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APPLICATION OF FRACTIONAL ORDER DIFFUSION MODEL IN ANALYSIS OF DIFFUSION-WEIGHTED MAGNETIC RESONANCE IMAGING DATA

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Abstract. This study explores the application of a fractional diffusion equation in diffusion-weighted magnetic resonance imaging (DW-MRI or DWI) analysis, aiming to validate and extend previous research based on an open-access dataset. A fractional-order model using the Mittag-Leffler function is implemented and validated by reproducing results presented in existing literature. The method is then applied to an open-access Connectome Diffusion Microstructure Dataset (CDMD) to analyze real brain imaging data. The computed parameter maps reveal improved contrast between white matter and gray matter, confirming the model's potential for distinguishing tissue properties. The performance of the fractional diffusion model is compared with the conventional mono-exponential model, demonstrating improved accuracy in fitting diffusion signal attenuations in terms of root mean squared error (RMSE). This research establishes a reproducible baseline for future studies on fractional diffusion modeling in MRI and suggests expanding the study to larger datasets and exploring refinements in parameter estimation to further enhance diagnostic capabilities.

Keywords: fractional order derivative, fractional diffusion equation, anomalous diffusion, Mittag-Leffler function, entropy, kurtosis, Python, MRI, DWI.

Introduction

Diffusion-weighted imaging (DWI) is a powerful modality in magnetic resonance imaging (MRI) that enables the characterization of tissue microstructure by capturing the diffusion properties of water molecules. It plays a crucial role in medical diagnostics, particularly in identifying pathological conditions such as ischemic stroke, brain tumors, and neurodegenerative diseases. Traditional DWI analysis relies on the mono-exponential model, which assumes Gaussian diffusion, but this simplification often fails to account for the complexity of biological tissues.

Fractional order diffusion models have been increasingly recognized as powerful tools for characterizing complex diffusion processes in biological systems. Particularly, some promising applications in DWI were proposed. However, these methods usually require more complex calculations and impose specific requirements on data and thus as far as we know they were only verified in laboratory conditions on very limited data. While recently some large open-access DWI datasets were published that may provide valuable information on applicability of these approaches.

The primary objective of this study is to implement and validate a fractional-order diffusion model for DWI analysis. It involves reproducing results from existing fractional diffusion studies, applying the methodology to an open-access Connectome Diffusion Microstructure Dataset (CDMD), and evaluating the model's effectiveness. The study aims to establish a reproducible baseline for future enhancements in diffusion MRI analysis.

Objectives and Problems of Research

The object of the study is the analysis of diffusion-weighted magnetic resonance tomography data.

The subject of the study is fractional models in the context of analysis of DWI data.

The main objective of this work is to develop software and algorithms for analysis of anomalous diffusion in DWI based on the fractional diffusion equation and to lay the foundations for further improvements of existing methods. To achieve this goal, the following tasks were performed:

• The existing fractional calculus-based models for DWI analysis were examined.

• One of such models was implemented in Python and results obtained in the original paper were reproduced on artificial data.

• A DWI dataset suitable for application of implemented method was selected.

• The algorithm was applied to the selected dataset. The results were compared with the ones obtained by authors of the approach for a different dataset and with classical DWI processing method.

Scientific novelty of this research is in the analysis of data obtained with fractional diffusion model for CDMD dataset, because as far as we know the considered method has not been applied to such data before, and our results demonstrate the possibility of such application.

The practical significance is in the software developed during this research that provides a framework for further investigations. Additionally, because results are obtained for the open-access dataset they can be used as a baseline for further improvements in the investigated method.

Review of Modern Information Sources on the Subject of the Paper

Diffusion-weighted imaging is a form of magnetic resonance imaging that relies on measurement of random motion of water molecules within a tissue. The diffusion of water molecules can be hindered by tissue microstructure. Therefore, DWI allows to differentiate between tissues and distinguish regions affected by diseases such as ischemic stroke or brain tumor [1].

