COMP0118 Coursework 1: Parametric Models

1.1 Parameter Estimation and Mapping

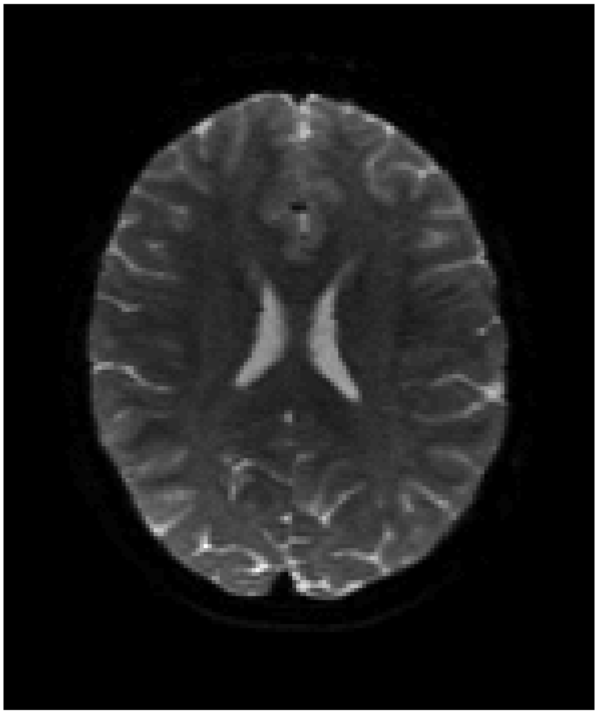
Load and Inspect Data

I first load the data from the file `data.mat`.

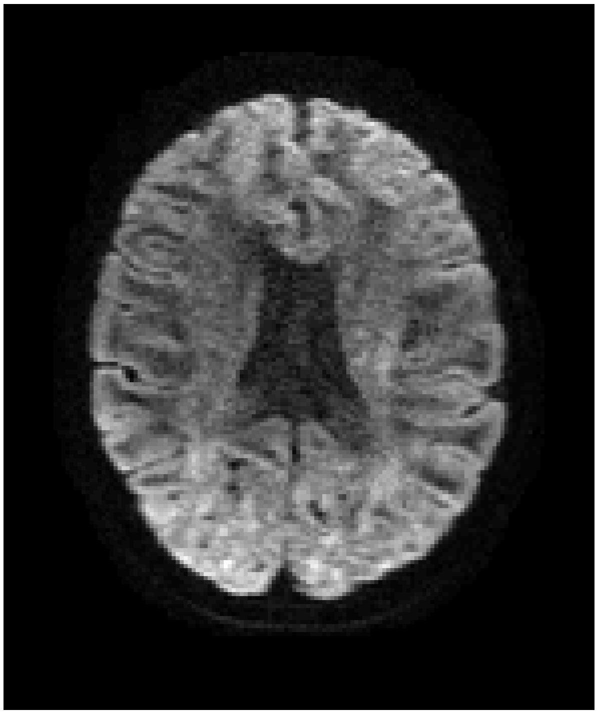
```
%loading data into matlab
load('data_p1/data.mat');
dwis = double(dwis);
dwis=permute(dwis, [4, 1, 2, 3]);
```

I now display a single image slice to check that the image has been loaded correctly.

```
% middle slice of the 1st image volume, had b=0
imshow(flipud(squeeze(dwis(1, :, :, 72))'), []);
```



```
% Middle slice of the 2nd image volume, which has b=1000
imshow(flipud(squeeze(dwis(2,:,:,72))'), []);
```



Next, I load the gradient directions stored in the file bvecs.

```
qhat = load('data_p1/bvecs');
% and the bvalue array
bvals = 1000*sum(qhat.*qhat);
```

Core Questions

Q1.1.1 - Implementing linear diffusion tensor estimation and using it to map the mean diffusivity and fractional anisotropy over one slide of an image.

Perform fitting for a single voxel

```
% Select a single voxel
Avox = dwis(:, 92, 65, 72);

% Create the design matrix
G = [ones(1, 108); -bvals.*qhat(1, :).^2; -2*bvals.*qhat(1,:).*qhat(2,:); -2*bvals.*qha

% Compute parameter vector x
x = G\log(Avox);
```

Perform for all voxels

```
% Store diffusion tensor mapping here
dt_map72 = zeros(7, 145, 174);

% Precompute the design matrix
G = [ones(1, 108); -bvals.*qhat(1, :).^2; -2*bvals.*qhat(1,:).*qhat(2,:); -2*bvals.*qha

% Repeat process for every voxel in slice
tic;
for i=1:145
    for j=1:174
        % Select voxel
        Avox = dwis(:, i, j, 72);

        if min(Avox) > 0
            % Compute x
            dt_map72(:, i, j) = G \ log(Avox);
        end
    end
end
toc;

md_map72 = zeros(145, 174);
fa_map72 = zeros(145, 174);
cmap72 = zeros(145, 174, 3);

% Create the mean diffusivity map using dt_map72
for i=1:145
    for j=1:174

        % Select params for voxel
        x = dt_map72(:, i, j);

        % Get diffusion tensor
        D = [[x(2) x(3) x(4)]; [x(3) x(5) x(6)]; [x(4) x(6) x(7)]];

        % Compute eigenvectors and eigenvalues of D
        [V, L] = eig(D);
        Lbar = trace(L)/3;

        % Compute mean diffusivity
        md = (x(2, :) + x(5, :) + x(7, :)) / 3;
        md_map72(i, j) = md;

        % Compute fractional anisotropy map
        numerator = 0;
        denominator = 0;
        for k=1:3
            numerator = numerator + (L(k, k) - Lbar)^2;
            denominator = denominator + L(k, k)^2;
        end
        fa = sqrt((3/2) * numerator/denominator);
        fa_map72(i, j) = fa;
```

```
        % Find principal eigenvector
        [max_eigenval, idx] = max(diag(L));
        principal_e = V(:, idx);
        cmap72(i, j, :) = fa * abs(principal_e);
    end
end

% Visualize mean diffusion, fractional anisotropy and color maps
figure
imshow(flipud(md_map72'), [])
figure
imshow(flipud(fa_map72'), [])
figure
imshow(flipud(permute(cmap72, [2, 1, 3])), [])
```

Q1.1.2 - Implement Ball-and-stick model to measure the density of axon fibres, indirectly, in each voxel.

