# Appendix

to the article

## Robust and fast Monte Carlo Markov Chain sampling of diffusion MRI microstructure models

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### 1 MCMC priors

The priors used during MCMC sampling.

| **Parameter** | **Prior** |
|---|---|
| $S_0$ | $U(0, 1 \cdot 10^{10})$ |
| $w_i$ | $U(0, 1)$ |
| $d_{\parallel}$ (or $d$) | $U(3 \cdot 10^{-11}, 1 \cdot 10^{-8})$ |
| $d_{\perp_1}$, $d_{\perp_2}$ | $U(0, 1 \cdot 10^{-8})$ |
| $\theta$, $\phi$ | $U(0, \pi)$ |
| $\psi$ | $U(0, \pi)$ |
| $\kappa$ | $U(0, 2\pi)$ |

Table 1: The priors $p_i(\mathbf{x}_i)$ per model parameter. These priors are combined with the model specific parameters in table 2 to form the complete model priors. For parameter usage and specification see table 3 in the article.

| **Model ($M$)** | **Prior** |
|---|---|
| BallStick_in[$n$], NODDI, CHARMED_in[$n$] | $p_j(\mathbf{x}, M) = 1$ if $\sum_{k=0}^{n-1} \mathrm{w}_k <= 1$, else $p_j(\mathbf{x}, M) = 0$ |
| Tensor, CHARMED_in[$n$] (extra axonal compartment) | $p_j(\mathbf{x}, M) = 1$ if $d > d_{\perp_0} > d_{\perp_1}$, else $p_j(\mathbf{x}, M) = 0$ |

Table 2: The model priors $p_j(\mathbf{x}|M)$ for model $M$. Each of these priors should be interpreted as a boolean, that is, they return a value of 1 if the condition is fulfilled, else they return 0. These priors are combined with the parameter specific priors in table 1 to form the complete model priors.

## 2 MCMC proposal distributions

The default proposal distributions used in MCMC sampling.

| **Parameter** | **Proposal distribution** |
|---|---|
| $S_0$ | $\mathcal{N}(\mathbf{X}_i^{(t)}, 10)$ |
| $w_i$ | $\mathcal{N}(\mathbf{X}_i^{(t)}, 0.01)$ |
| $d$, $d_\parallel$, $d_{\perp_1}$, $d_{\perp_2}$ | $\mathcal{N}(\mathbf{X}_i^{(t)}, 1 \cdot 10^{-10})$ |
| $\psi$ | $\mathcal{N}(\mathbf{X}_i^{(t)}, 0.1) \mod \pi$ |
| $\theta$, $\phi$ | $\mathcal{N}(\mathbf{X}_i^{(t)}, 0.1)$ |
| $\kappa$ | $\mathcal{N}(\mathbf{X}_i^{(t)}, 0.01)$ |

Table 3: The proposal distributions $q_i(\mathbf{X}^{(t+1)^*}|\cdot)$ per model parameter with their default proposal standard deviations. For parameter usage and specification see table 3 in the article.

## 3 Default starting point

The following table lists the default initialization point when not initializing with an Maximum Likelihood Estimator.

| Parameter | Default starting value |
|---|---|
| $S_0$ | $1 \cdot 10^4$ |
| $w_i$ | $0.5$ |
| $d_\parallel$ (or $d$) | $1.7 \cdot 10^{-9}$ |
| $d_{\perp_1}$ | $1.7 \cdot 10^{-10}$ |
| $d_{\perp_2}$ | $1.7 \cdot 10^{-11}$ |
| $\theta$, $\phi$, $\psi$ | $\pi/2$ |
| $\kappa$ | $1$ |

Table 4: The default starting points for the MCMC sampler, used only when the sampler is not initialized with a maximum likelihood estimator.