DWI is based on the application of diffusion-sensitizing gradients in an MRI sequence, typically using a spin-echo echo-planar sequence (SE-EPI). The degree of diffusion weighting is characterized by b-value, expressed in units of s/mm^2, which is calculated as:

$$b = \gamma^2 G^2 \delta^2 (\Delta - \delta/3) = q^2 \bar{\Delta}, \quad (1)$$

where γ is the gyromagnetic ratio of a Hydrogen atom, G – magnitude of the diffusion weighted gradient pulse, δ – width of applied gradient pulses, Δ – time between two paired gradient pulses [2].

Formula (1) can also be expressed as:

$$b = q^2 \bar{\Delta}, \quad (2)$$

where $q = \gamma G \delta$ is a diffusion gradient strength sensitization (mm^{-1}), $\bar{\Delta} = \Delta - \delta/3$ is an effective diffusion time (ms) [3].

To qualitatively evaluate impedance of water molecules diffusion the apparent diffusion coefficient (ADC) is computed based on DWI data. ADC is expressed in units of mm^2/s. This can be done by analyzing signals obtained with varying b-values.

The conventional model used to describe diffusion in biological tissues is the mono-exponential model, where signal attenuation follows:

$$S(b)/S_0 = exp(-bD_m), \quad (3)$$

where $S(b)$ is the signal intensity at a given b-value, S_0 is the signal without diffusion weighting, and D_m is the ADC [4]. With this model ADC can be directly computed given two DWI signals, one obtained without diffusion weighting S_0, and the other at a given b-value (e.g. b = 1000 s/mm^2):

$$D_m = \frac{log\big(S(b)\big) - log(S_0)}{-b} = -\frac{1}{b} \cdot log\left(\frac{S(b)}{S_0}\right). \quad (4)$$

This model assumes Gaussian diffusion, which can be described according to the second-order partial differential equation:

$$\frac{\partial P(x,t)}{\partial t} = D\frac{\partial^2 P(x,t)}{\partial x^2}, \tag{5}$$

where D is diffusion coefficient and $P(x, t)$ is the diffusion propagator, which provides the probability density of finding a molecule at position x at time t. The solution to this equation is the familiar Gaussian PDF:

$$P(x,t) = \frac{1}{\sqrt{4\pi Dt}}\exp\left(-\frac{x^2}{4Dt}\right). \tag{6}$$

Equation (5) describes Random Walk (RW) stochastic process, where mean square displacement (MSD) grows linearly with time:

$$\langle x^2(t)\rangle \sim t. \tag{7}$$

In RW model each diffusing particle waits a fixed time interval between steps. While complex environments with heterogenous or porous structures can obstruct particle movement and make it wait random times between steps. Therefore, this model is often inadequate for describing complex tissues with heterogeneous microstructure.

Continuous time random walk (CTRW) model generalizes the RW model, by relaxing assumption of discrete time intervals between steps. In this model both step lengths and intervals between steps are random and are governed by arbitrary and independent probability distributions. The MSD no longer increases with a linear dependence on time, but in many cases follows power law:

$$\langle x^2(t)\rangle \sim t^{\gamma}. \tag{8}$$

Diffusion based on such model is called anomalous. Two variants of such diffusion are distinguished based on value of anomalous diffusion exponent γ. If $\gamma > 1$ the diffusion process is called “superdiffusive” and when $0 < \gamma < 1$ it is “subdiffusive”, while with $\gamma = 1$ it is normal diffusion [5, 6].

In recent years, fractal analysis methods are being actively developed. They often demonstrate superior to classical methods results in describing complex systems [7, 8]. One of fields where this feature may be especially useful is medicine. Consequently, many applications of fractal methods to medical data were proposed. For example, in [9] the effect of Riesz fractional order derivative-based operator on the task of intracranial hemorrhage segmentation is investigated.

One of the main ideas in fractal analysis of DWI data is that fractional order models can better consider anomalous diffusion. Such models are proposed in papers [3, 5].

In [3] it was proposed to model diffusion in neural tissue based on CTRW theory and fractional calculus. The experiments were performed on fixed rat brain and demonstrated that this model can provide new information regarding the anomalous diffusion.