First, I implement the Ball and stick model for a single voxel.

```
% Select a single voxel
Avox = dwis(:,92,65,72);

% Define a starting point for the non-linear fit
startx_noisy = [3.5e+00 3e-03 2.5e-01 0 0];

% Define various options for the non-linear fitting
% algorithm.
h=optimset('MaxFunEvals',20000,...
 'Algorithm','quasi-newton',...
 'TolX',1e-10,...
 'TolFun',1e-10);

% Now run the fitting
[parameter_hat,RESNORM,~,~]=fminunc('BallStickSSD',startx_noisy,h,Avox,bvals,qhat);

format short e
parameter_hat
RESNORM
```

Now I implement the model on all voxels of the middle slice.

```
% Store fitted parameters for each voxel here
fitted_params_unconstrained_model = zeros(145, 174, 5);

tic;
for i=1:145
    for j=1:174
        % Select a single voxel
```

```
        Avox = dwis(:,i,j,72);

        if min(Avox) > 0
            % Define a starting point for the non-linear fit
            startx_noisy = [3.5e+00 3e-03 2.5e-01 0 0];

            % Define various options for the non-linear fitting
            % algorithm.
            h=optimset('MaxFunEvals',20000,...
             'Algorithm','quasi-newton',...
             'TolX',1e-10,...
             'TolFun',1e-10);

            % Now run the fitting
            [parameter_hat,RESNORM,~,~]=fminunc('BallStickSSD',startx_noisy,h,Avox,bval

            % Store parameter values in parameter_hat
            fitted_params_unconstrained_model(i, j, :) = parameter_hat;
        end
    end
end
toc;
```

Evaluating the results by comparing the MRI signal predicted using the fitted parameter model result with the true signal values.

```
% Select results for the middle voxel
Avox = dwis(:, 92, 65, 72);
[S, SSD] = BallStickEval(fitted_params_unconstrained_model(92, 65, :), Avox, bvals, qha

% Plotted predicted values vs true values
figure
set(gcf, 'Position', [10, 10, 900, 500])
plot(Avox, ' bs', 'MarkerSize', 16, 'LineWidth', 4);
hold on;
plot(S, ' rx', 'MarkerSize', 16, 'LineWidth', 4);
xlabel('q index');
ylabel('S');
legend('Data','Model');
xlim([0,110]);
title(sprintf('Comparison of Model predicted signal S (red) and true measurement in Avo
```

Q1.1.3 - Adapt the implementation from 1.1.2 using the transformation method with `fminunc` to allow for only realistic settings of parameters.

Implement on a single voxel

```
% Select a single voxel
Avox = dwis(:,92,65,72);
```

```
% Define a starting point for the non-linear fit
startx_noisy = [sqrt(3.5e+00) sqrt(3e-03) sqrt(-log(2.5e-01)) 0 0];

% Define various options for the non-linear fitting
% algorithm.
h=optimset('MaxFunEvals',20000,...
 'Algorithm','quasi-newton',...
 'TolX',1e-10,...
 'TolFun',1e-10);

% Now run the fitting
[parameter_hat,RESNORM,EXITFLAG,OUTPUT]=fminunc('BallStickSSD_transformation',startx_nc

% Transform parameters back to original values
parameter_hat(:, 1) = parameter_hat(:, 1)^2;
parameter_hat(:, 2) = parameter_hat(:, 2)^2;
parameter_hat(:, 3) = exp(-1 * parameter_hat(:, 3)^2);

format short e
parameter_hat
RESNORM
```

Implement for all voxels

```
% Store fitted params for transformation model here
fitted_params_transformation_model = zeros(145, 174, 5);

tic;
for i=1:145
    for j=1:174
        % Select a single voxel
        Avox = dwis(:,i,j,72);

        if min(Avox) > 0
            % Define a starting point for the non-linear fit
            startx_noisy = [sqrt(3.5e+00) sqrt(3e-03) sqrt(-log(2.5e-01)) 0 0];

            % Define various options for the non-linear fitting
            % algorithm.
            h=optimset('MaxFunEvals',20000,...
             'Algorithm','quasi-newton',...
             'TolX',1e-10,...
             'TolFun',1e-10);

            % Now run the fitting
            [parameter_hat,RESNORM,EXITFLAG,OUTPUT]=fminunc('BallStickSSD_transformatic

            % Transform parameters back to original values
            parameter_hat(:, 1) = parameter_hat(:, 1)^2;
            parameter_hat(:, 2) = parameter_hat(:, 2)^2;
            parameter_hat(:, 3) = exp(-1 * parameter_hat(:, 3)^2);
```

```
            % Store parameter values in parameter_hat
            fitted_params_transformation_model(i, j, :) = parameter_hat;
        end
    end
end
toc;
```

Evaluating the results by comparing the MRI signal predicted using the fitted parameter model result with the true signal values.

```
% Select results for the middle voxel
Avox = dwis(:, 92, 65, 72);
[S, SSD] = BallStickEval(fitted_params_transformation_model(92, 65, :), Avox, bvals, qh

% Plotted predicted values vs true values
figure
set(gcf, 'Position', [10, 10, 900, 500])
plot(Avox, ' bs', 'MarkerSize', 16, 'LineWidth', 4);
hold on;
plot(S, ' rx', 'MarkerSize', 16, 'LineWidth', 4);
xlabel('q index');
ylabel('S');
legend('Data','Model');
xlim([0,110]);
title(sprintf('Comparison of Model predicted signal S (red) and true measurement in Avo
```

