Computational Modelling for Biomedical Imaging - Coursework 1

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Q1.1.1

From eyeballing the data in fig. 1 we notice that the fit is very poor, especially for the 3 entries where the b-value is 0, having a $\Delta S > 7 * 10^5$. The other entries don't fit the data well either.

The final value of RESNORM (1.2242e+12) is clearly above the kind of value we would normally expect. The fit is poor probably because the search strategy got stuck in a local minima.

The expected value of RESNORM would be given by the formula:

$$E\left[\sum_{i=1}^{33}(X_i - \bar{X}_i)^2\right] = E\left[\sum_{i=1}^{33}\sigma_i^2\right] = 33 * \sigma^2$$

Since sigma is between 5000-6000 this means that $8.25 * 10^8 < RESNORM < 1.188 * 10^9$.

Some of the parameter values we obtain are not sensible. For example, the value of f is negative, meaning that we have negative intra-axonal diffusion, which is not physically possible. The value of S0 is also really high, when in fact it should be around $1.1 * 10^5$.

Q1.1.2

I did the following transformations:

- $S0 \to S0^2$
- $d \to d^2$
- $f \to (1 + e^{-f})^{-1}$ (sigmoid)

This time the algorithm converges to the following parameters: $S0 = 1.132129e + 05, d = 1.534e - 03f = 0.575, \theta = -1.03, \phi = -0.11$ with a RESNORM of 1.33e+09. These parameter values are realistic and give us a RESNORM that is around 1000 times smaller. Note that we this time the starting parameters were changed to more realistic values ($S0 = 1.5e + 05, d = 3e - 03f = 0.5, \theta = 0, \phi = 0$). The reason we gett better parameters and RESNORM is because we introduced the transformations that keep the parameters within reasonable limits and because we used a better starting position.

Q1.1.3

Running the same procedure for gaussian-distributed starting points and for three different pixels gives us the following parameters:

Voxel	S0	d	f	θ	ϕ	GlobalMinCounter(out of 100)
(52,62,25)	1.132e+05	1.534e+03	0.575	2.10	6.17	89
(63,40,18)	1.121e+05	1.829e+03	0.5125	1.19	5.43	83
(50,64,23)	1.214e-05	7.208e-04	0.1955	5.05	5.02	87

GlobalMinCounter represents the number of times the global minimum was found was found. We are quite confident that those are the global minimums, since we made sure that the covariance of the gaussian distribution from which we sample the starting position is large enough to cover a wide area of the space. If we consider the probability p of finding the global minimum in one run, then after k runs the probability of **not** having found the global minimum would be $(1 - p)^k$ where k is the number of runs. Then, the minimum number of runs in order to be 95% confident that we will find the global minimum is $\arg\min_k 0.05 > (1 - p)^k$. Since $p \approx 0.86$ then $k = 2$, meaning that 2 runs are enough to be 95% confident.

Q1.1.4

The maps for $S0$, d, f, $RESNORM$ and the fibre direction n are shown in figures 2a, 2b, 3a, 3b and 4 respectively.

Q1.1.5

I implemented the DTI model and used the following mappings to get to the parameters of the BallStick model:

1. $d = mean(D)$, $f = 0.5(|\lambda'_1 - \lambda'_2| + |\lambda'_1 - \lambda'_3| + |\lambda'_2 - \lambda'_3|)$ where $\lambda'_i = \lambda_i/(\lambda_1 + \lambda_2 + \lambda_3)$ for $i \in 1..3$
2. $d = tr(D)/3$, f as above
3. $d = max(D)$, $f = 0.5((\lambda'_1 - \lambda'_2)^2 + (\lambda'_1 - \lambda'_3)^2 + (\lambda'_2 - \lambda'_3)^2)$, for λ'_i as above

The most efficient was method 1, for which the global minimum was found in approximatively 93/100 runs. The parameters I got using method 1 are:$S0 = 1.13184e + 05$, $Dxx = 0.00125$, $Dxy = -0.00013$, $Dxz = -0.00053$, $Dyy = 0.00043$, $Dyz = 0.00011$ and $Dzz = 0.000782$ with a $RESNORM = 1.4458e + 09$.

Q1.1.6

The computation time for `fmincon` is around 9x slower when compared to `fminunc` (averaged over 100 trials, `fmincon`=6.68sec, `fminunc`=56.28sec). Nevertheless, the global minimum is almost always found by both functions (87/100 runs). The parameters and $RESNORM$ it converges to are the same as in Q1.1.2.

