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| **Supplementary Table S1** | | | |
| **Block A: Biophysical Models representing Microstructural features** | | | |
| **Biophysical Models** | | **Biophysical Parameters relating Microstructural features** | **Protocol feasibility** |
| (Pasternak *et al.*, 2009) | FWE-DTI | FW, DTensor, FA, MD, AD, RD | Single/Multishell |
| (Zhang *et al.*, 2012) | NODDI | ODI, NDI, fISO | Multishell |
| (Kaden *et al.*, 2016; Kaden, Kruggel and Alexander, 2016) | Spherical Mean Technique (SMT) | SMT\_FA (FA), SMT\_MD, LDC (Longitudinal Diffusion Coefficient), TDC (Transverse DC), Anisotropy Index (FA= LDC/TDC) | Multishell |
| (Palombo *et al.*, 2020) | SANDI (Ball, Stick, Sphere model) | f\_in, f\_ec, f\_is, D\_in, D\_ec, r\_s | Multishell (b-value>3000s/mm2) |
| (Novikov *et al.*, 2018) | Standard Model | f, Da, De\_perp, De\_parallel. | Multishell |
| (Ning, Westin and Rathi, 2015) | SHORE | RTOP, MSD | Multishell |

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| **Supplementary Table S2** | | | | | | | |
| **Block B: diffusion MRI data mapping with AI (ML/DL) agnostic to q-space Geometry** | | | | | | | |
| **AI Models** | | **General architecture** | **Dataset  Total# (Train#:Test#: Validation#)** | **Loss/ Optimizer** | **Total gradient directions (b-vectors)** | **b-value (s/mm2)** | **Task** |
| (Zheng, Zheng, *et al.*, 2022) | AEME | LSTM | HCP Young Adult  **26** (17:2:81); HCP **10** (27:3:70) | MSE/ Adam | 60, 36, 24 | 1000, 2000 | NODDI |
| (Zheng, Sun, *et al.*, 2022) | METSC (Adapted from ViT) | Transformer (Encoder- Decoder) | HCP **26** (17:2:81); Private IVIM **24** (56:6:38) | MSE/ Adam | 60, 36, 24 | ­­1000, 2000 | NODDI |
| (Tian *et al.*, 2022) | SDnDTI | Modified U-net | HCP **20**; HCP in Aging **20** | MAE/ Adam | 186, 93, 18, 12 | 1500, 1500 | dMRI denoising |
| (Karimi and Gholipour, 2022b) | Transformer | Transformer (Attention) | HCP **200** (67:17:17), PING **20 (0:0:100),** VOGM **7 (0:0:100)** | MSE/ Adam | 88 | 1000 | DTI |
| (Karimi and Gholipour, 2022a) | ADL (Atlas powered DL) | U-net++ | Developing HCP **300** (77:0:23) | L2-norm/Adam | FA(88,12,6),ODI(300,30, 12) | FA(1000) ODI( 1000, 2600) | FA, ODI |
| (Jha *et al.*, 2022) | VRfRNet\* | GAN | HCP **30** (80:3:17) | Mixed loss= adversarial+L1+total variational/ Adam | 90, 28, 15, 6 | 1000 | fODF |
| (Reisert *et al.*, 2017) | Bayesian | Bayesian ML | HCP **1** | Rician\_Loglikelihood/NA | HCP (90) | HCP (1000.2000,3000) | Any, NODDI |
| (Ma and Peng, 2021) | IQT with Auto-Encoder | Residual Network | HCP **72** (N/A) | MSE+VGG Loss/ Adam | N/A | 1000 | DTI Super-resolution |
| (Tian *et al.*, 2021) | SRDTI | CNN (3D) | HCP **200** (72:18:10) | L2 Loss/ Adam | 90 | 1000 | DTI Super resolution |
| (Qin *et al.*, 2021) | Multimodal SRqDL | CNN (3D) | HCP-MGH **32** (16:0:84) | MSE/ Adam | 512 | 1000, 3000, 5000, 10000 | NODDI, SMT Super-resolution |
| (Qin *et al.*, 2021) | Super resolved q-space DL (SRqDL) | CNN | HCP-WuMinn **25** (20:0:80); HCP-MGH | MSE/ Adam | 270, 36 | 1000, 2000, 3000 | NODDI |
| (Li *et al.*, 2021) | SuperDTI | U-Net | HCP Young Adult **50** (60:20:20) | MSE/ Adam | 270, 36, 18, 6 | 1000, 2000, 3000 | DTI |
| (Karimi, Jaimes, *et al.*, 2021) | Fetal MRI | CNN + Residual Block | dHCP **102** (80:0:20) | MSE/Adam | 88 | 400, 500, 1000, 2600 | DTI |
| (Tian *et al.*, 2020) | DeepDTI | CNN | HCP WU-Minn-Ox | MSE/ Adam | 90 | 1000 | DTI |
| (Koppers *et al.*, 2019) | SHResNet | CNN + Residual Block | CDMRI Harmonization Challenge **10** (N/A) | MSE/ Adam+SGD | 30 | 1200 | DWI harmonization |
| (Ye, Li and Chen, 2019) | MESC-Net | LSTM | HCP **25** (20:0:80) | MSE/ Adam | 270, 90, 60 | 1000, 2000, 3000 | SMT, NODDI, SHORE |
| (Gibbons *et al.*, 2019) | CNN-NODDI | CNN (2D) | Private **48** (70:18:12) | MAE/ Adam | 128, 64, 24, 8 | 400, 1000, 2000 | NODDI, GFA |
| (Blumberg *et al.*, 2018) | Deeper IQT with RevNet | ML | HCP | RMSE/Adam | 90 | 1000 | DTI super-resolution |
| (Ye, 2017) | MEDN/ PMEDN (Dictionary based learner) | Adapted MLP | HCP **25** (20:0:80) | MSE/ Adam | 270, 60 | 1000, 2000, 3000 | NODDI |
| (Alexander *et al.*, 2017) | IQT | ML (Regression Forest) | HCP **24** (67:0:33), HCP Lifespan **26** (0:0:100), Private **13** | maximize *information gain* at nodes | HCP (270), HCP Lifespan (N/A), Monkey (N/A) | HCP (1000, 2000, 3000), HCP Lifespan (1000, 2500), Monkey (2000, 3000, 9500) | NODDI, SMT |
| (Nedjati-Gilani *et al.*, 2017) | Trained Random Forest | ML (Regression Forest) | Private **4** (N/A) | maximise the *information gain* at nodes | 23, 23, 23, 23 | 1622, 1718, 3611, 4031  (Δ 0.102, 0.412, 0.406, 0.169s) | Permeability |
| (Golkov *et al.*, 2016) | q-DL | MLP | HCP **2** (N/A); Private Datasets **12** (N/A) | MSE/ SGD | 288, 158, 75, 40, 30, 25, 12, 8 | 600, 750, 1070, 1200, 1800, 2400, 3000 | DKI, NODDI |