Q1.1.4 - Perform experiments now with many different starting points to assess if we really have converged to global minimum.

```
n_runs = 100;
% Store errors per run here
errors_per_run = zeros(1, n_runs);

% Select a single voxel
i = 100;
j = 80;
Avox = dwis(:,i,j,72);

% Visualize where it is in the brain
figure
imshow(flipud(squeeze(dwis(1, :, :, 72))'), []);
axis on;
hold on;
plot(92, 65, 'r+', 'MarkerSize', 10, 'LineWidth', 2);
plot(72, 95, 'g+', 'MarkerSize', 10, 'LineWidth', 2);
plot(52, 88, 'b+', 'MarkerSize', 10, 'LineWidth', 2);
plot(100, 110, 'c+', 'MarkerSize', 10, 'LineWidth', 2);
plot(60, 50, 'm+', 'MarkerSize', 10, 'LineWidth', 2);
plot(72, 47, 'y+', 'MarkerSize', 10, 'LineWidth', 2);
```

```
plot(60, 120, 'w+', 'MarkerSize', 10, 'LineWidth', 2);
% plot(100, 80, 'w+', 'MarkerSize', 10, 'LineWidth', 2);

n = 1;
while n <= n_runs

    % Define a starting point for the non-linear fit
    startx = [3.5e+00 3e-03 2.5e-01 0 0];

    % Add gaussian noise to each of parameters
    startx_noisy(:, 1) = startx(:, 1) + 1e+03*randn;
    startx_noisy(:, 2) = startx(:, 2) + 1e-03*randn;
    while any(startx_noisy(:, 1:2) < 0)
        startx_noisy(:, 1) = startx(:, 1) + 1e+03*randn;
        startx_noisy(:, 2) = startx(:, 2) + 1e-03*randn;
    end
    startx_noisy(:, 3) = startx(:, 3) + 1e-01*randn;
    while startx_noisy(:, 3) > 1 || startx_noisy(:, 3) < 0
        startx_noisy(:, 3) = startx(:, 3) + 1e-01*randn;
    end
    startx_noisy(:, 4) = startx(:, 4) + 1e-01*randn;
    startx_noisy(:, 5) = startx(:, 5) + 1e-01*randn;

    % Perform inverse transformation on first three parameters
    startx_noisy(:, 1:2) = sqrt(startx_noisy(:, 1:2));
    startx_noisy(:, 3) = sqrt(-log(startx_noisy(:, 3)));

    % Define various options for the non-linear fitting
    % algorithm.
    h=optimset('MaxFunEvals',20000,...
     'Algorithm','quasi-newton',...
     'TolX',1e-10,...
     'TolFun',1e-10, 'Display', 'off');

    % Now run the fitting
    try
        [parameter_hat,RESNORM,EXITFLAG,OUTPUT]=fminunc('BallStickSSD_transformation',s
    catch
        continue;
    end

    % Perform transformation back on parameters
    parameter_hat(:, 1) = parameter_hat(:, 1)^2;
    parameter_hat(:, 2) = parameter_hat(:, 2)^2;
    parameter_hat(:, 3) = exp(-parameter_hat(:, 3)^2);

    % Store
    errors_per_run(:, n) = RESNORM;

    n = n + 1;
end
```

Plot the errors per run

```
figure
plot(n_runs)
hold on;
plot(errors_per_run)
xlabel('Iterations')
ylabel('Error')
title('Errors on every iteration')
```

```
% Find proportion of trials with smallest value of RESNORM
min_error = min(errors_per_run)
count = 0;
tolerance = 0.1;
for n=1:n_runs
    if (errors_per_run(n) - min_error <= tolerance)
        count = count + 1;
    end
end

proportion = count / n_runs

% proportion = p(the run will find a global min) = p
% p(atleast 1 global min in n runs) = 1 - p(no global min in N runs)
% 0.95 = 1 - nC0*p^0*(1-p)^n
n_runs = log(0.05)/log(1-proportion)
```

Q1.1.5 - Create parameter maps over image slice for S0, d, f and RESNORM. Also Create a fibre direction map.

```
% Select 72nd image slice
image = dwis(:, :, :, 72);

% Compute feature maps for this slice
parameter_maps = createParameterMaps(image, bvals, qhat, 10);
```

```
% Select parameter maps
S0_map72 = parameter_maps(:, :, 1);
d_map72 = parameter_maps(:, :, 2);
f_map72 = parameter_maps(:, :, 3);
theta_map72 = parameter_maps(:, :, 4);
phi_map72 = parameter_maps(:, :, 5);
RESNORM_map72 = parameter_maps(:, :, 6);

% Visualize the feature maps
figure
imshow(flipud(S0_map72'), [])

figure
imshow(flipud(d_map72'), [])
```

```
figure
imshow(flipud(f_map72'), [])

figure
imshow(flipud(RESNORM_map72'), [])

% compute fibre direction map
figure
set(gcf, 'Position', [10, 10, 450, 500])
fibredir_map72 = zeros(145, 174, 2);
for i=1:145
    for j=1:174
        fibredir_map72(i, j, :) = f_map72(i, j) .* [cos(theta_map72(i, j))*sin(theta_ma
    end
end
quiver(flipud(fibredir_map72(:, :, 1)'), flipud(fibredir_map72(:, :, 2)'))
```

```
Unrecognized function or variable 'finBestFit'.

Error in generateDataSet (line 14)
            [parameter_hat, ~] = finBestFit(3, Avox, bvals, qhat);
Warning: NEWFF used in an obsolete way.
          See help for NEWFF to update calls to the new argument list.

net =

    Neural Network

              name: 'Custom Neural Network'
          userdata: (your custom info)

    dimensions:

         numInputs: 1
         numLayers: 2
        numOutputs: 1
    numInputDelays: 0
    numLayerDelays: 0
 numFeedbackDelays: 0
 numWeightElements: 1145
        sampleTime: 1

    connections:

       biasConnect: [1; 1]
      inputConnect: [1; 0]
      layerConnect: [0 0; 1 0]
     outputConnect: [0 1]

    subobjects:

             input: Equivalent to inputs{1}
            output: Equivalent to outputs{2}

            inputs: {1x1 cell array of 1 input}
            layers: {2x1 cell array of 2 layers}
           outputs: {1x2 cell array of 1 output}
            biases: {2x1 cell array of 2 biases}
      inputWeights: {2x1 cell array of 1 weight}
      layerWeights: {2x2 cell array of 1 weight}

    functions:
```