Q1.1.7

Q1.1.8

Q1.2.1

The histogram of $p(x|A)$ along with the 2σ and 95% ranges are shown for parameters $S0$, d and f in figures 5, 6 and 7 respectively. These have been computed for the voxel (52,62,25). Parameter estimates for various other voxels are given in table 1. A better visualisation[1] of the parameter intervals for $S0$, d and f is given in figures 8, 9, 10. The 2σ and 95% confidence ranges all agree with each other and have roughly the same mean. In table 1 all voxels have similar ranges for $S0$, however voxel (70,64,14) has different ranges for d and f, probably because it is a CSF or gray matter voxel. In figures 8, 9, 10 we notice that the 2σ range is always smaller than the 95% confidence interval, for all parameters.

Q1.2.2

The 2σ and 95% confidence ranges for MCMC are given in figures 8, 9, 10. Ranges reported by MCMC have the same mean as the ranges generated by the parametric bootstrap, but they are larger, suggesting that MCMC covers a larger parameter space.

[1] plot contains two other methods apart from parametric bootstrap: MCMC and Laplace

Q1.2.3

I only managed to implement Laplace's method.

Q1.3.1

The parameters that I found are: $S0 = 0.9231$, $d = 1.1355e-09$, $f = 0.49$, $\theta = 4.704$, $\phi = 0.038$ with a $RESNORM = 3.8681$. The predicted signal is plotted against the measurements in figure 11. The parameters have been found by applying `fmincon` for reveral rounds of 100 times, with random starting positions sampled from a gaussian distribution with mean μ. Parameter vector μ was updated at each iteration with the global minimum found in the previous round.

Q1.3.2

For fitting these models I decided to switch to `fminunc` because it is faster and slightly more efficient at finding the global minimum. For the Zeppelin-Stick model I actually made implementations with both functions and realised that for the same starting position, `fminunc` was converging to better parameters and $RESNORM$ than `fmincon`. The fit for these models can be visualised in figures 12, 13 and 14. The best model was the Zeppelin-Stick, with a $RESNORM = 1.1784$, followed by Zeppelin-Stick with tortuosity, Ball-stick and DTI having $RESNORMS$ of 2.1337, 3.8681 and 20.5832 respectively. The main reason the Zeppelin-Stick model outperforms the others is because it is more general than ZeppelinStick with tortuosity and Ball-Stick, having more parameters. It is therefore expected to perform at least as good as the others.

Q1.3.3

	Zeppelin-Stick	Zeppelin-Stick Tort	Ball-Stick	Diffusion Tensor
AIC	750	1345	2427	12878
BIC	785	1375	2452	12913

The AIC and BIC scores show that the Zeppelin-Stick model is the one performing best (having the lowest scores), followed by Zeppelin-Stick with tortuosity, Ball-Stick and DTI. AIC and BIC rankings are consistent across the models.

Q1.4.1

Q1.4.2

Images

Q1.1.1

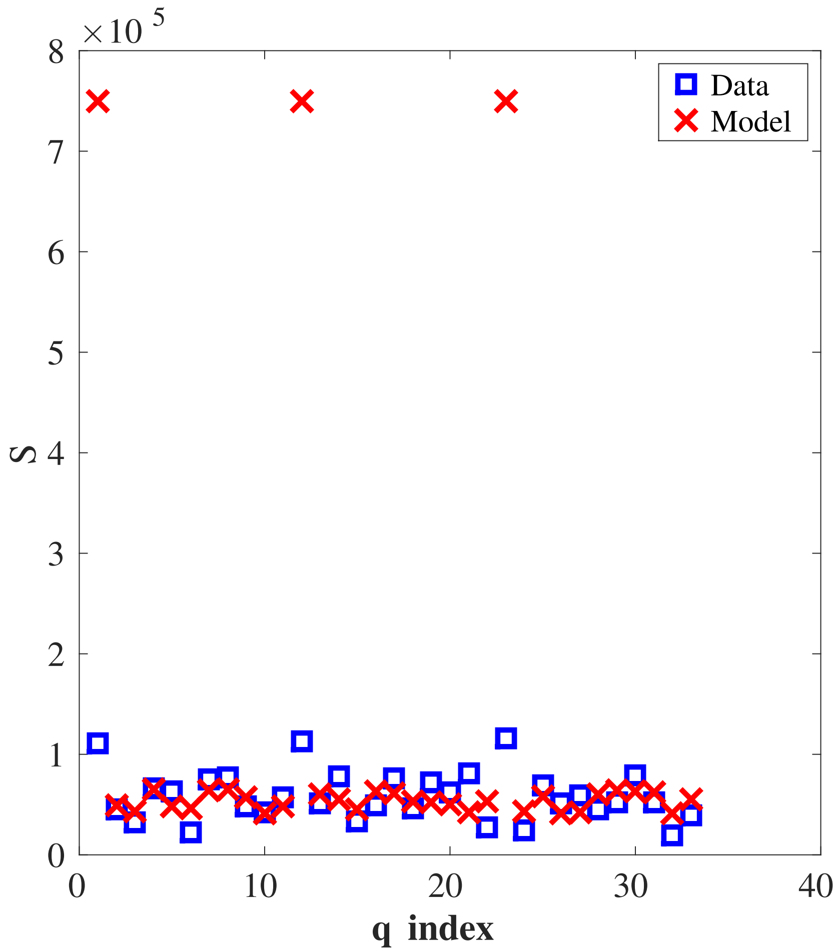
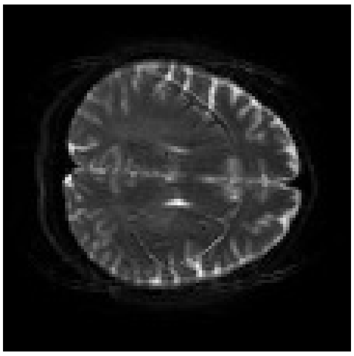
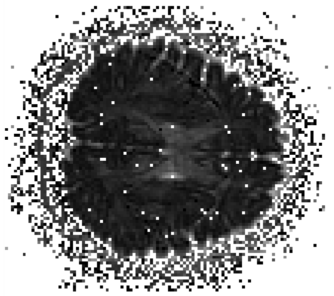


