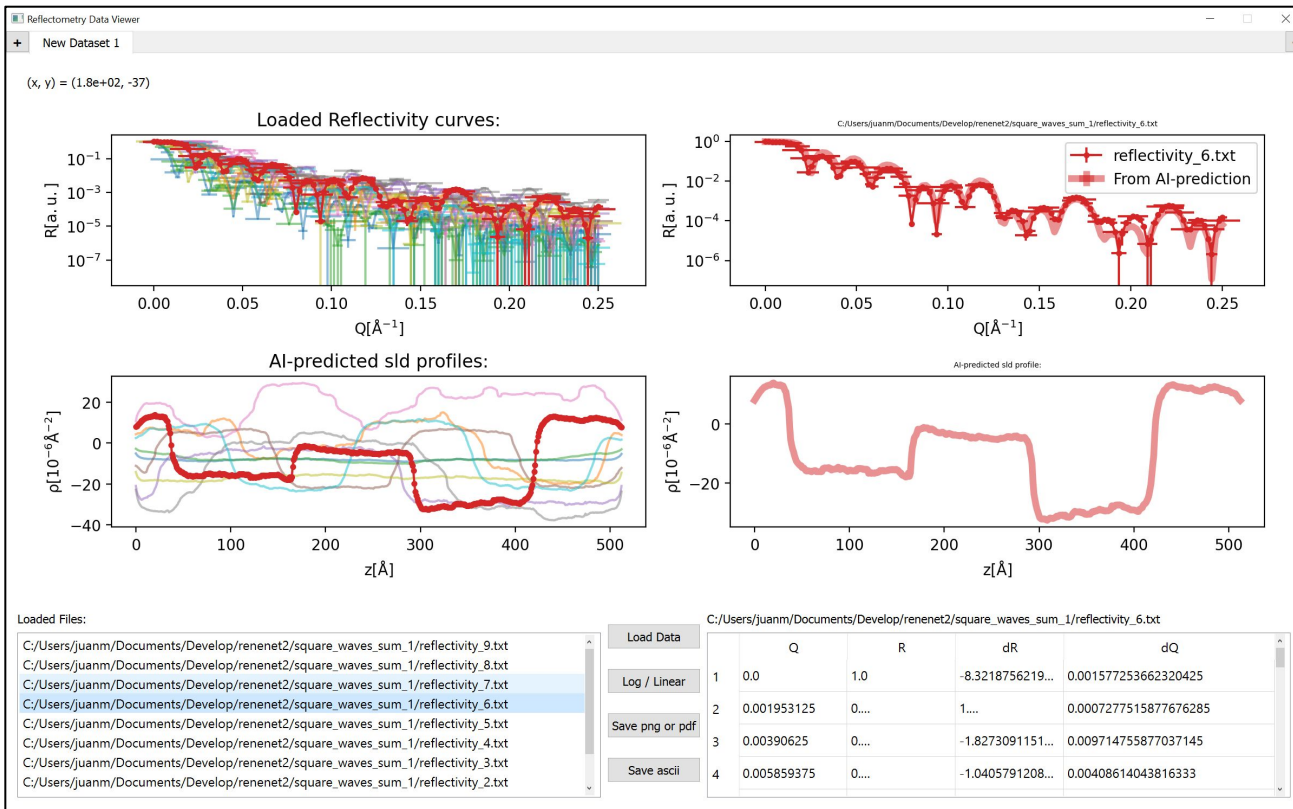
"Square root analogy"



