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Microstructure Mapping Lab

Optimizing parameter estimation for the NEXI gray matter microstructure model

MIML – Microstructure Imaging meets Machine Learning

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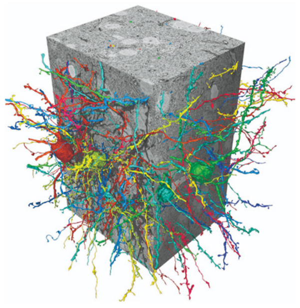
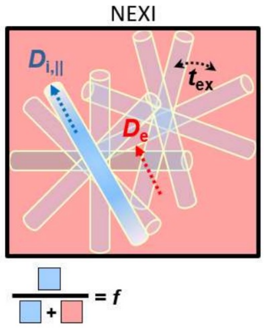
The Neurite Exchange Imaging model



Grey matter microstructure (under the electron microscope)



Intra-axonal space (IAS)

Extra-axonal space (EAS)

Kernel:	$\mathcal{K}\left(q,t,\mathbf{g}\cdot\mathbf{n};\ f,D_{i,\|},D_e,t_{ex}\right) = f' e^{-q^2 t D_i'} + (1-f') e^{-q^2 t D_e'}$
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):	$S(q,t) = S\big\|_{q=0} \cdot \int_0^1 \mathcal{K}(q,t,\mathbf{g}\cdot\mathbf{n};\mathbf{p})\,d(\mathbf{g}\cdot\mathbf{n})$

Source : Jelescu et al. 2022. ArXiv

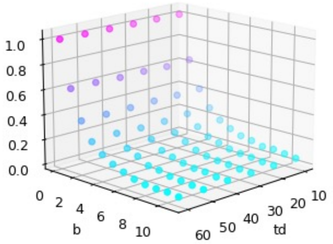
Synthetic data generation

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



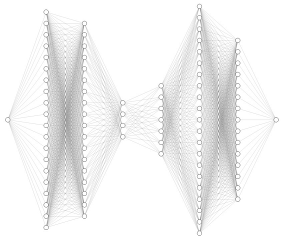
Add noise

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

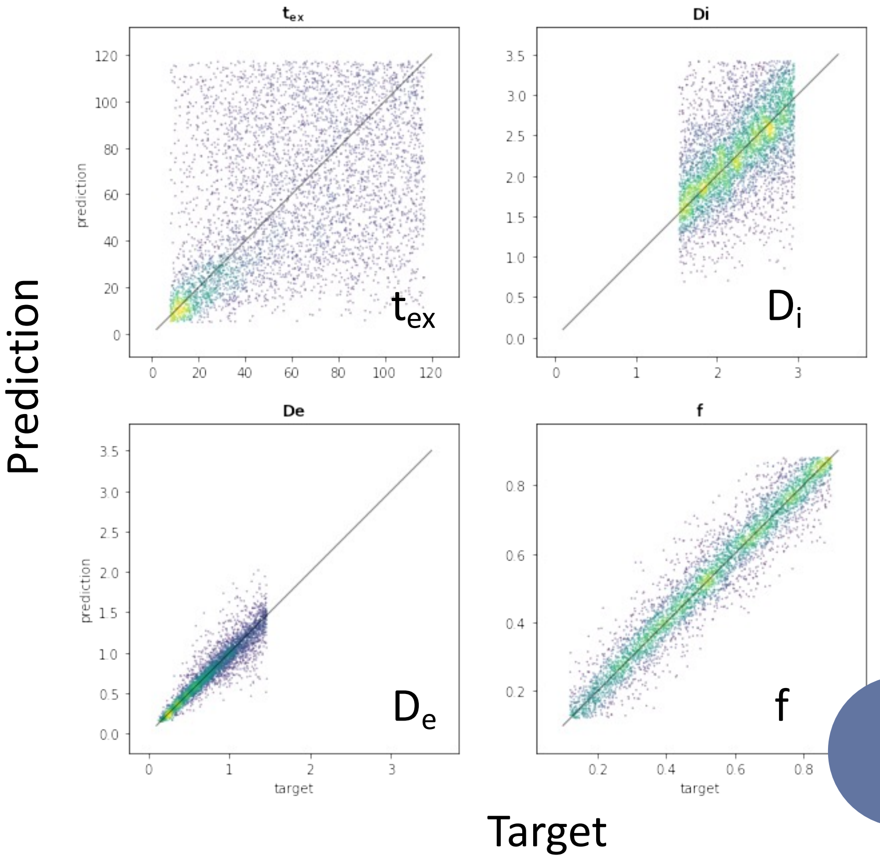
Nonlinear Least Squares VS. Machine Learning results