Figure 1: Estimated of the Ball-Stick model for the voxel at position $(52, 62, 25)$

Q1.1.4

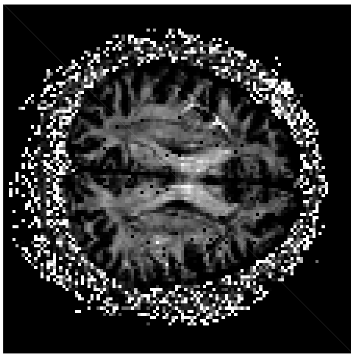


(a) $S0$ map

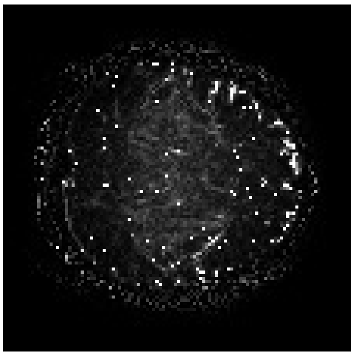


(b) D map

Figure 2



(a) F map



(b) $RESNORM$ map

Figure 3

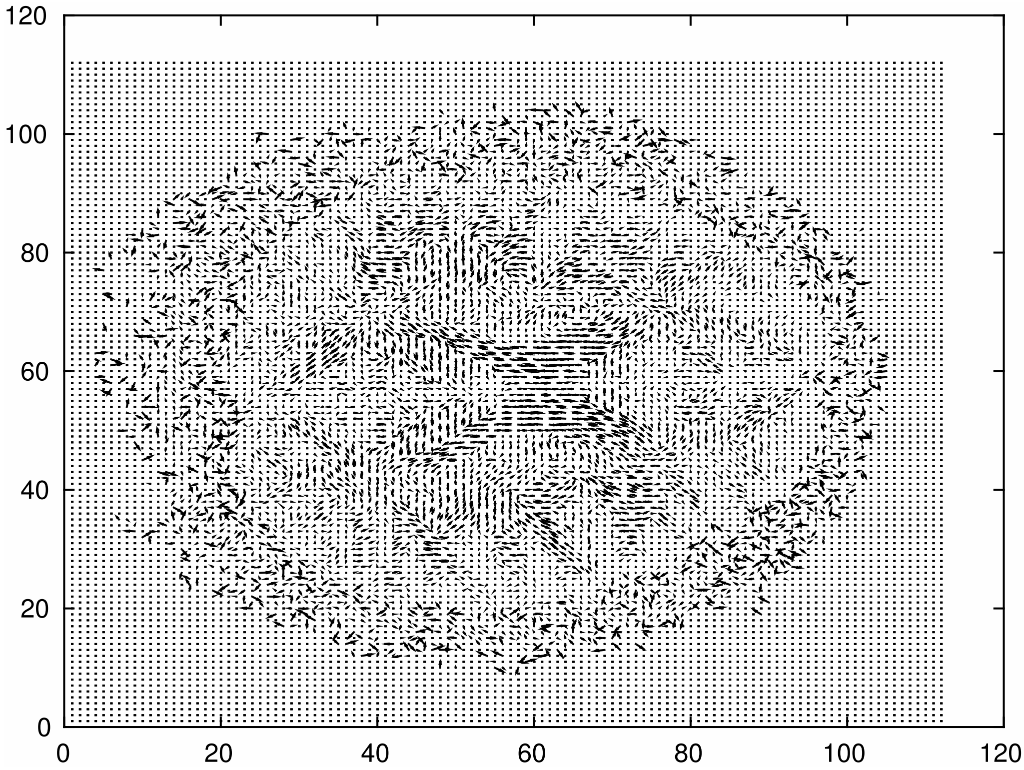


Figure 4: Fibre direction map

Q1.2.1

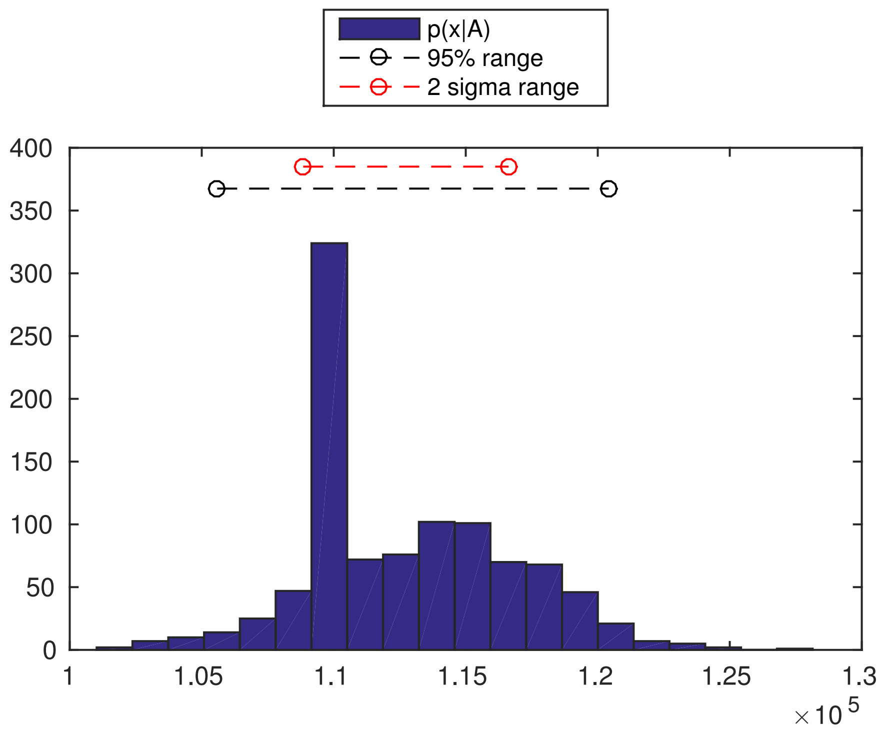


Figure 5: Parametric bootstrap for $S0$ using voxel (52,62,25)

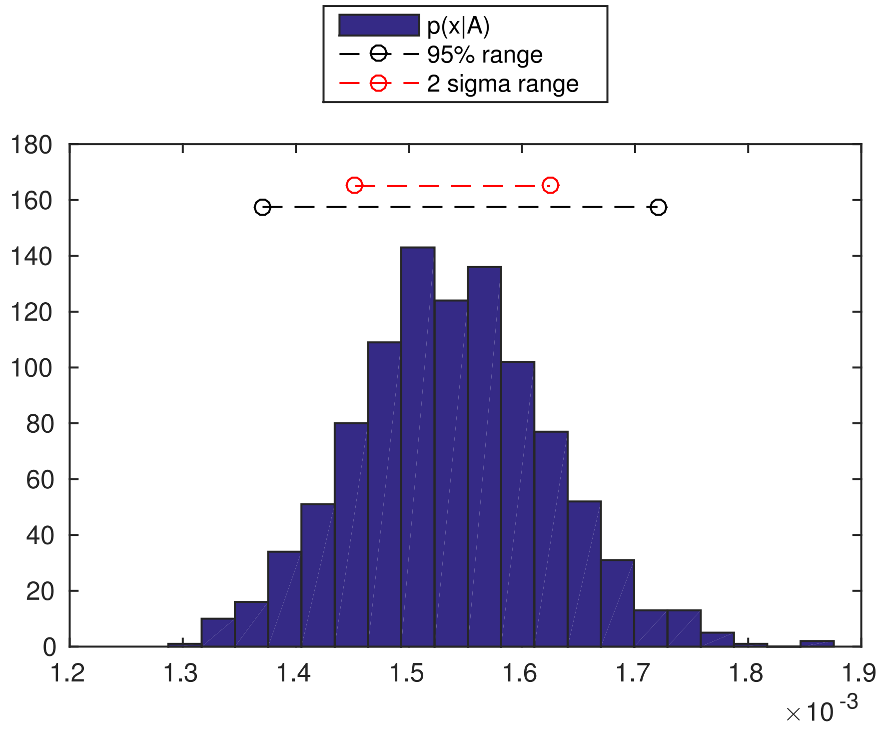


Figure 6: Parametric bootstrap for d using voxel (52,62,25)