In [5] a similar model was applied to diffusion weighted magnetic resonance imaging in the brain of a chronic ischemic stroke patient. Specifically, it was shown that entropy and kurtosis computed based on this model can provide valuable insights into tissue microstructure.

However, as far as we know this approach was not investigated on larger datasets. Therefore, the main objective of this research is to apply method proposed in [3] to open access DWI dataset, to provide a baseline that can be used to evaluate further improvements of this approach.

To consider anomalous diffusion in DWI analysis, some promising approaches based on continuous time random walk theory were proposed [3, 5, 6]. The key idea of CTRW theory is to extend the diffusion equation with operators of fractional order, that allows describing both Gaussian and anomalous diffusion:

$$\frac{\partial^{\alpha} P(x,t)}{\partial t^{\alpha}} = D_{\alpha,\beta}\frac{\partial^{\beta} P(x,t)}{\partial |x|^{\beta}}. \tag{9}$$

where $\partial^{\alpha}/\partial t^{\alpha}$ is the Caputo fractional derivative in time for $0 < \alpha \leq 1$, $\partial^{\beta}/\partial|x|^{\beta}$ is the Riesz fractional derivative in space for $1 < \beta \leq 2$ and $D_{\alpha,\beta}$ is the generalized diffusion constant (distance$^{\beta}$/time$^{\alpha}$).

Utilizing Fourier and Laplace transforms equation (3) can be expressed as:

$$p(k,s) = \frac{1}{s + D_{\alpha,\beta} s^{1-\alpha} |k|^{\beta}}. \quad (10)$$

By applying inverse Laplace transform the following characteristic function is obtained:

$$p(k,t) = E_{\alpha}\left(-D_{\alpha,\beta}|k|^{\beta} t^{\alpha}\right), \quad (11)$$

where E_{α} is the single-parameter Mittag-Leffler function (MLF)

$$E_{\alpha}(z) = \sum_{k=1}^{\infty} \frac{z^k}{\Gamma(\alpha k + 1)}. \quad (12)$$

When $\alpha = 1$ and $\beta = 2$ equation (11) becomes a mono-exponential function, suitable for modelling Gaussian diffusion:

$$p(k,t) = E_1\left(-D_{1,2}|k|^2 t^1\right) = exp(-D_{1,2}|k|^2 t). \quad (13)$$

While for $0 < \alpha \leq 1$ and $\beta = 2$ it can be used to model time-fractional subdiffusion:

$$p(k,t) = E_{\alpha}\left(-D_{\alpha,2}|k|^2 t^{\alpha}\right). \quad (14)$$

In [3] it is proposed to use (14) as a model for DWI signal attenuation. Because b-value can be represented as (2), parameters q and $\bar{\Delta}$ can be used for k and t respectively in equation (14)

$$S(b)/S_0 = p(q,\bar{\Delta}) = E_{\alpha}\left(-D_{\alpha,2}|q|^2 \bar{\Delta}^{\alpha}\right). \quad (15)$$

We cannot directly compute ADC from this model, however having data for multiple b-values we can fit it to (14) to estimate parameters *D* and *α*.

Additionally, spectral entropy and excess kurtosis computed based on *D* and *α* demonstrated valuable information for brain tissues analysis.

The spectral entropy measures the uncertainty of a characteristic function and can be computed by inserting equation (14) into (16).

$$H[\hat{p}(q,\bar{\Delta})] = -\sum_{i=1}^{N} \frac{\hat{p}(q,\bar{\Delta})_i ln(\hat{p}(q,\bar{\Delta})_i)}{ln(N)}, \quad (16)$$

where $\hat{p}(k_i) = p(k_i)p^*(k_i)$.

Main Material Presentation

Connectome Diffusion Microstructure Dataset (CDMD). Application of fractional order model proposed in [3] requires specific data. It must contain DWI signal measurements for a wide range of b-values and pulse sequence parameters δ and Δ need to be specified. While in public datasets often only one b-value is provided, which is enough for simpler models such as the mono-exponential one.