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| **Supplementary Table S3** | | | | | | | |
| **Block C: AI data mapping with active use of q-space Geometry** | | | | | | | |
| **Models** | | **General architecture** | **Dataset  Total# (Train#:Test#: Validation#)** | **Loss/ Optimizer** | **Total gradient directions (b-vectors)** | **b-value (s/mm2)** | **Task** |
| (Diao and Jelescu, 2023) | ED-RNN | RNN based Encoder- Decoder | HCP **6** (80:10:10); Rat model of Alzheimer’s disease (Tristão Pereira et al., 2021) | MSE/ Adam | 90 | 1000, 2000 | WMTI-Watson |
| (Chen *et al.*, 2022) | HGT (based on TAGCN(Du *et al.*, 2018) + RDT) | Two different stages: GCN and Transformer (Attention) | HCP **21** (48:5:48) | MSE/ Adam | 60, 30 | 1000, 2000 | NODDI |
| (Faiyaz, Uddin and Schifitto, 2022) | HemiHex-MLP | Adapted MLP | Quad 22 Challenge Data **160** (2:3:95) | MSE/ SGD, Adam, RMSprop | 61, 21 | 1000 | DTI |
| (Sedlar *et al.*, 2021) | Spherical CNN\*\* | CNN | HCP **50** (60:20:20) | MSE/ Adam | 270 | 1000, 2000, 3000 | NODDI Super angular resolution |
| (Nath *et al.*, 2021) | Bottleneck DL\* Adapted SHResNet and M-heads(Lee *et al.*, 2015; Koppers *et al.*, 2019) | CNN + Residual Block | HCP **89** (45:27:28) | MSE/ RMSprop | 270, 90 | 1000, 2000, 3000 | DTI, Ball & Stick, IVIM, SMT, NODDI |
| (Karimi, Vasung, *et al.*, 2021) | q-space feature-based MLP | MLP | dHCP **95** (79:0:21) | MSE/ Adam | 88 | 1000 | fODF |
| (Ren *et al.*, 2021) | q-space conditioned DWI Generator | U-Net, GAN | HCP500 **19** (47:5:47) | L1+L2 Loss/ Adam | [253, 270] | 1000, 2000, 3000 | NODDI, SHORE, DKI, fODF |
| (Chen *et al.*, 2020) | GCNN | GCN | BCP **13** (38:0:62) | L1 Loss/ Adam | 144 | 500, 1000, 1500, 2000, 2500, 3000 | NODDI |
| (Lin *et al.*, 2019) | CNN\* | CNN (3D) | HCP **30** (72:8:20) | MSE/ Adam | 270,120, 95, 90, 85, 75, 65, 60, 55, 45, 40, 35, 30, 25, 20 | 1000, 2000, 3000 | fODF |

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| **Supplementary Table S4** | | | | | | | |
| **Block D: Models leveraging AI and Maximum Likelihood Estimation (MLE) frameworks** | | | | | | | |
| **Recent trends in AI models** | | **AI-MLE Integrated architecture** | **Dataset  Total# (Train#:Test#: Validation#)** | **Loss/ Optimizer** | **Total gradient directions (b-vectors)** | **b-value (s/mm2)** | **Task** |
| (Faiyaz *et al.*, 2021, 2022) | DL prior NODDI (DLpN) | Modified MLP initializes MLE | HCP **8** (23:3:75); Private CSVD **16** (11:1:88) | MSE+Rician-Loglikelihood/ Adam | 270, 180, 90 | 1000, 2000, 3000 | Single Shell NODDI |
| (Ting *et al.*, 2022) | DL-MLE | Modified MLP initializes MLE | Private **5** (N/A) | MSE+Rician- Loglikelihood/ (N/A) | 90 | 711, 2855 | NODDI |
| (Sabidussi *et al.*, 2023) | dtiRIM | Modified RNN calculating MLE gradient update | NFG Simulation; | Modified MSE/ Adam | 90, [68, 7] | 1000 | DTI |

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