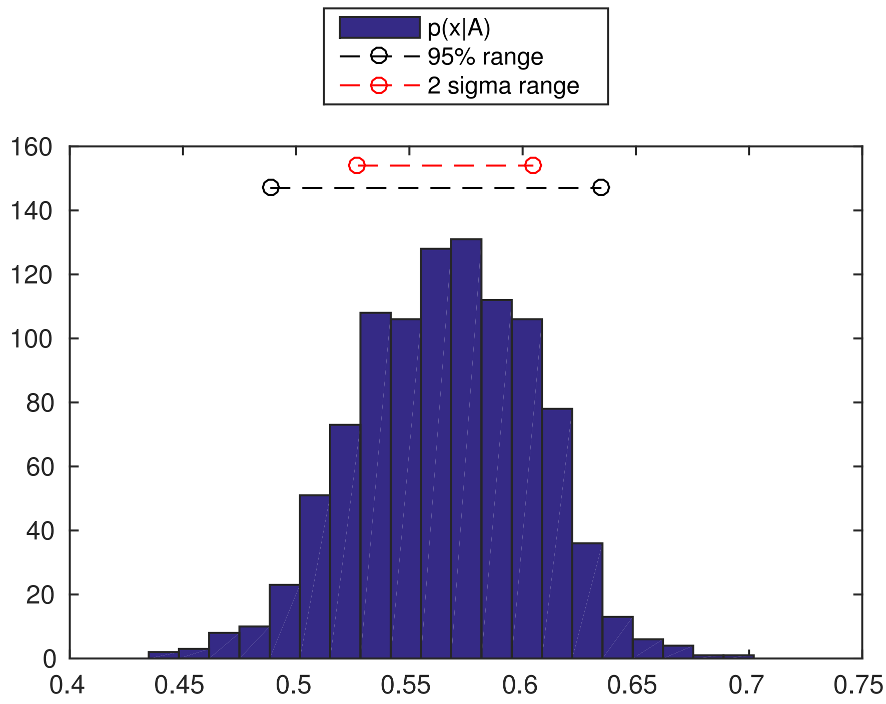


Figure 7: Parametric bootstrap for f using voxel (52,62,25)

2-sigma ranges

Voxel	$S0$		d		f	
(52,62,25)	1.088e+05	1.166e+05	1.452e-03	1.624e-03	0.527	0.604
(63,40,18)	1.017e+05	1.229e+05	1.026e-03	1.397e-03	0.136	0.326
(70,64,14)	1.022e+05	1.112e+05	7.584e-04	8.928e-04	0.078	0.185

95% confidence intervals

(52,62,25)	1.055e+05	1.204e+05	1.370e-03	1.719e-03	0.488	0.634
(63,40,18)	0.918e+05	1.330e+05	0.870e-03	1.608e-03	0.000	0.404
(70,64,14)	0.976e+05	1.152e+05	6.888e-04	9.507e-04	0.000	0.231

Table 1: 2-sigma and 95% confidence intervals for voxel (52,62,25) using Parametric bootstrap

Q1.2.2 & Q1.2.3

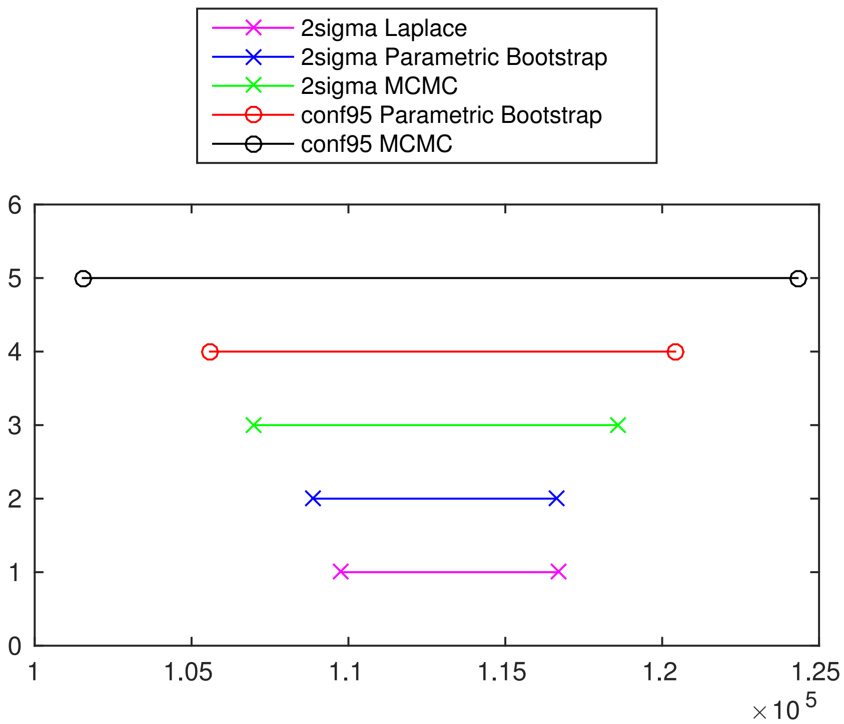


Figure 8: 2σ and 95% confidence intervals on parameter $S0$ using three different methods: parametric bootstrap, MCMC and Laplace. Voxel used was (52,62,25)