# Artificial Neural Network Batch Fitting

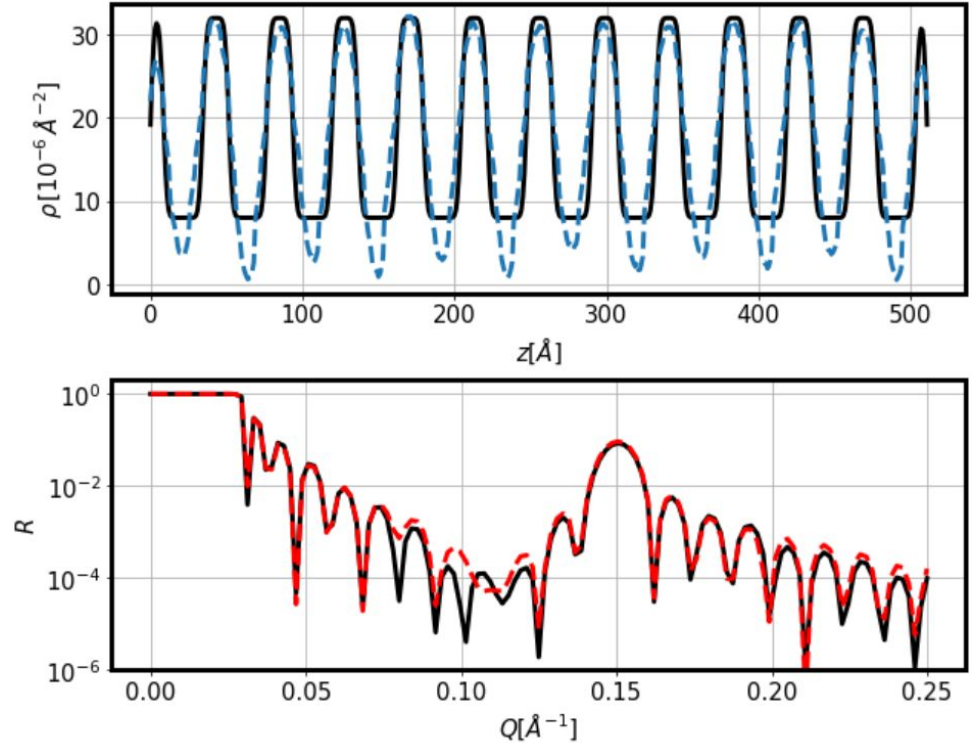
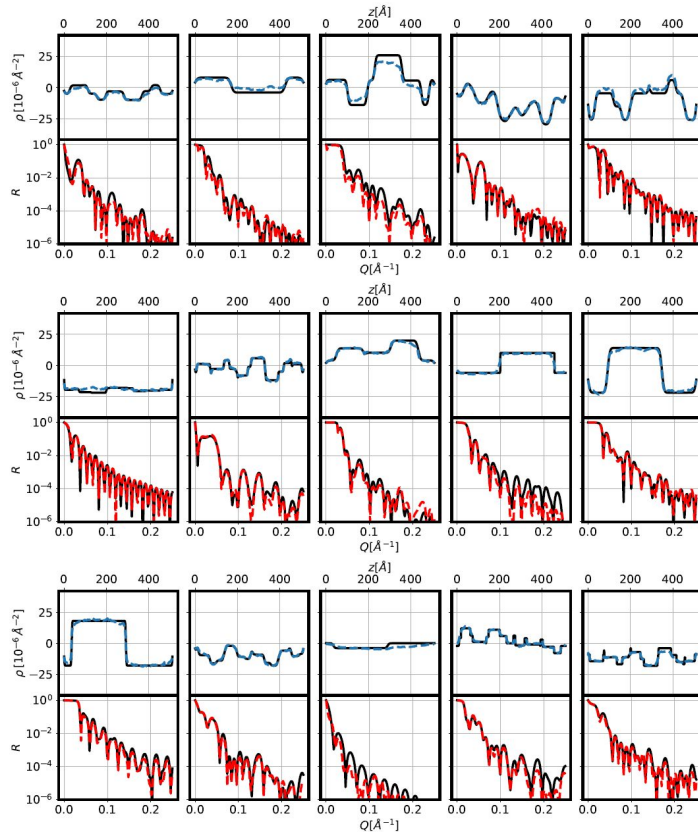