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

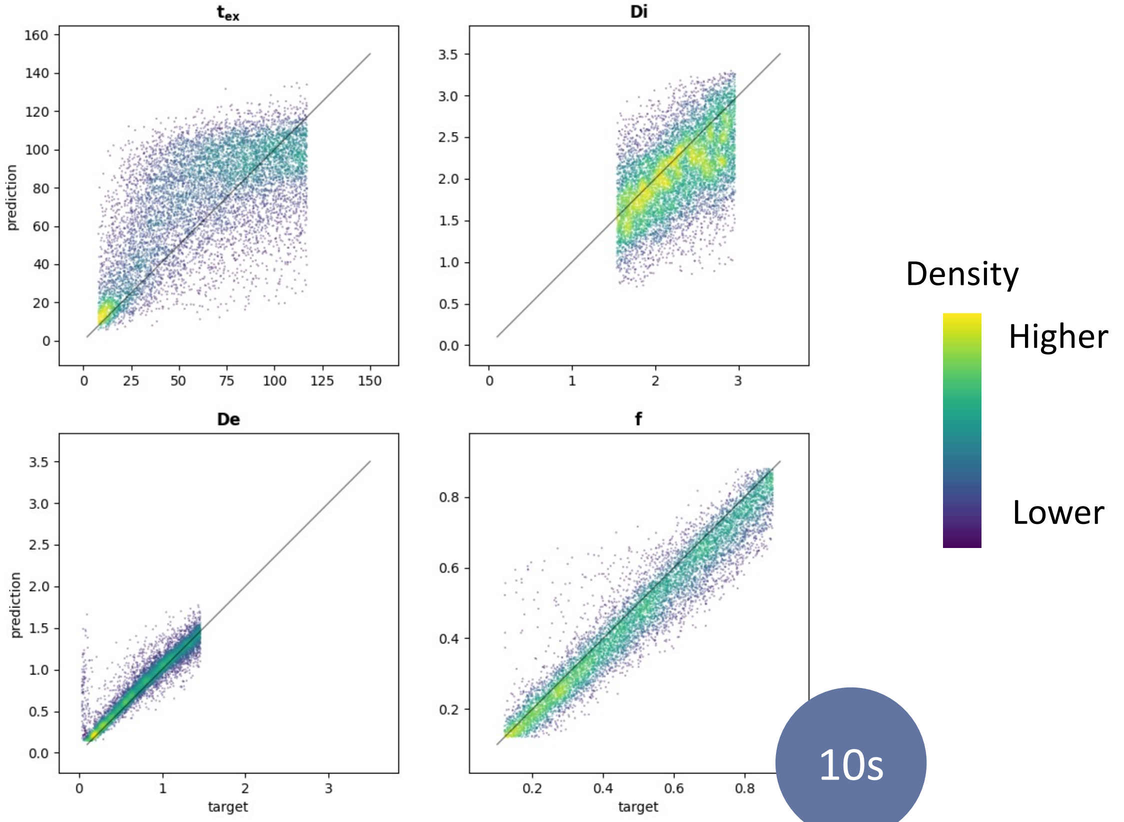
- Optimized by Optuna
- Hidden layers # of neurons :
530, 481, 112, 200, 547, 406



On a noisy dataset
(σ_{noise} =0,01)



1h



10s

With the help of Nicolas Albert

The Cramer-Rao Lower Bound

$$Var_{dMRI\ config}(\hat{\mathbf{p}}_i) \geq \left(\sum_{\substack{(b,t_d)\ couples \\ in\ dMRI\ config}} \mathcal{J}^{-1}(b, t_d, \mathbf{p}) \right)_{i,i} = CRLB_i$$