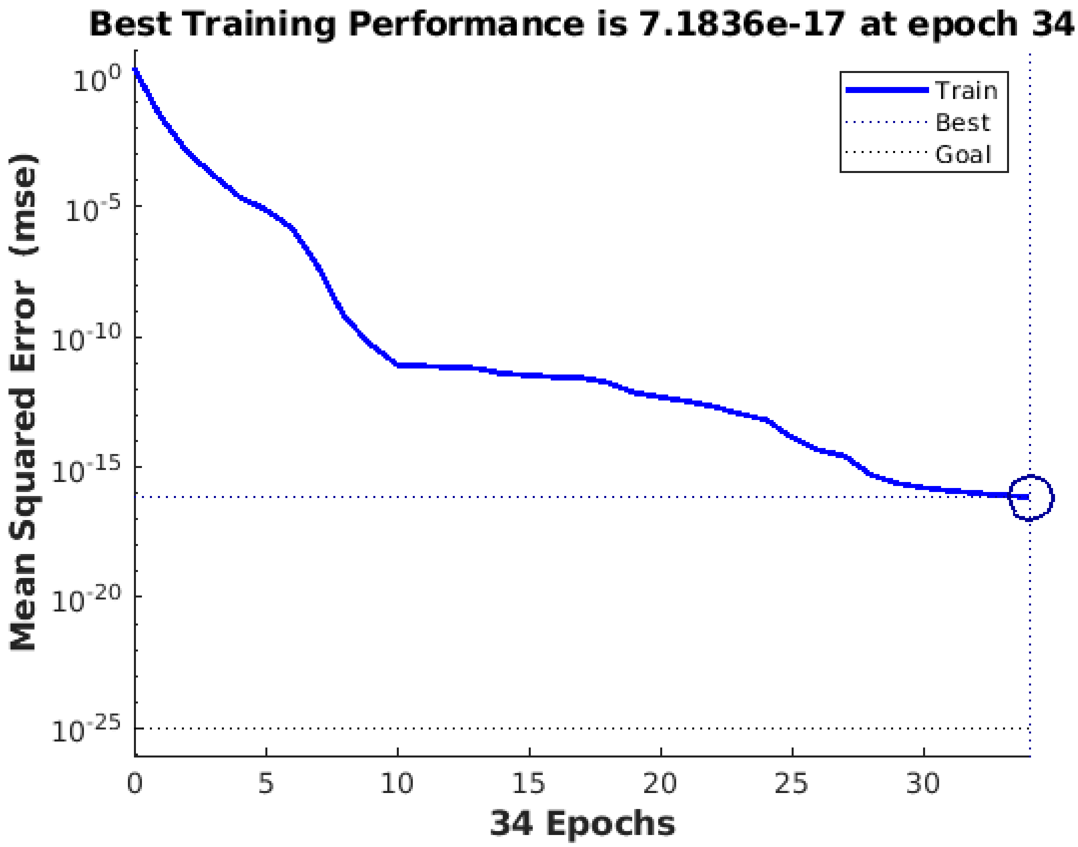
```
      adaptFcn: 'adaptwb'
    adaptParam: (none)
      derivFcn: 'defaultderiv'
     divideFcn: (none)
   divideParam: (none)
    divideMode: 'sample'
       initFcn: 'initlay'
    performFcn: 'mse'
  performParam: .regularization, .normalization
      plotFcns: {'plotperform', 'plottrainstate',
                'plotregression'}
    plotParams: {1x3 cell array of 3 params}
      trainFcn: 'trainlm'
    trainParam: .showWindow, .showCommandLine, .show, .epochs,
                .time, .goal, .min_grad, .max_fail, .mu, .mu_dec,
                .mu_inc, .mu_max, .lr

weight and bias values:

            IW: {2x1 cell} containing 1 input weight matrix
            LW: {2x2 cell} containing 1 layer weight matrix
             b: {2x1 cell} containing 2 bias vectors

methods:

         adapt: Learn while in continuous use
     configure: Configure inputs & outputs
        gensim: Generate Simulink model
          init: Initialize weights & biases
       perform: Calculate performance
           sim: Evaluate network outputs given inputs
         train: Train network with examples
          view: View diagram
   unconfigure: Unconfigure inputs & outputs
```




```
net =

    Neural Network

              name: 'Custom Neural Network'
          userdata: (your custom info)

    dimensions:

         numInputs: 1
         numLayers: 2
        numOutputs: 1
    numInputDelays: 0
    numLayerDelays: 0
 numFeedbackDelays: 0
 numWeightElements: 1145
        sampleTime: 1

    connections:

       biasConnect: [1; 1]
      inputConnect: [1; 0]
      layerConnect: [0 0; 1 0]
     outputConnect: [0 1]

    subobjects:

             input: Equivalent to inputs{1}
            output: Equivalent to outputs{2}

            inputs: {1x1 cell array of 1 input}
            layers: {2x1 cell array of 2 layers}
           outputs: {1x2 cell array of 1 output}
            biases: {2x1 cell array of 2 biases}
```

```
      inputWeights: {2x1 cell array of 1 weight}
      layerWeights: {2x2 cell array of 1 weight}

    functions:

          adaptFcn: 'adaptwb'
        adaptParam: (none)
          derivFcn: 'defaultderiv'
         divideFcn: (none)
       divideParam: (none)
        divideMode: 'sample'
           initFcn: 'initlay'
        performFcn: 'mse'
      performParam: .regularization, .normalization
          plotFcns: {'plotperform', 'plottrainstate',
                    'plotregression'}
        plotParams: {1x3 cell array of 3 params}
          trainFcn: 'trainlm'
        trainParam: .showWindow, .showCommandLine, .show, .epochs,
                    .time, .goal, .min_grad, .max_fail, .mu, .mu_dec,
                    .mu_inc, .mu_max, .lr

    weight and bias values:

                IW: {2x1 cell} containing 1 input weight matrix
                LW: {2x2 cell} containing 1 layer weight matrix
                 b: {2x1 cell} containing 2 bias vectors

    methods:

             adapt: Learn while in continuous use
         configure: Configure inputs & outputs
            gensim: Generate Simulink model
              init: Initialize weights & biases
           perform: Calculate performance
               sim: Evaluate network outputs given inputs
             train: Train network with examples
              view: View diagram
       unconfigure: Unconfigure inputs & outputs

y = 5×1
10^-10  ×
   -0.1387
   -0.3083
    0.3747
    0.0654
   -0.4293
ans = 5×1
     0
     0
     0
     0
     0
Error using bsxfun
Non-singleton dimensions of the two input arrays must match each other.

Error in gsubtract>calc_general (line 40)
    c = bsxfun(@minus,a,b);

Error in gsubtract>calc_cell (line 60)
  for i=1:numel(a), c{i} = calc_general(a{i},b); end

Error in gsubtract (line 24)
  c = calc_cell(a,b);
```

```
Error in nncalc.perform (line 17)
e = gsubtract(t,y);

Error in network/perform (line 33)
perf = nncalc.perform(net,t,y,ew,net.performParam);
```

```
[trainX, trainY] = generateDataSet(dwis, bvals, qhat);
```

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Index in position 4 exceeds array bounds (must not exceed 1).