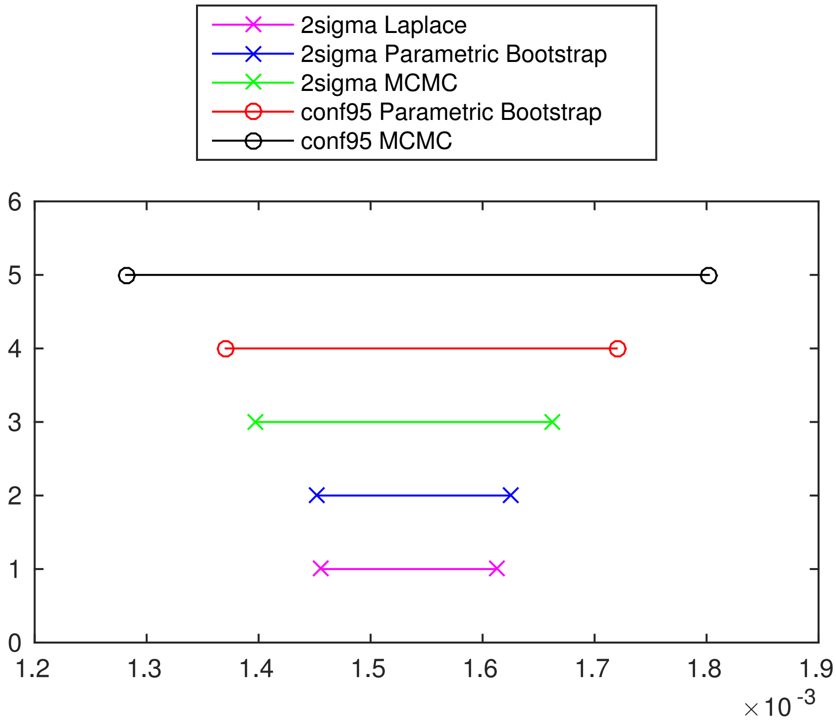


Figure 9: 2σ and 95% confidence intervals on parameter d using three different methods: parametric bootstrap, MCMC and Laplace. Voxel used was (52,62,25)

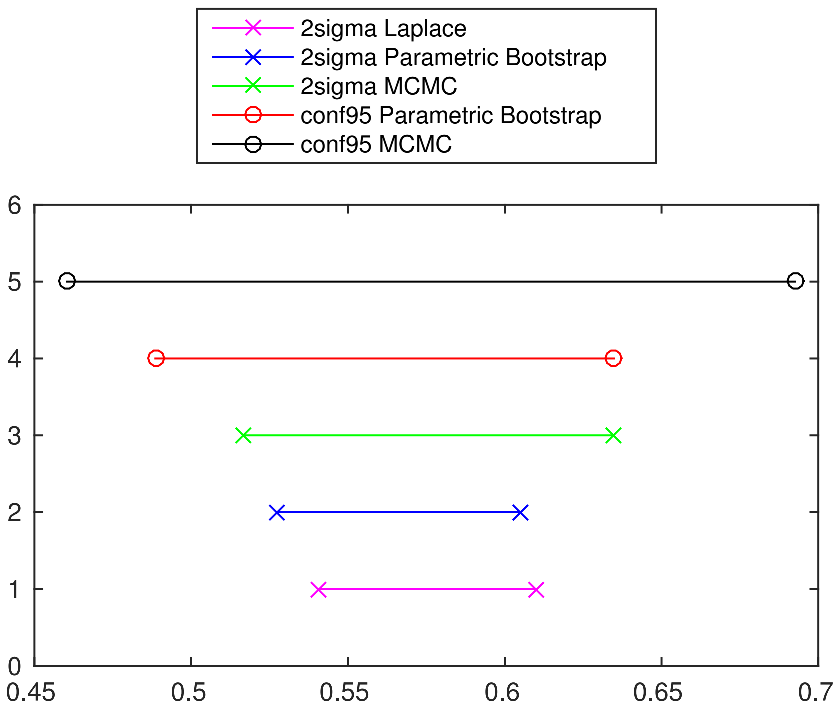


Figure 10: 2σ and 95% confidence intervals on parameter f using three different methods: parametric bootstrap, MCMC and Laplace. Voxel used was (52,62,25)

