Optimizing parameter estimation for the NEXI gray matter microstructure model

MIML – Microstructure Imaging meets Machine Learning

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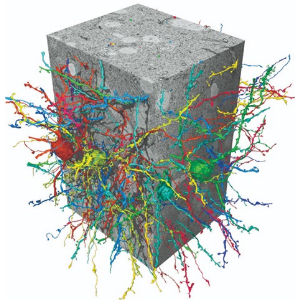
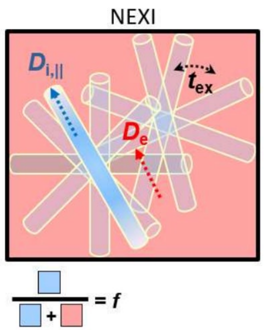
Microstructure Mapping Lab

The Neurite Exchange Imaging model



Grey matter microstructure
(under the electron microscope)



Intra-axonal space (IAS)

Extra-axonal space (EAS)

Objective: invert this function ! (difficult)

Kernel:	$\mathcal{K}(q,t,\mathbf{g}\cdot\mathbf{n};\ f, D_{i,\|}, D_e, t_{ex}) = f' e^{-q^2 t D_i'} + (1-f') e^{-q^2 t D_e'}$
Where: "apparent" diffusivities	$D'_{i/e} = \frac{1}{2}\left\{ D_{i,\|}(\mathbf{g}\cdot\mathbf{n})^2 + D_e + \frac{1}{q^2 t_{ex}} \mp \left[\left[D_e - D_{i,\|}(\mathbf{g}\cdot\mathbf{n})^2 + \frac{2f-1}{q^2 t_{ex}}\right]^2 + \frac{4f(1-f)}{q^4 t_{ex}^2}\right]^{\frac{1}{2}}\right\}$
"apparent" fraction	$f' = \frac{1}{D_i' - D_e'}\left[f D_{i,\|}(\mathbf{g}\cdot\mathbf{n})^2 + (1-f)D_e - D_e'\right]$
Powder average (over directions):	$\bar{S}(q,t) = S\big\|_{q=0} \cdot \int_0^1 \mathcal{K}(q,t,\mathbf{g}\cdot\mathbf{n};\mathbf{p})\,d(\mathbf{g}\cdot\mathbf{n})$

Source : Jelescu et al. 2022. NeuroImage

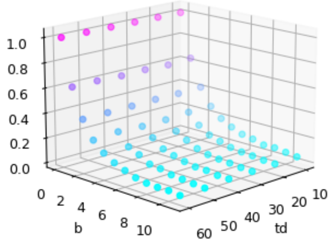
Synthetic data generation

Random brain voxel parameters
[t_{ex}, Di, De, f]

Different sequences (with different b-values and diffusion times)

Create signals
S(b, t_d, t_{ex}, Di, De, f)

N (n_{shells} $\times$ n_{td}) times



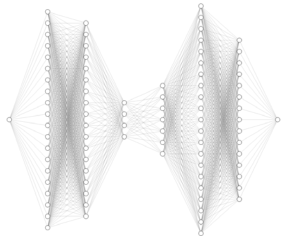
Add noise

Predict
[t_{ex}, Di, De, f]

