COMP0118: Coursework 1

Mingzhou Hu

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Note:

All the figures referenced in this report are in another file(Figure.pdf).

Q1.1.1

We can know that from the Figure Q1.1.1, the fit is not very good. The average of actual signal is $(2.352 \pm 0.938) \times 10^3$ units, while the average of predicted signal in this case is $(2.361 \pm 0.772) \times 10^3$ units.The expected value of RESNORM should be $108 \times \sigma^2(200^2) = 4.32 \times 10^6$ units, however, the actual value of RESNORM in this case is 2.88×10^7 units. The actual value of RESNORM is quite larger than the expected value, so this is a poor fitting. The parameter values we obtained in this case are: $S0 = 3.520 \times 10^3, diff = -4.979 \times 10^{-6}, f = 1.201 \times 10^2, theta = 0.887, phi = 1.557$. The value of S0 is physically realistic, so it is sensible. The value of diff is not sensible, because it is negative. The value of f is out of [0,1], so it is not sensible. The values of theta and phi are sensible.

Q1.1.2

I used following transformation method to allow only physically realistic settings of the parameters:$S0 \rightarrow S0^2, diff \rightarrow diff^2, f \rightarrow \frac{1}{1+e^{-f}}$, theta and phi do not need constraints. The final parameter values we obtained in the case are: $S0 = 4.258 \times 10^3, diff = 1.141 \times 10^{-3}, f = 0.357, theta = -0.981, phi = 0.579$. It is clear that the values are sensible, since S0 and diff are positive and f is in [0,1]. From Figure Q1.1.2, we can see that the fit is better than that in Q1.1.1. The actual RESNORM in this case is 5.87×10^6 units, which is closer than that in Q1.1.1. The reason is that we use transformation to keep the parameters physically realistic and constraining the search space close to the global minimum.

Q1.1.3

The fitting procedure repeats for 1000 times from different starting points in this case, the proportion that we find the solution with the smallest value of RESNORM(5.872×10^6) is in 83.9% of trials. We consider that the probability p is finding the global minimum in one trial, so 1-p is not finding the global minimum in one trial. we need to be 95% sure we find the global minimum, so $1-(1-p)^n \geq 0.95$. Now we know that p=0.839 and n must be a positive integer, so n is 2, which means 2 runs we need to be 95% sure we find the global minimum. I tried another voxel(83,56,92) and found that the result is similar to that of above voxel. The propotion is 84.1% and runs are still 2.

Q1.1.4

In order to create parameter maps over one slice of the image volume, we need to repeat the fitting procedure in each voxel of the slice. Firstly, we need to compute the global minimum for each voxel. According to the calculation in Q1.1.3, we can compute that we need at least 5 times to find the global minimum for each voxel. The maps of S0, d, f and RESNORM are shown in Figure Q1.1.4(S0), Q1.1.4(d), Q1.1.4(f) and Q1.1.4(RESNORM) and the maps of fibre direction and coherent fibre direction are shown in Figure Q1.1.4(fd) and Q1.1.4(cfd). The comments for each figure are in Figures.pdf file.

Q1.1.6

The computation time of fmincon function is faster than that of fminunc function. They are 0.1500 seconds and 0.2300 seconds respectively. However, the values of parameters and RESNORM(5.872×10^6) are same in these two cases.

Q1.1.8

The formula to compute the sum of square differences in Rician noise model is: $sumRes = \sum_{i=1}^{N} \frac{(A_i - \sqrt{S_i^2 + \sigma^2})^2}{\sigma^2}$, N is the number of measurement(108) in the signal, A is actual signal, S is predicted signal and sigma(200) is the standard deviation of the noise.
I used fminunc function to run the fitting procedure. We can see that from Figure Q1.1.8 the fit is related good in this case and very similar to Q1.1.2. The parameter estimates($S0 = 4.253 \times 10^3, diff = 1.150 \times 10^{-3}, f = 0.358, theta = -8.443, phi = -8.846$) are not affected by this new implementation, which are quite similar to those in Q1.1.2. However, the computation time is quite faster than that in Q1.1.2, which are 0.0800 seconds and 0.2300 seconds respectively. The RESNORM in this case is 146.823 units.

Q1.2.1

The formula to estimate a noise parameter is: $\sigma^2 = \frac{1}{K-N} \sum_{k=1}^{K} R_k^2$, K is the number of measurements(108), N is the number of parameters(5) and R is Residuals(RESNORM). The procedure of parametric bootstrap repeats for 5000 times. The Figure Q1.2.1(S0), Q1.2.1(d) and Q1.2.1(f) show the histogram of $p(x \mid A)$ along with 2σ and 95% ranges for S0, d and f respectively. From these figures, we found that 2σ range is always a bit bigger than 95% range for all parameters in this case. The 2σ ranges for S0, d and f are $[4.144 \times 10^3, 4.369 \times 10^3]$,

[1.067×10^{-3}, 1.221×10^{-3}] and [0.314, 0.405] respectively. The 95% ranges for S0, d and f are [4.146×10^3, 4.367×10^3], [1.071×10^{-3}, 1.221×10^{-3}] and [0.315, 0.403] respectively. I tried another voxel(56,39,48) and found that from Figure Q1.2.1(S0)(2), Q1.2.1(d)(2) and Q1.2.1(f)(2) the ranges for S0, d and f are very different from voxel(92,65,72). Voxel(56,39,48) has higher S0, but lower diffusivity and f value, the reason may be that the position is in some gyrus.