Q1.3.1

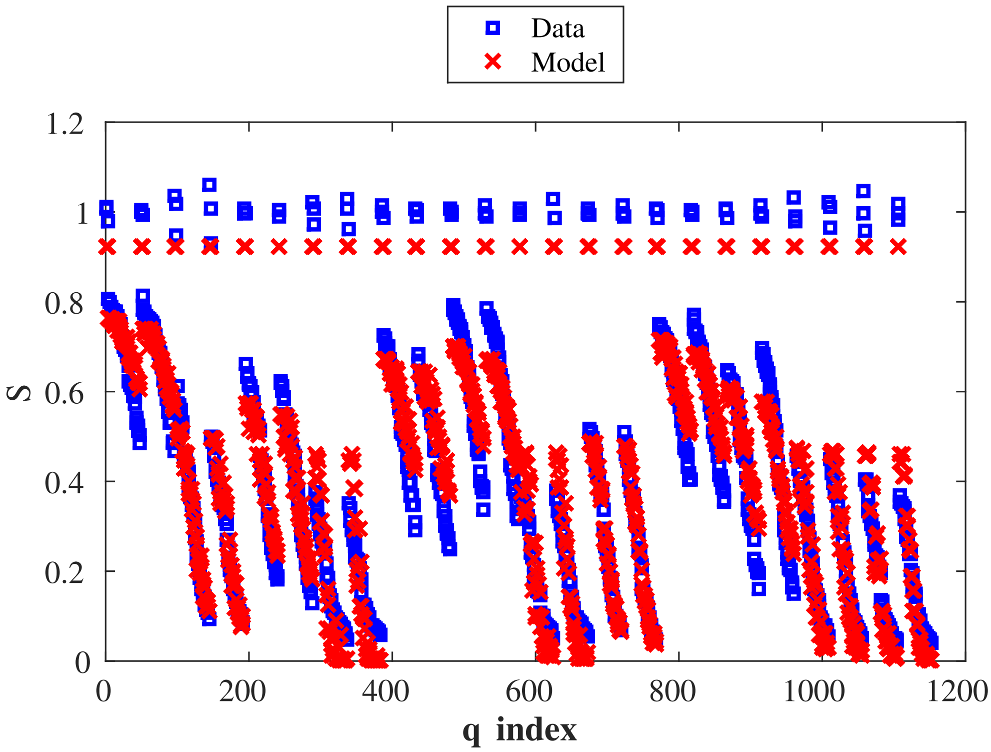


Figure 11: Estimated fit for the Ball-Stick model for the given voxel. RESNORM=3.8681

Q1.3.2

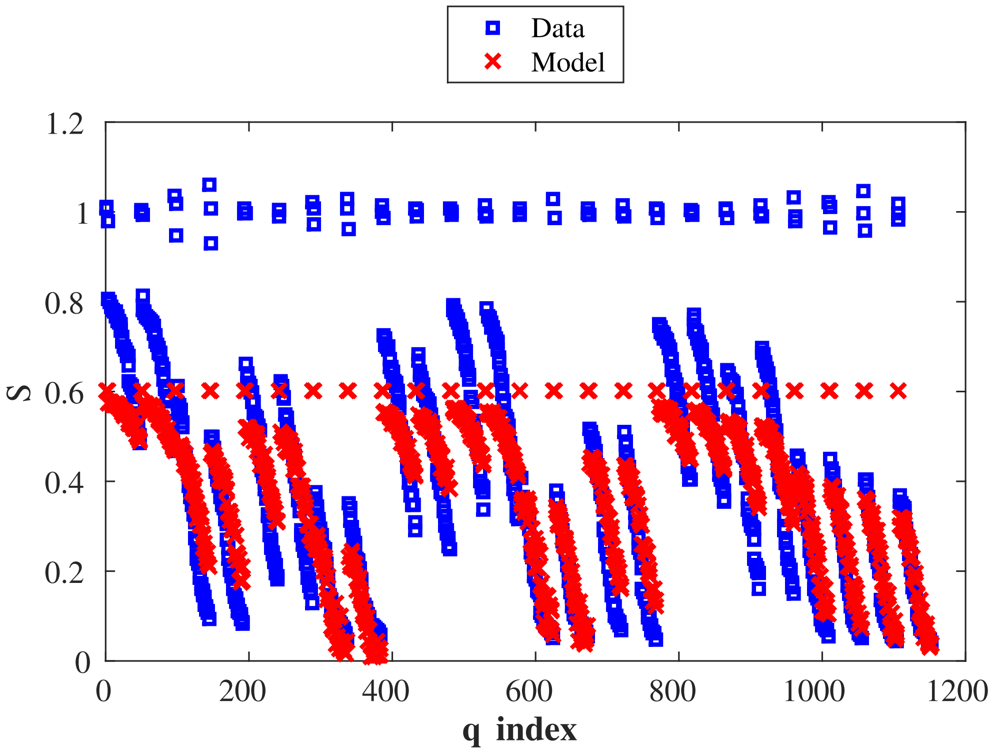


Figure 12: Estimated fit for Diffusion Tensor model for the given voxel. RESNORM=20.5832