Error in generateDataSet (line 10)
        Avox = dwis(:, i, j, 72);
```

1.2 Confidence and Uncertainty

Core Questions:

Q1.2.1 - Using parametric bootstrap to estimate 2-sigma range and 95% range for S0, d and f in ball-and-stick model.

```
% Select a voxel
Avox = dwis(:, 70, 90, 72); floor()
format short e
% Generate bootstrap samples
bootstrap_samples = PBootstrap(Avox, bvals, qhat, 10, 1000);
```

```
k = 100×100
    90  -114    93   -49   145   -77  -129   188   -80    33    91    48    15 ...
    30    71  -110  -210    78   -16   153     3    -4   -29    57    66   -37
  -196  -125    48    69   -95    22  -290  -112    41    42  -217   -46  -157
   -52   120    39    61    64   -17   -53   227  -201   -42  -117   261  -135
   194   125   -26   -87    60    51   150  -124  -253    -6  -100  -121   -20
   -58  -192    79    38   113   -63   -86    12   -83    -4    44   -37   -21
     2   114    54   159   -78    87   145    -5    40    64  -162   -69   -70
   -95    35    57    60    14   -90    66   128    44   137   -73    69    14
   208    96    18    64   -59    51     0  -118   -92    79  -157     0   113
   -60  -213  -109   -81   -51    -4   259  -143   153    50    13     7   -29
     ⋮
Index in position 1 is invalid. Array indices must be positive integers or logical values.

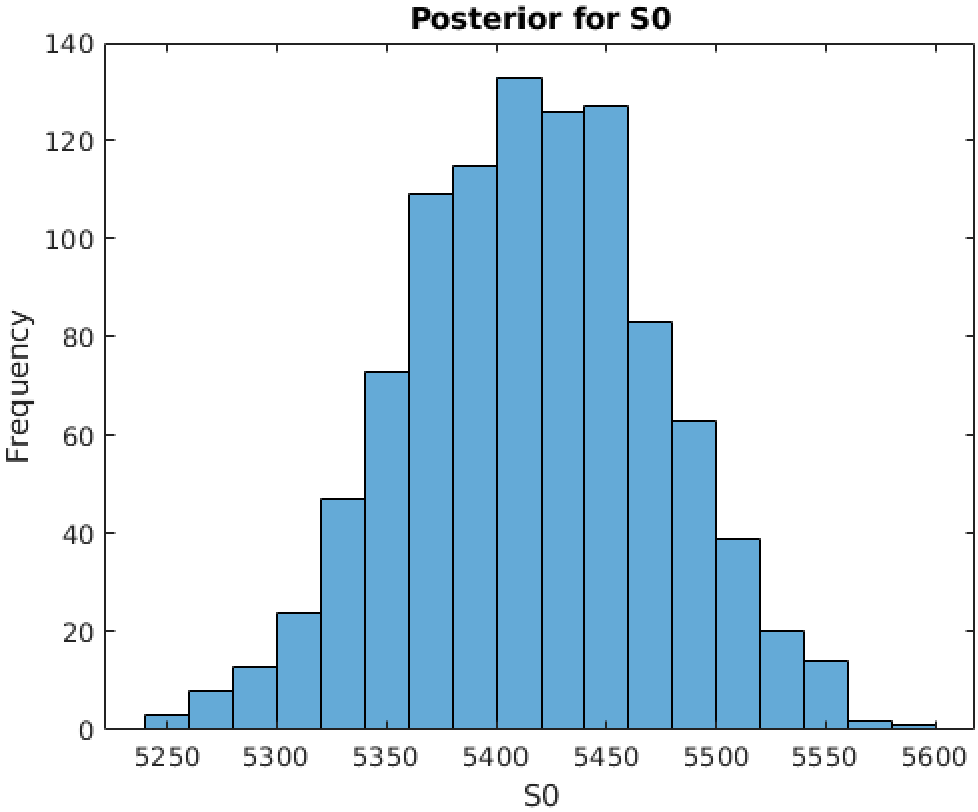
Error in ClassicBootstrap (line 28)
    Ahat = Avox(k, :);
```

Plot histograms of each parameter

```
bootstrap_samples_sorted = sort(bootstrap_samples, 2, 'ascend');

figure;
histogram(bootstrap_samples(1, :));
```

```
xlabel('S0');
ylabel('Frequency');
title('Posterior for S0');
hold on;
```




```
two_sigma_range_S0_high = mean(bootstrap_samples(1,:)) + 2*std(bootstrap_samples(1,:))
```

```
two_sigma_range_S0_high =
   5.5323e+03
```

```
two_sigma_range_S0_low = mean(bootstrap_samples(1,:)) - 2*std(bootstrap_samples(1,:))
```