Q1.2.2

The formula to compute acceptance ratio is: $e^{\frac{oldRESNORM - newRESNORM}{2\times sigma^2}}$. The 2σ and 95% ranges for MCMC are given in Figure Q1.2.2(S0), Q1.2.2(d) and Q1.2.2(f). From these figures, we can see that the ranges for MCMC are a bit smaller than those parametric bootstrap, it means that MCMC covers a smaller parameter space. However, according to fact, MCMC should cover larger parameter space.

Q1.2.3

For Laplace's method, diagonal elements provide 2σ range and σ is in the diagonal of Hessian. Hessian can returned during fitting procedure by using fminunc function. The 2σ and 95% ranges for Laplace are given in Figure Q1.2.3(S0), Q1.2.3(d) and Q1.2.3(f). The range for S0 is smaller than that for parametric bootstrap and MCMC, while the ranges for d and f are larger than those for parametric bootstrap and MCMC.

Q1.3.1

We repeat the fitting procedure in Q1.1.2 and Q1.1.3 and we can see from Figure Q1.3.1 that the fit is quite good. The best parameters we obtained in the case are: $S0 = 1.005, diff = 3.784 \times 10^{-2}, f = 0.302, theta = -4.738, phi = 3.058$ and RESNORM is 15.106. We we find the solution with the smallest value of RESNORM(15.106) is 95.2%, so one trial is enough to be 95% sure we find the global minimum.

Q1.3.2

For zeppelin and stick model, we need two more parameters λ_1 and λ_2 ($\lambda_1 > \lambda_2$). We can see from Figure Q1.3.2(zs) that the fit is good. The min RESNORM here is 8.2893 and we find the solution with the smallest value of RESNORM(8.2893) is 10%. For zeppelin and stick with tortuosity model, we also need two more parameters λ_1 and λ_2 ($\lambda_2 = (1-f)\lambda_1$). The Figure Q1.3.2(zst) shows that the fit is good. The min RESNORM here is 11.5939 and we find the solution with the smallest value of RESNORM(11.5939) is only 6%. The Figure Q1.3.2(dt) shows that the result using diffusion tensor model and it seems like the fit is not good. The min RESNORM here is 53.7948 and we find the solution with the smallest value of RESNORM(53.7948) is 10%. In my opinion, zeppelin and stick model is the best model with smallest RESNORM, followed by ball and stick model and zeppelin and stick with tortuosity model, and the last one is diffusion tensor model.

Q1.3.3

The equation to compute AIC is: $AIC = 2N + Klog(K^{-1}\sum_{k=1}^{K}(S_k - A_k)^2)$, and the equation to compute BIC is: $BIC = NlogK + Klog(K^{-1}\sum_{k=1}^{K}(S_k - A_k)^2)$, K is the number of measurements(3612), N is the number of parameters and standard deviation of noise is 0.04 in this case. For ball and stick model, AIC=9.4513×10^3 and BIC=9.4822×10^3. For zeppelin and stick model, AIC=2.9138×10^4 and BIC=2.9191×10^4. For zeppelin and stick with tortuosity model, AIC=2.9146×10^4 and BIC=2.9183×10^4. We found from the results that the values for AIC and BIC are very similar. In this case, the best model is ball and stick model with the smallest values for AIC and BIC, and the results of another two model are very similar. The results show that the ranking from each criterion is not consistent.

Q1.3.4

We can see from Figure Q1.3.4 that the fit is good with ball and two stick model. The min RESNORM here is 11.7357 and we find the solution with the smallest value of RESNORM(11.7357) is 21%. As for the min RESNORM, the zeppelin and stick model is better than ball and two stick model, while as for the probability to find the global minimum, ball and two stick model is better than other models but worse than ball and stick model.

Q1.4.1

The Fisher information matrix with best parameters is below:

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[   251478.6,  -3177470.0,    204344.1, -22.59793,  1333.381]
[ -3177470.0,  1.326482e9, -21025022.0,   3073.03, -15464.94]
[   204344.1, -21025022.0,   2078105.0, -244.3286,  14760.42]
[  -22.59793,     3073.03,   -244.3286,   12437.0,  902.6487]
[   1333.381,   -15464.94,    14760.42,  902.6487,  4048.619]
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