As the result of available datasets analysis, a Connectome Diffusion Microstructure Dataset (CDMD) was considered the most suitable one for our research. It contains DWI data for 26 healthy participants acquired on the MGH-USC 3 T Connectome scanner with a maximum gradient strength of 300 mT/m and a custom-built 64-channel head coil [10]. For each participant, acquired data includes two diffusion times (19 and 49 ms), eight gradient strengths linearly spaced between 30 mT/m and 290 mT/m for each diffusion time, and 32 or 64 uniformly distributed directions.

Diffusion MRI data was acquired using a two-dimensional SE-EPI sequence. For each participant, 66–70 contiguous sagittal slices were acquired with the center slice placed along the midline corpus callosum to achieve symmetric whole brain coverage. The imaging was performed with the following parameters: repetition time (TR) = 3800 ms, echo time (TE) = 77 ms, field of view (FOV) = 216 × 216 mm, matrix size = 108 × 108, slice thickness = 2 mm, voxel size = 2 × 2 × 2 mm3, diffusion time (Δ) = 19 or 49 ms, pulse duration (δ) = 8 ms, eight diffusion-encoding gradient strengths evenly spaced between 30 and 290 mT/m (i.e., 31, 68, 105, 142, 179, 216, 253, 290 mT/m) for each diffusion time corresponding to 16 different b-values (i.e., 50, 350, 800, 1500, 2400, 3450, 4750, and 6000 s/mm2 for Δ = 19 ms; 200, 950, 2300, 4250, 6750, 9850, 13,500, 17,800 s/mm2 for Δ = 49 ms) [10].

Each sample of the dataset is stored in a separate directory and contains several files:

- the DWI data tensor of shape (70, 108, 108, 850) stored in NIfTI format;
- the brain mask of shape (70, 108, 108) stored in the same NIfTI format;
- text file with .bval extension providing b-values for each experiment;
- text file with .delta extension providing diffusion time (Δ) for each experiment.

Algorithm description

In this section we describe the algorithm for analysis of DWI data from CDMD based on [3] approach. In this research only data for participant #5 was analyzed. We considered only cases with diffusion time Δ = 19. Although, in CDMD scanning was performed by sagittal slices, because authors of [3] work with axial slices, we also extracted (70, 108) middle axial slice from (70, 108, 108) DWI tensor (Fig. 1).

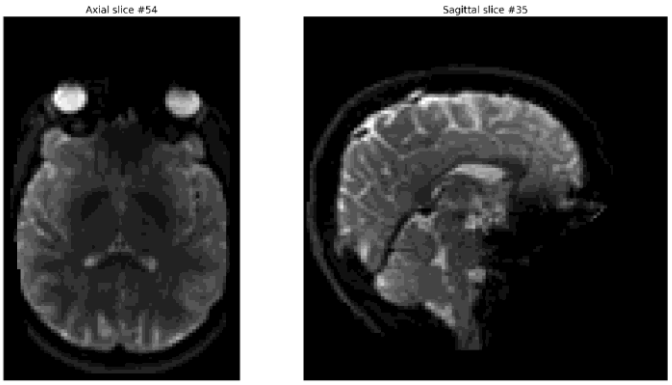

Fig. 1. Examples of middle axial (left) and sagittal (right) slices of a sample from CDMD

In [5] only one diffusion-weighted gradient direction was used, in [3] the three diffusion weighted directions were averaged, therefore in this study we decided to use the average of all 32 directions available for each b-value in the dataset.

After that only the region corresponding to brain was selected utilizing brain mask provided in CDMD (Fig. 2). By performing this preprocessing, we obtained an array of b-values b and an array of corresponding signal values $S(b)$ averaged by diffusion directions for each voxel of the brain.