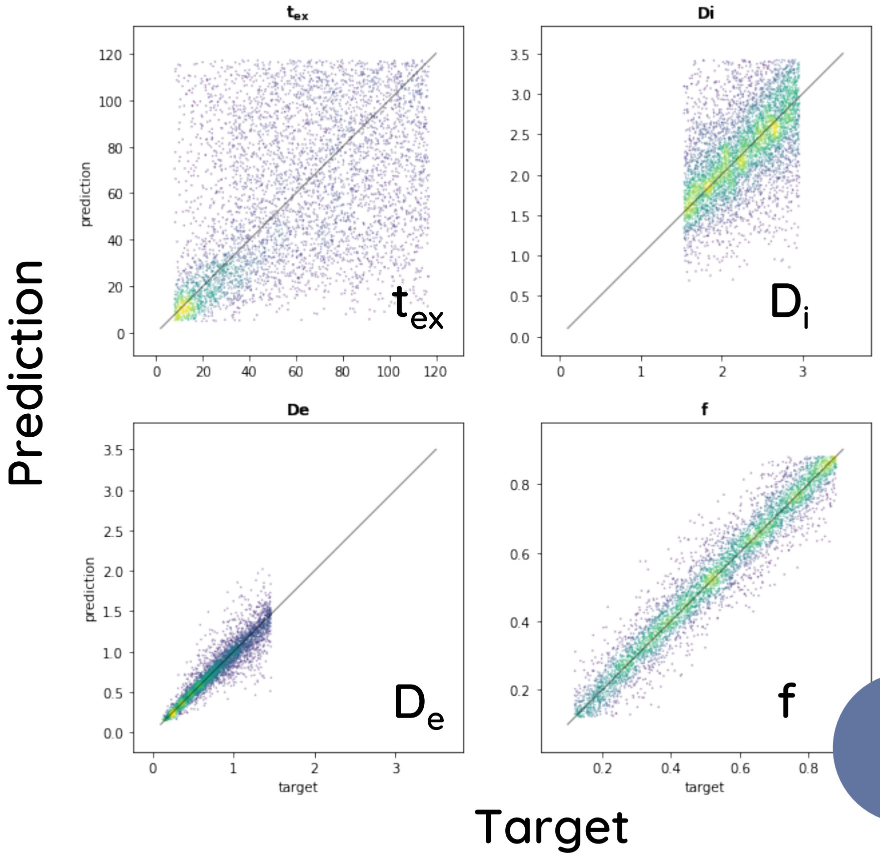
Nonlinear Least Squares VS. Machine Learning results

- L-BFGS-B bounded method
- Use of the Jacobian

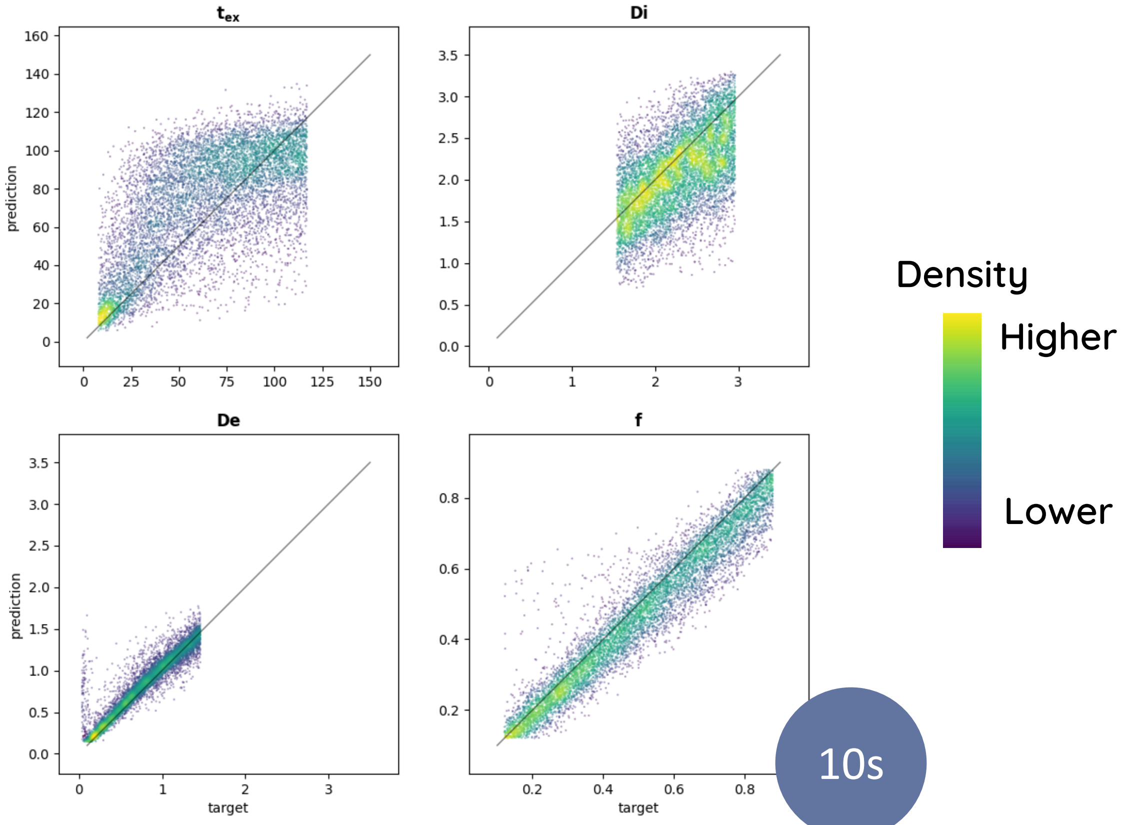
- Optimized by Optuna
- Hidden layers # of neurons : 530, 481, 112, 200, 547, 406