# ANN fitting - First implemented prototype



# Pros / promises:

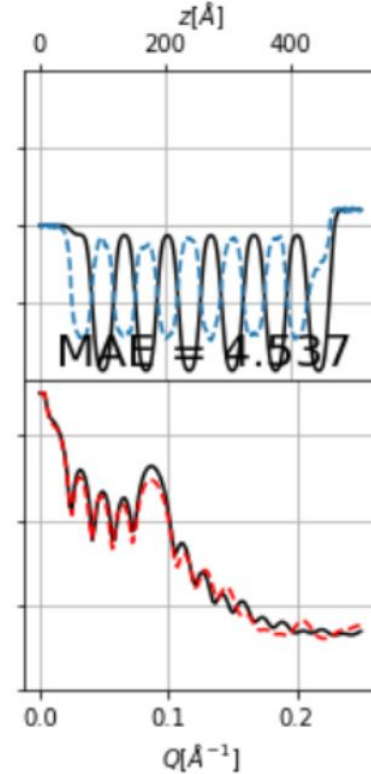
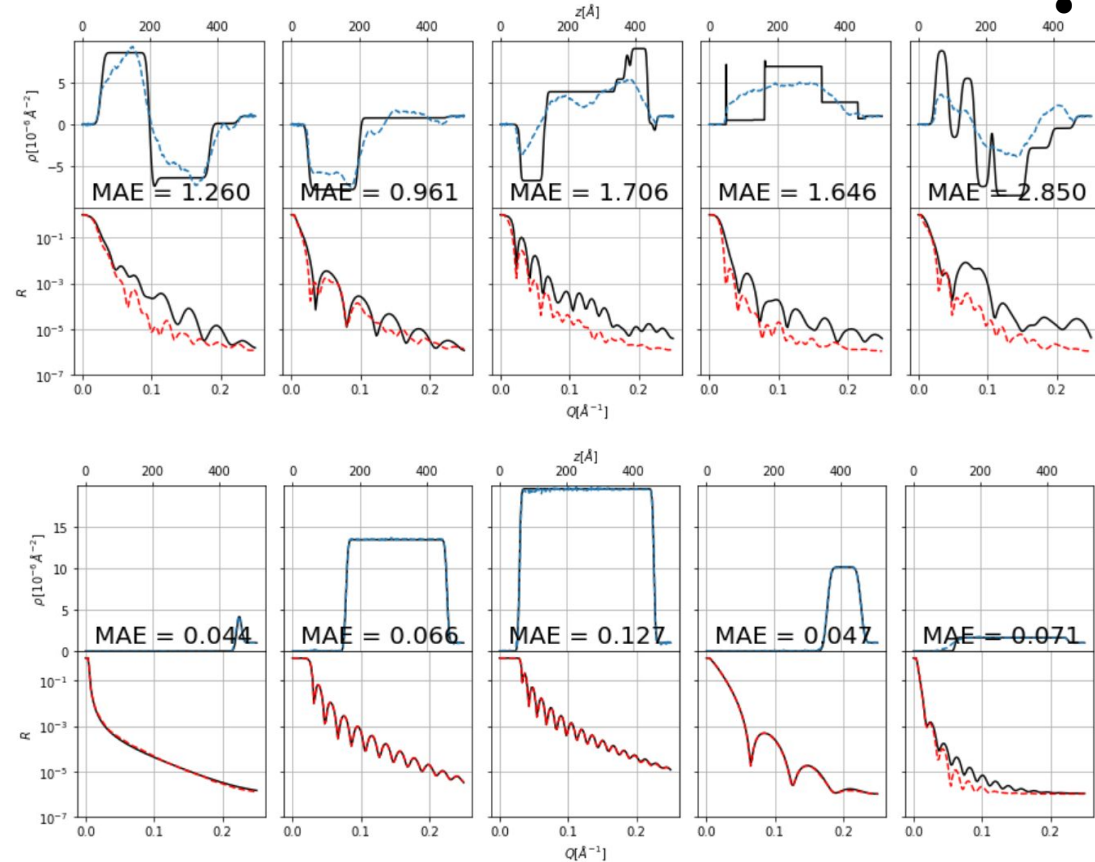
- Real time analyses possible
- One click preliminary results
- Provide a probable first guess, even if wrong
- Fast batch analyses





# Caveats and limitations:

- SLD family needed in advance
- Can return an sld that matches the reflectivity curve but that is nevertheless wrong
- User intervention to properly define the locations of the interfaces between layers



More info on the arXiv:

**Physics > Computational Physics**

*[Submitted on 15 Oct 2020]*

# **Towards Reflectivity profile inversion through Artificial Neural Networks**

Juan Manuel Carmona-Loaiza

Link: <https://arxiv.org/abs/2010.07634>

The image features the words "Thank You" in a large, black, cursive script font, centered horizontally. The background is white and filled with abstract, decorative elements in shades of light blue, teal, and pale lavender. These elements include thick, curved lines, solid circles of various sizes, and stylized, multi-lobed shapes that resemble atomic models or organic forms. The overall aesthetic is clean, modern, and celebratory.

Thank You