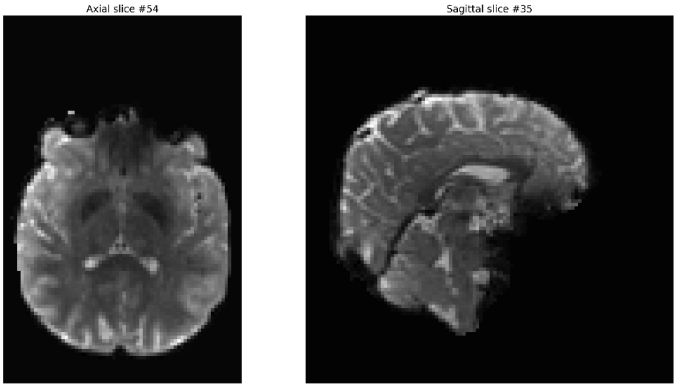

Fig. 2. Examples of the same middle axial (left) and sagittal (right) slices of a sample from CDMD after setting all voxels outside the brain mask to 0

To find D and α, this data was fit to equation (15) using Levenberg-Marquardt minimization algorithm for solving nonlinear least-squares problem with bounds on the variables. Initial guesses on independent variables are $D = 0.5$ and $\alpha = 0.5$. Variables are bounded with [0, 1] for D and [0.1, 1] for α.

After estimating D and α separately for each voxel, we used them for calculation of the entropy H according to formula (16) and the excess kurtosis K according to formula (17).

Software implementation. All experiments were performed in Python programming language.

Firstly, CDMDDataset class was implemented. It stores some dataset constant parameters and has one method load_sample that given a sample name, diffusion time Δ and slice index loads DWI data using nibabel library.

```
class CDMDDataset:
    def __init__(self, data_root: Path):
        self.data_root = data_root
        self.Gs = [31, 68, 105, 142, 179, 216, 253, 290]
        self.small_delta = 8

    def load_sample(
            self, sample: str, big_delta: float, slice_id: int) -> Sample
```

It returns a structure containing one DWI slice, brain mask and corresponding metadata.

```
@dataclass
class Sample:
    image: np.ndarray
    bvalues: np.ndarray
    mask: np.ndarray
    delta: float
```

Fitting pipeline is based on the source code of dwilib repository. A custom model based on equation (15) was added. For MLF calculation numfracpy library was used that implements approach proposed in [11].

```
from numfracpy import Mittag_Leffler_one

def adc_mlf_alpha(ADCs, alpha, b, delta):
    results = []
    for b_i in b:
        q = np.sqrt(b_i / delta)
        k, t = q, delta
        f = -ADCs * np.abs(k)**2 * t**alpha
        result = Mittag_Leffler_one(f, alpha)
        results.append(result)
    return np.asarray(results)
```

Because this model involves more complex computations than the standard ones and each voxel is fit independently, the library source code was modified to support parallel fitting of each voxel using tqdm's process_map that is based on multiprocessing standard library module. Also to avoid unnecessary calculations only voxels covered by the brain mask are considered, and the results are reshaped to the original image size using the following function:

```
def restore_masked_result(result: np.ndarray, mask: np.ndarray) -> np.ndarray:
    restored_results = []
    for i in range(result.shape[-1]):
        img = np.zeros_like(mask, dtype=np.float64)
        img[mask != 0] = result[:, i].flatten()
        restored_results.append(img)
    return np.dstack(restored_results)
```

For entropy and excess kurtosis calculation the next two functions were implemented:

```
def compute_entropy(sample: Sample, D: np.ndarray, alpha: np.ndarray) -> np.ndarray:
    entropy = np.zeros_like(D)
    for i, j in np.argwhere(sample.mask != 0):
        p = adc_mlf_alpha(D[i, j], alpha[i, j], sample.bvalues, sample.delta)
        p_hat = p * np.conjugate(p)
        entropy[i, j] = stats.entropy(p_hat, base=len(p_hat), axis=0)
    return entropy

def compute_kurtosis(sample: Sample, alpha: np.ndarray) -> np.ndarray:
    K = 6 * (gamma(alpha + 1)**2 / gamma(2 * alpha + 1)) - 3
    K[sample.mask == 0] = 0
    return K
```

Finally, matplotlib and plotly libraries are used for visualizations and data analysis.

Results and Discussions

Verification on artificial data. To verify correctness of implemented algorithm, experiment from [3] was performed. The entropy was computed for cases of $0 < \alpha \leq 2$ and $0 < \beta \leq 4$. The diffusion coefficient was fixed as D=1, diffusion time set to t=1, and N=500 wavenumbers k_i from 0 to 5 were considered. On Fig. 3 the resulting entropy surface plot is shown.