On a noisy dataset (σ_{noise} =0,01)



1h



10s

With the help of Nicolas Albert

The Cramer-Rao Lower Bound

$$Var_{dMRI\ config}(\hat{\mathbf{p}}_i) \quad \geq \quad \left(I^{-1}(\mathbf{p})\right)_{i,i} = CRLB_i$$

Where the Fisher information matrix is : $I(\mathbf{p}) = \frac{1}{\sigma^2} . \mathcal{J}^T * \mathcal{J}$

and the jacobian of the signal : $\mathcal{J} = \partial S(b, t_d, \mathbf{p}) / \partial \boldsymbol{p}$

$\mathcal{J}$ is a vector of size (# of (b,t_d) couples in dMRI config, # of parameters)

and $\begin{pmatrix} \mathbf{p}_0 \\ \mathbf{p}_1 \\ \mathbf{p}_2 \\ \mathbf{p}_3 \end{pmatrix} = \begin{pmatrix} t_{ex} \\ D_i \\ D_e \\ f \end{pmatrix}$

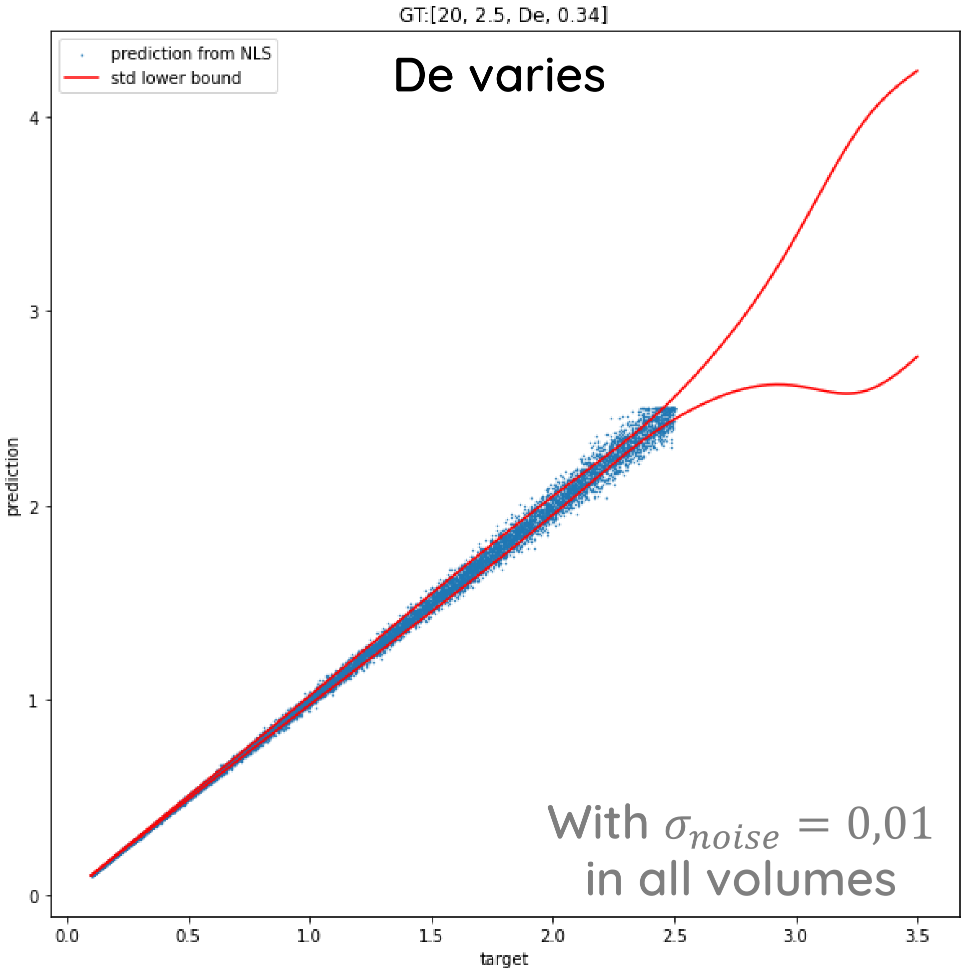
➡ Optimize the dMRI configuration (best b-td couples)