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

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

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

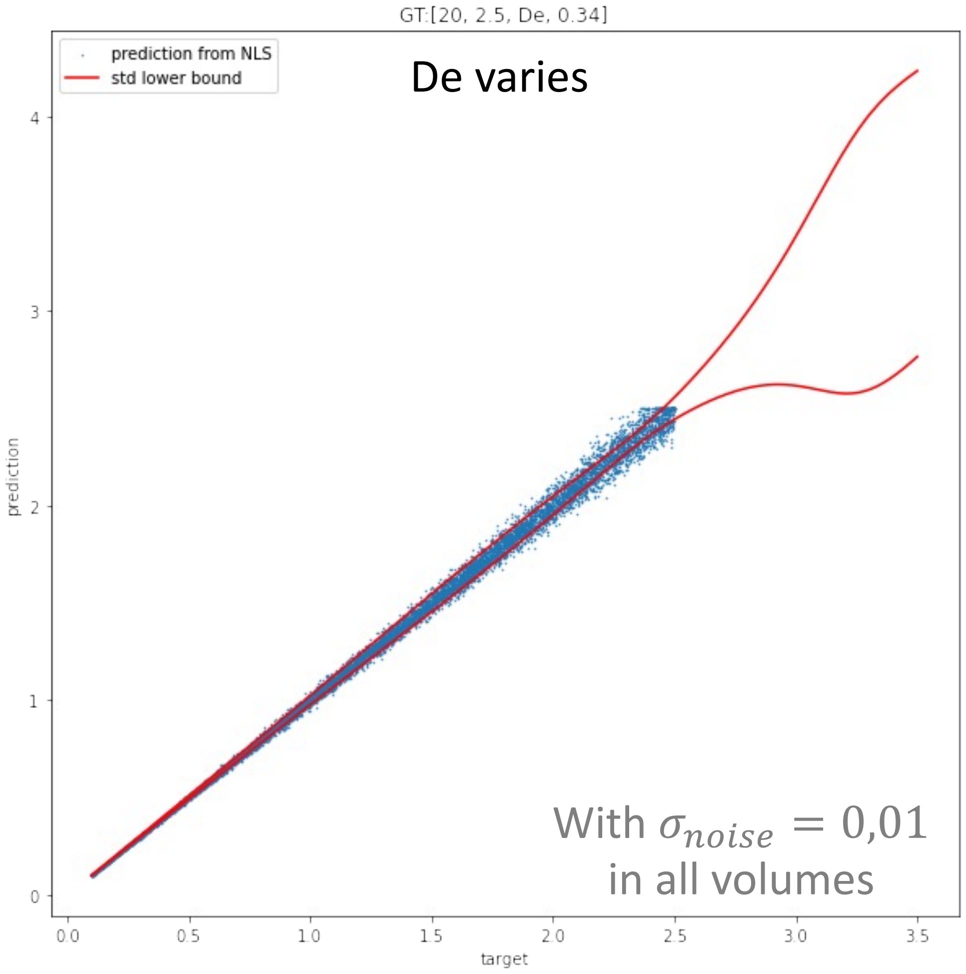
→ Optimize the dMRI configuration (best b-td couples)

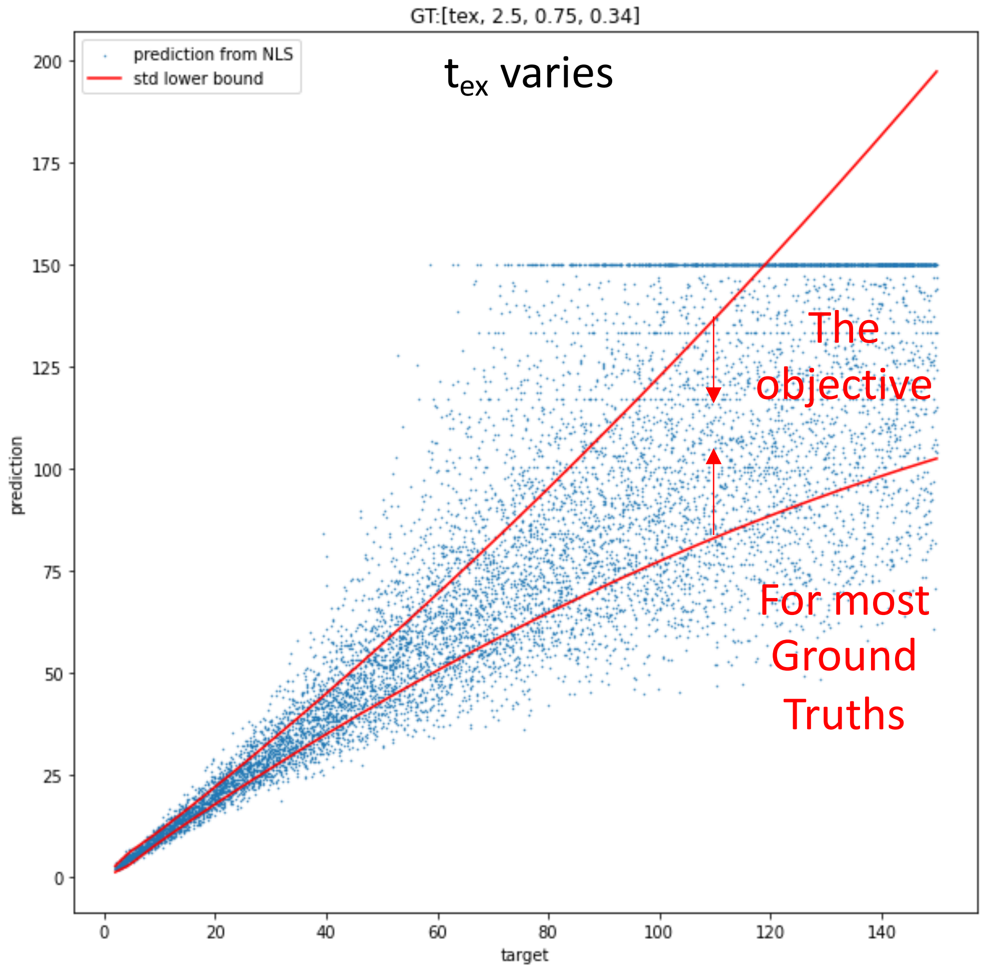
→ Compute the lower limit of the variance of our estimations

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





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Thank you for your attention !
Any question ?

Contact : quentin.uhl@chuv.ch