```
two_sigma_range_S0_low =
   5.2996e+03
```

```
ninety_five_percent_range_S0_high = bootstrap_samples_sorted(1, ceil(length(bootstrap_s
```

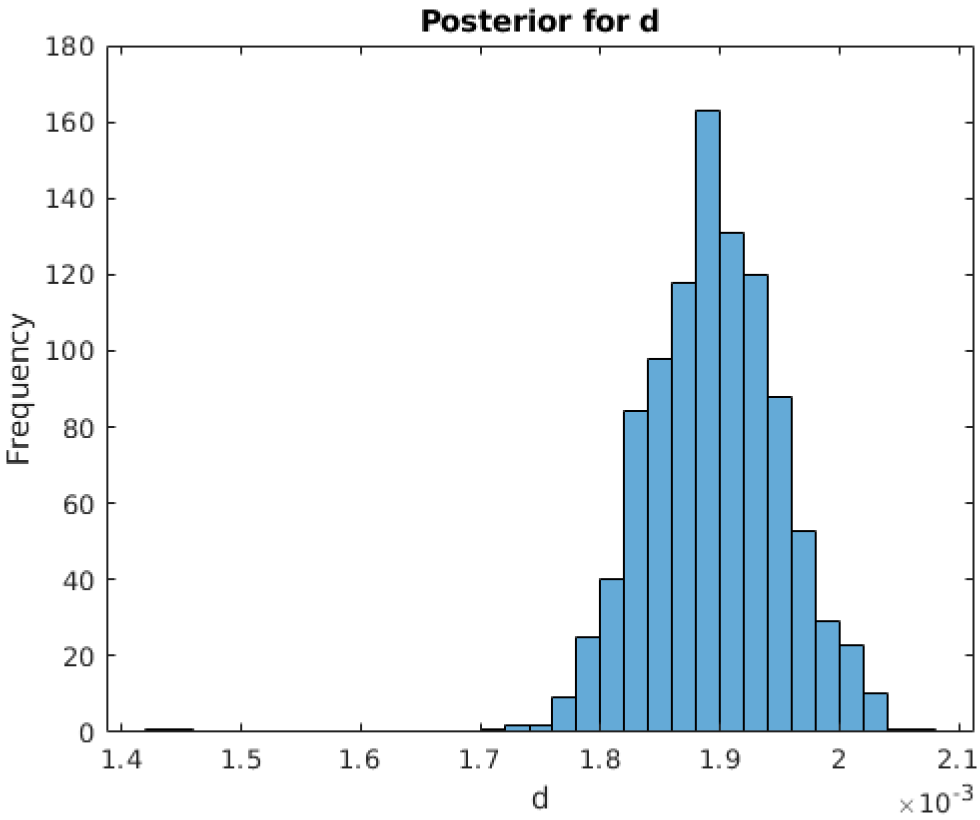
```
ninety_five_percent_range_S0_high =
   5.5272e+03
```

```
ninety_five_percent_range_S0_low = bootstrap_samples_sorted(1, ceil(length(bootstrap_sa
```

```
ninety_five_percent_range_S0_low =
   5.3002e+03
```

```
figure;
histogram(bootstrap_samples(2, :));
xlabel('d');
```

```
ylabel('Frequency');
title('Posterior for d');
```




```
two_sigma_range_d_high = mean(bootstrap_samples(2,:)) + 2*std(bootstrap_samples(2,:))
```

```
two_sigma_range_d_high =
   2.0116e-03
```

```
two_sigma_range_d_low = mean(bootstrap_samples(2,:)) - 2*std(bootstrap_samples(2,:))
```

```
two_sigma_range_d_low =
   1.7782e-03
```

```
ninety_five_percent_range_d_high = bootstrap_samples_sorted(2, ceil(length(bootstrap_sa
```

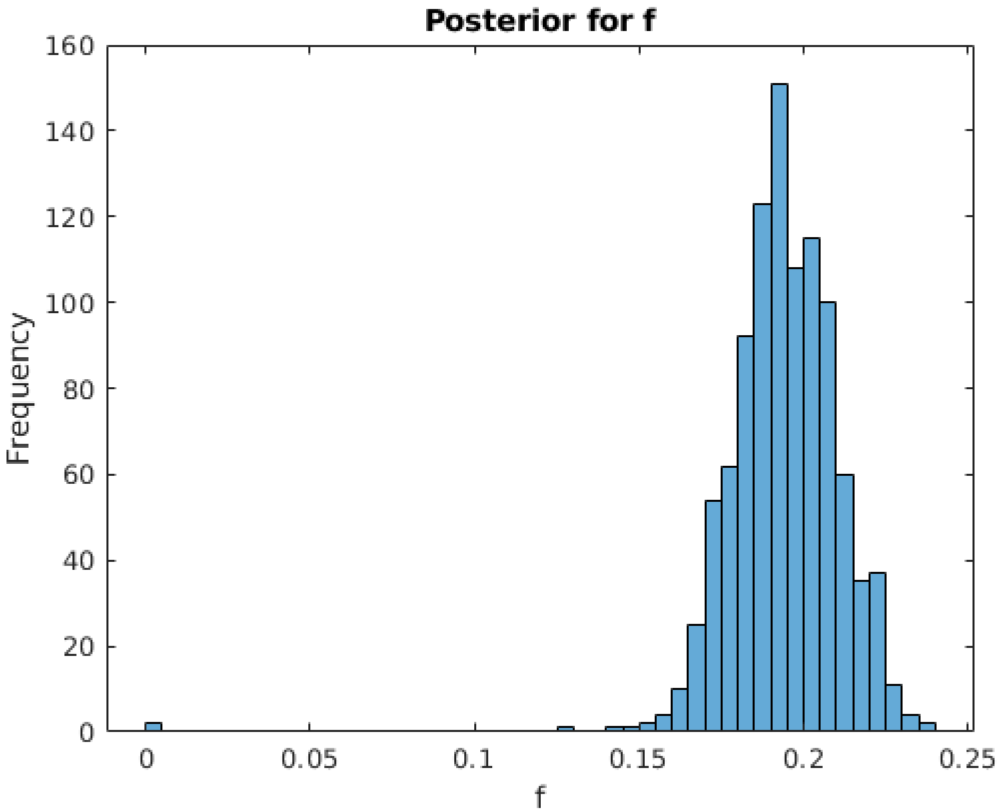
```
ninety_five_percent_range_d_high =
   2.0075e-03
```

```
ninety_five_percent_range_d_low = bootstrap_samples_sorted(2, ceil(length(bootstrap_sam
```

```
ninety_five_percent_range_d_low =
   1.7897e-03
```

```
figure;
histogram(bootstrap_samples(3, :));
xlabel('f');
ylabel('Frequency');
```

```
title('Posterior for f');
```




```
two_sigma_range_f_high = mean(bootstrap_samples(3,:)) + 2*std(bootstrap_samples(3,:))
```

```
two_sigma_range_f_high =
   2.2886e-01
```

```
two_sigma_range_f_low = mean(bootstrap_samples(3,:)) - 2*std(bootstrap_samples(3,:))
```

```
two_sigma_range_f_low =
   1.5971e-01
```

```
ninety_five_percent_range_f_high = bootstrap_samples_sorted(3, ceil(length(bootstrap_sa
```

```
ninety_five_percent_range_f_high =
   2.2356e-01
```

```
ninety_five_percent_range_f_low = bootstrap_samples_sorted(3, ceil(length(bootstrap_sam
```

```
ninety_five_percent_range_f_low =
   1.6574e-01
```

Q1.2.2 - Using Markov Chain Monte-Carlo (MCMC) to provide another estimate of 2-sigma range and 95% range for paramters.