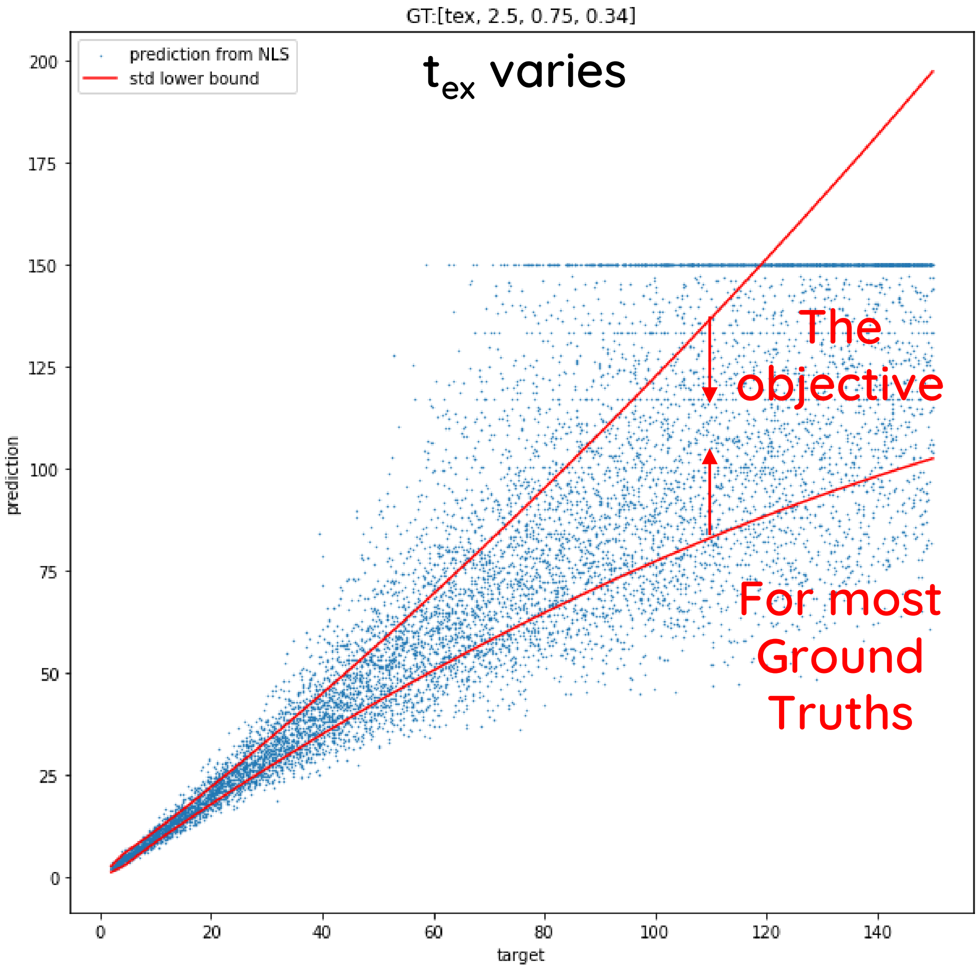
➡ Compute the lower limit of the variance of our estimations

Credit : Aurélien Bustin, Ruud B. van Heeswijk

$\sqrt{CRLB}$: the lower bound of the standard deviation

In each of these datasets, 3 parameters are set, only 1 varies





Thank you for your attention !
Any question ?

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