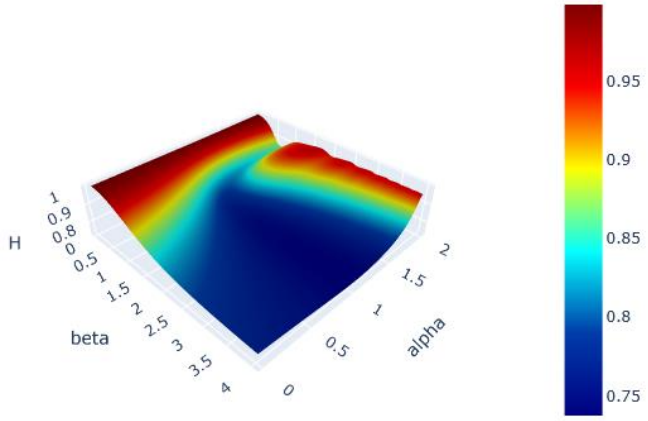

Fig. 3. MLF spectral entropy surface plot

This plot corresponds to the one presented in [3] and confirms that our implementation matches the original method.

Analysis of parameter maps. The obtained D_{MLF} has some outliers with very high values and therefore extremely poor contrast, as can be seen on the Fig. 4. Because of that we clipped all values larger than 0.1.

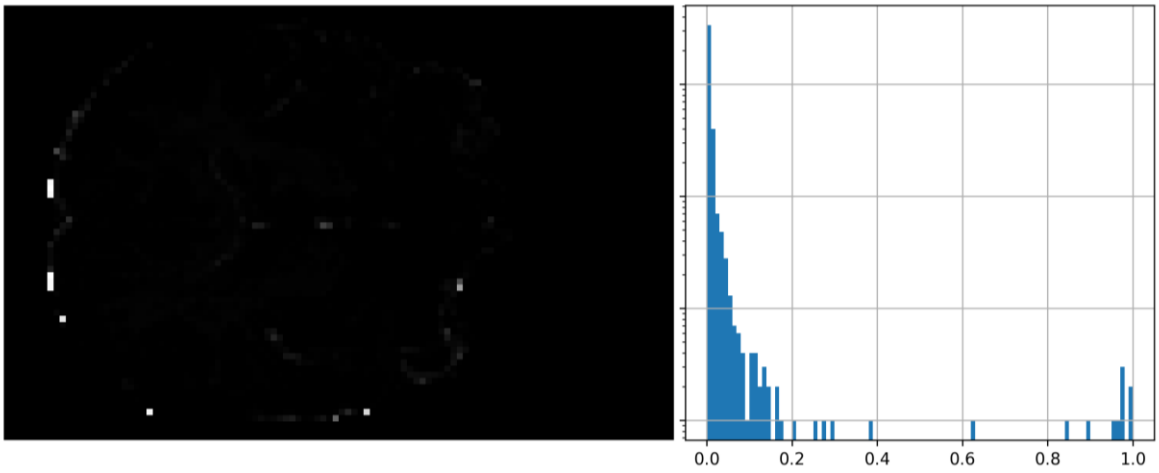

Fig. 4. D_{MLF} parameter plot (left) and its histogram (right). The histogram's y axis is in logarithmic scale

On Fig. 5 four parameter maps are shown. D_{MLF} is already clipped to exclude outliers and improve contrast. However, still D_{MLF} has an unexpectedly wide range of values. In the paper [3] D_{MLF} had a dynamic range of (0, 0.003) while in our case there are many voxels with $D_{MLF} > 0.003$. The reason for this may be different non-linear fitting parameters, because they are not specified in the original paper.

On the other hand, excess kurtosis K provides a good contrast between white matter (WM) and gray matter (GM), which aligns with the results in the paper [3]. Also, the same nearly inverse relationship between K and α can be observed.