```
% Select a voxel
Avox = dwis(:, 92, 65, 72);
```

```
rng(1)
% Generate bootstrap samples - 50 and 700
mcmc_samples = MCMC(Avox, bvals, qhat, 40, 450, 10000);
```

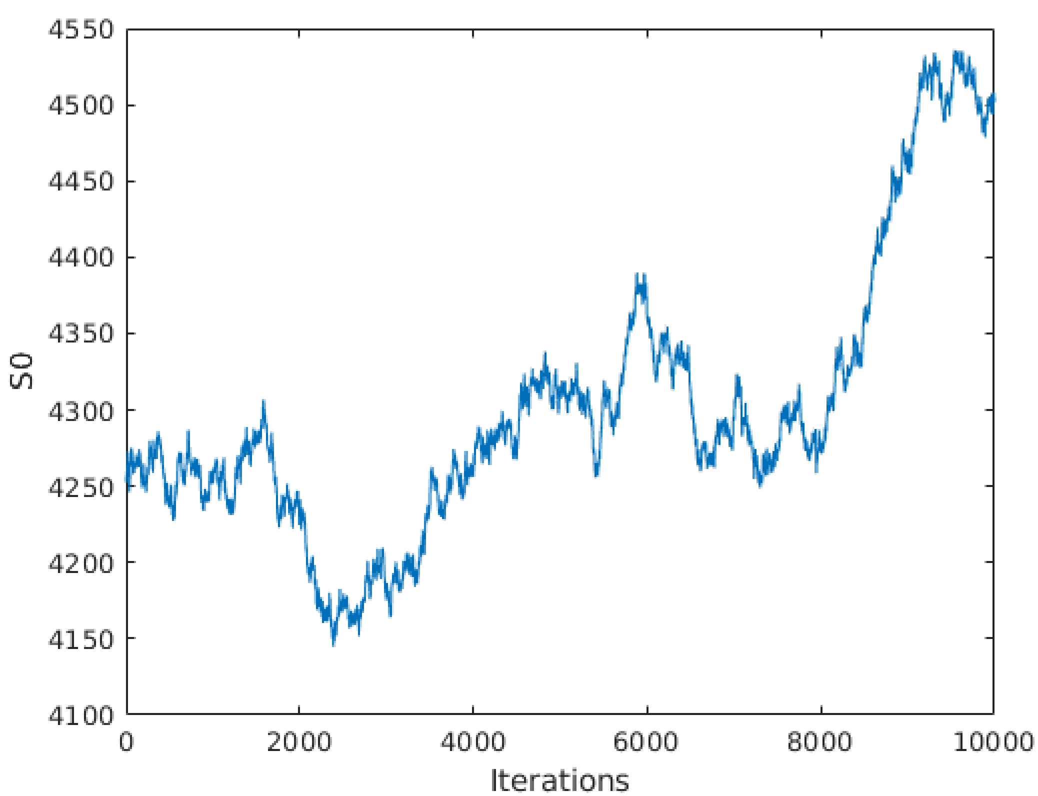
```
Local minimum possible.

fminunc stopped because it cannot decrease the objective function
along the current search direction.

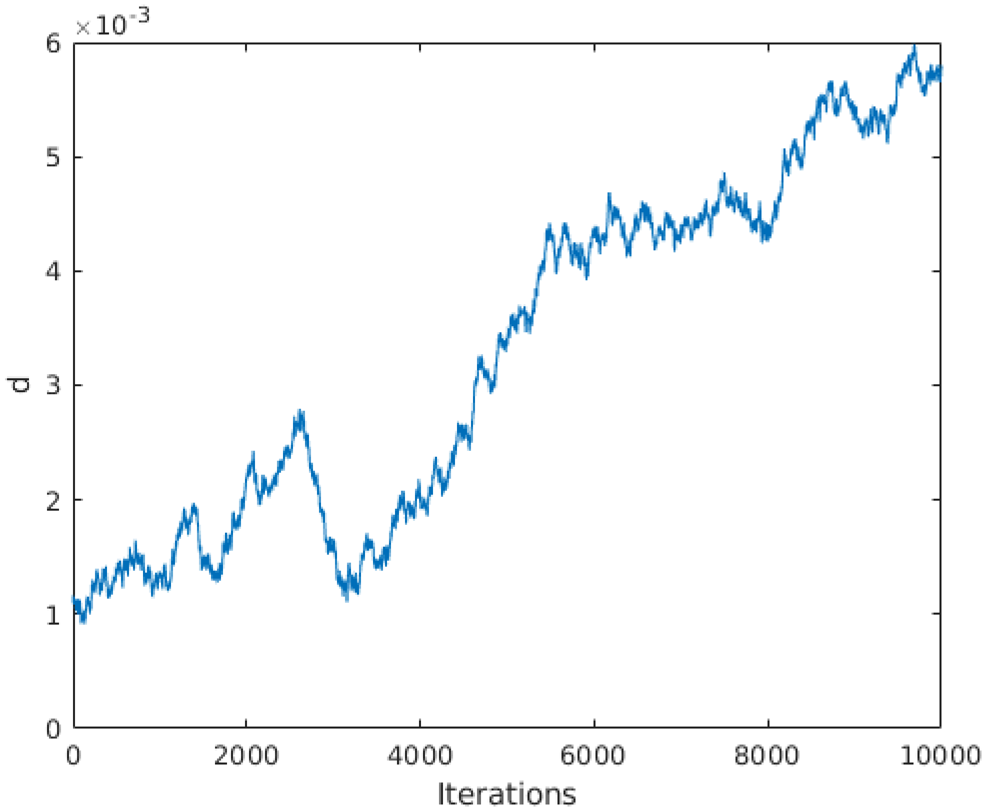
<stopping criteria details>
```

Plot parameter values over iterations

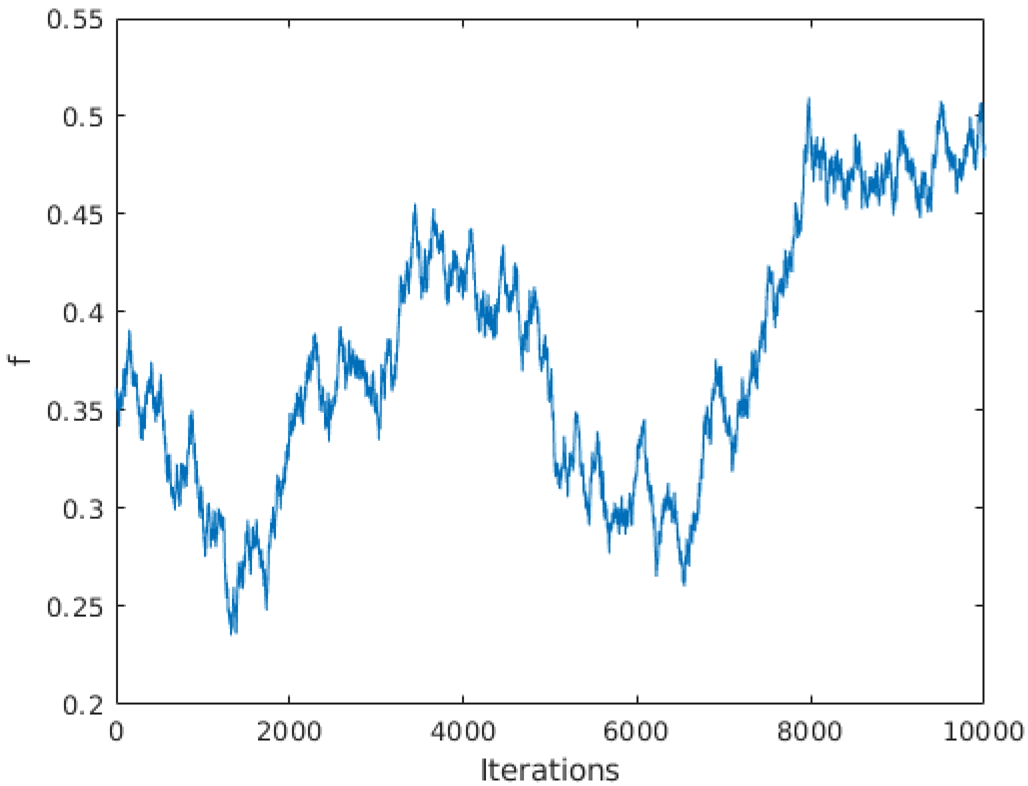
```
figure
plot(mcmc_samples(:, 1))
% ylim([4100, 4500])
xlabel('Iterations')
ylabel('S0')
```