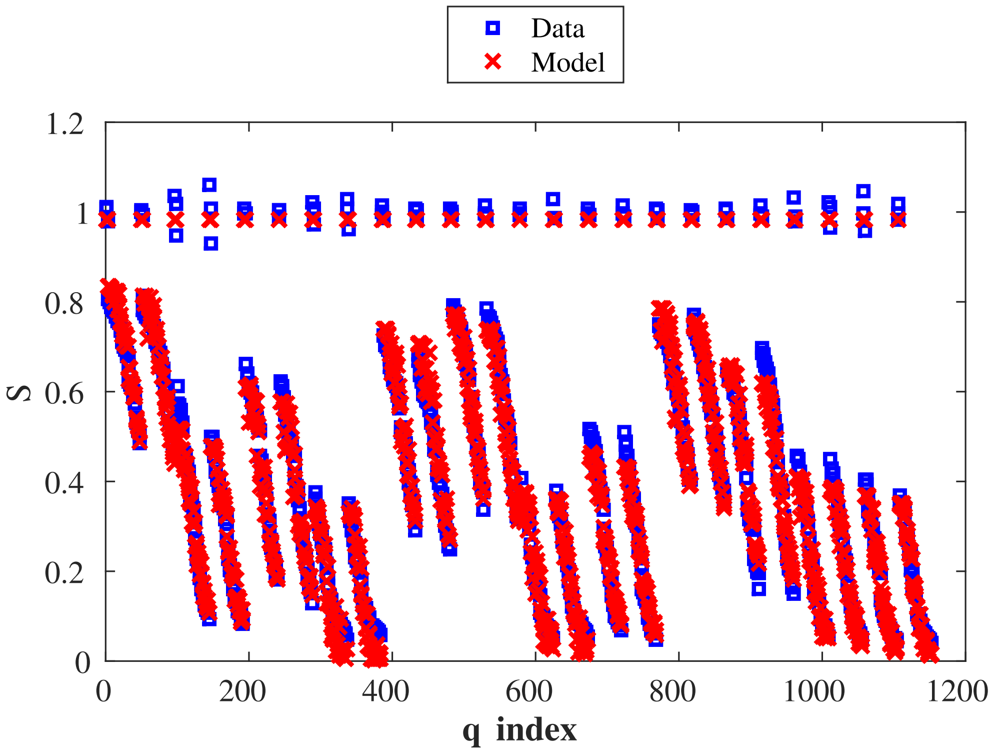


Figure 13: Estimated fit for Zeppelin-Stick model for the given voxel. RESNORM=1.1784

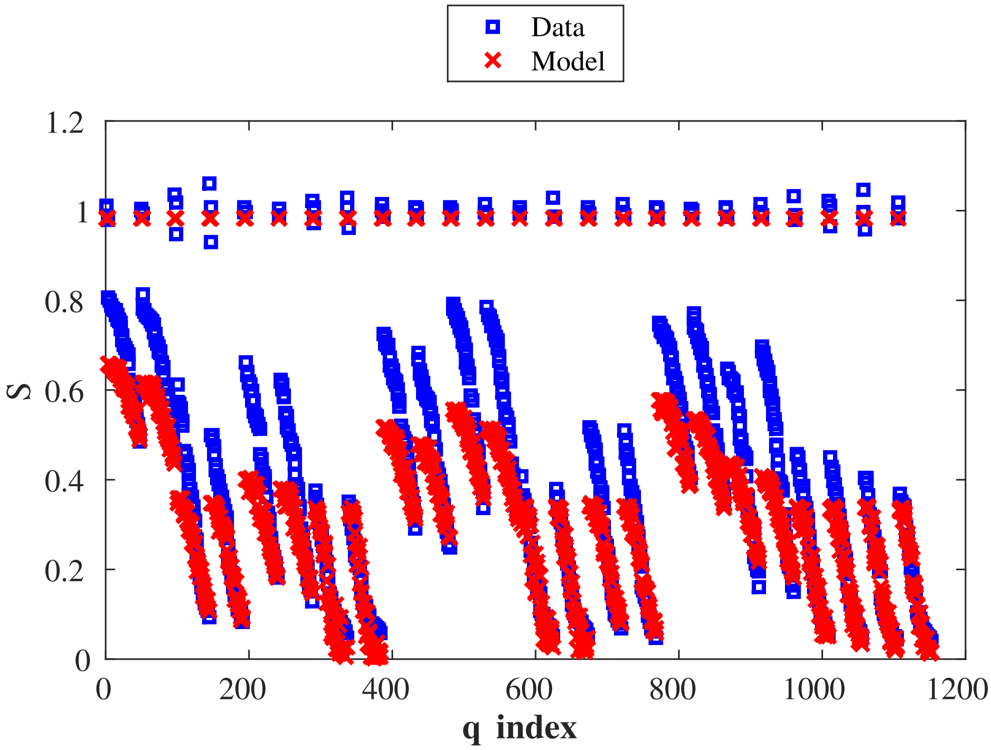


Figure 14: Estimated fit for Zeppelin-Stick with tortuosity model for the given voxel. RESNORM=2.1337