Entropy (H) parameters map contrast is rather low, with most values concentrated around 0.7. In [3] the situation is similar for healthy regions of the brain, while the main advantage entropy provides is a

good segmentation of ischemic tissue. Because in our case all patients in the dataset are healthy, entropy may not be that useful, but still, it can help to distinguish some brain tissues.

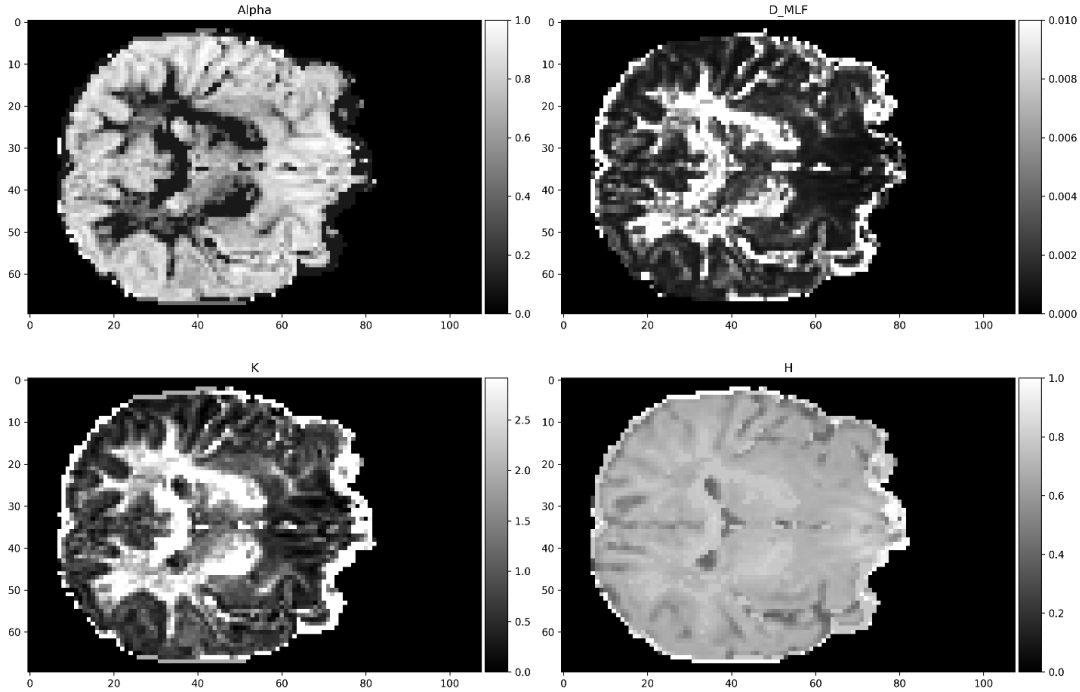

Fig. 5. Resulting parameter maps for MLF model: α, D_{MLF}, excess kurtosis (K), spectral entropy (H)

Comparison with mono-exponential model. To assess the effectiveness of the MLF-based approach, four parameter maps (Fig. 5) were compared with the conventional ADC map (Fig. 6). For this comparison, the DWI signal data from the same slice were also fitted to a mono-exponential model.

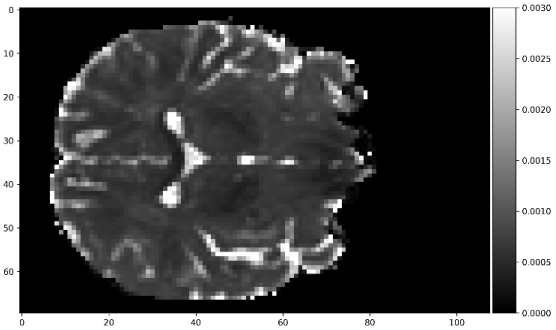

Fig. 6. Resulting ADC parameter map for mono-exponential model

ADC parameters map has worse contrast between WM and GM than K and α of the MLF model. Some similarity with entropy can be observed, regions with lower entropy have higher ADC value. Also, parameter map values are in range from 0 to 0.003 which is expected for classical ADC.

To quantitatively evaluate accuracy of both models Root Mean Squared Error (RMSE) between fitted function and data was computed for each voxel. To exclude outliers with very high errors, 1% of voxels with highest RMSE was ignored. These outliers are probably due to noise in the data, because they are observed with both models. Then average RMSE for all voxels fit with MLF model is 0.03, while for mono-exponential model it is 0.06. Thus, we can confirm that by considering subdiffusion MLF model better fits DWI data. Fig. 7 provides more information on distribution of errors.

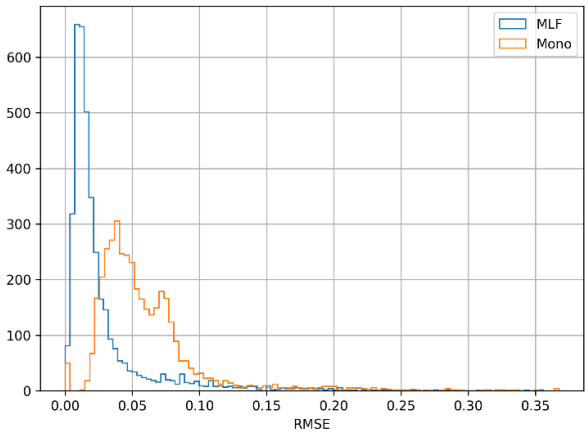

Fig. 7. RMSE histograms for voxels fit to MLF and mono-exponential models

Conclusions

In this study fractional order approach to DWI analysis is investigated. Specifically, a method based on CTRW theory proposed in [3] was implemented and validated on open-access dataset. The main results obtained in this paper are as follows:

• A Python software was developed that implements the discussed method and provides some research tools for conveniently applying it to samples from CDMD dataset and results analysis.

• It was verified that the method can be applied to data from CDMD dataset, and the results were compared with the ones reported in the original paper. They mostly align, except D_{MLF} having too wide dynamic range.

• The results obtained with MLF model were compared with the classical mono-exponential approach. The accuracy of fitting data to each model was evaluated with RMSE and it demonstrated that MLF model has twice lower error than the mono-exponential one (0.03 vs 0.06 respectively).

It is worth noting that these experiments were performed for a single sample from CDMD dataset, therefore one of the future research directions is to repeat this research for the whole dataset. The results of this research provide a baseline that can be used for testing further improvements of an investigated approach. For example, a case when both α and β are changing can be considered.

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ЗАСТОСУВАННЯ МОДЕЛІ ДИФУЗІЇ ДРОБОВОГО ПОРЯДКУ В АНАЛІЗІ ДАНИХ ДИФУЗІЙНО-ЗВАЖЕНОЇ МАГНІТНО-РЕЗОНАНСНОЇ ТОМОГРАФІЇ

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Анотація. У цьому дослідженні розглядається застосування рівняння дифузії дробового порядку для аналізу дифузійно-зваженої магнітно-резонансної томографії (DW-MRI або DWI) з метою валідації та розширення попередніх досліджень на основі відкритого набору даних. Було реалізовано модель дробового порядку з використанням функції Міттага-Леффлера та перевірено її коректність шляхом відтворення результатів, представлених у науковій літературі. Далі метод був застосований до відкритого набору даних Connectome Diffusion Microstructure Dataset (CDMD) для аналізу реальних зображень головного мозку. Отримані карти параметрів показали покращений контраст між білою та сірою речовиною, що підтвердило потенціал моделі для розрізнення властивостей тканин мозку. Ефективність моделі дробової дифузії була порівняна з традиційною моноекспоненційною моделлю, демонструючи вищу точність у відтворенні затухання дифузійного сигналу за критерієм середньоквадратичної похибки (RMSE). Це дослідження встановлює відтворювану базу для майбутніх робіт у галузі моделювання дробової дифузії в МРТ та пропонує розширення дослідження на більші набори даних, а також вдосконалення методів оцінювання параметрів для покращення діагностичних можливостей.

Ключові слова: дробова похідна, дробове рівняння дифузії, аномальна дифузія, функція Міттаг-Леффлера, ентропія, ексцес, Python, MRI, DWI.