```
figure
plot(mcmc_samples(:, 2))
% ylim([0.3, 0.42])
xlabel('Iterations')
ylabel('d')
```



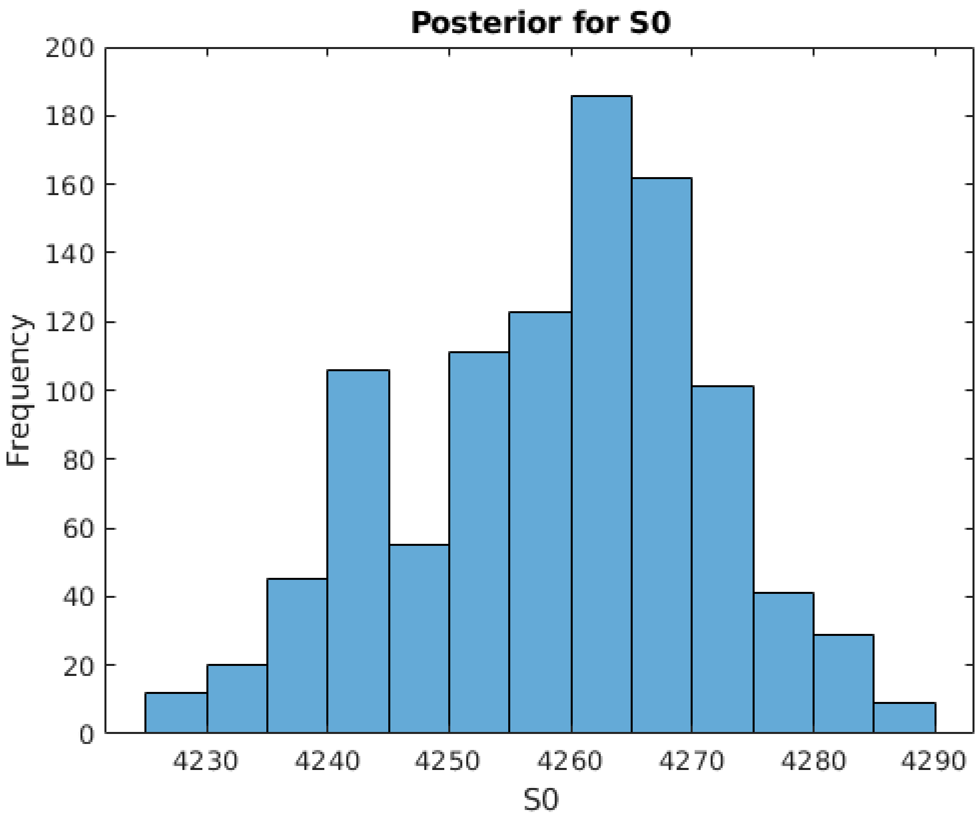

```
figure
plot(mcmc_samples(:, 3))
% ylim([1e-03, 1.3e-03])
xlabel('Iterations')
ylabel('f')
```



Plot histograms of parameter samples

```
mcmc_samples_sorted = sort(mcmc_samples, 1, 'ascend');

figure
histogram(mcmc_samples(:, 1))
xlabel('S0');
ylabel('Frequency');
title('Posterior for S0');
```




```
two_sigma_range_S0_high = mean(mcmc_samples(:, 1)) + 2*std(mcmc_samples(:, 1))
```

```
two_sigma_range_S0_high =
   4.2839e+03
```

```
two_sigma_range_S0_low = mean(mcmc_samples(:, 1)) - 2*std(mcmc_samples(:, 1))
```

```
two_sigma_range_S0_low =
   4.2340e+03
```

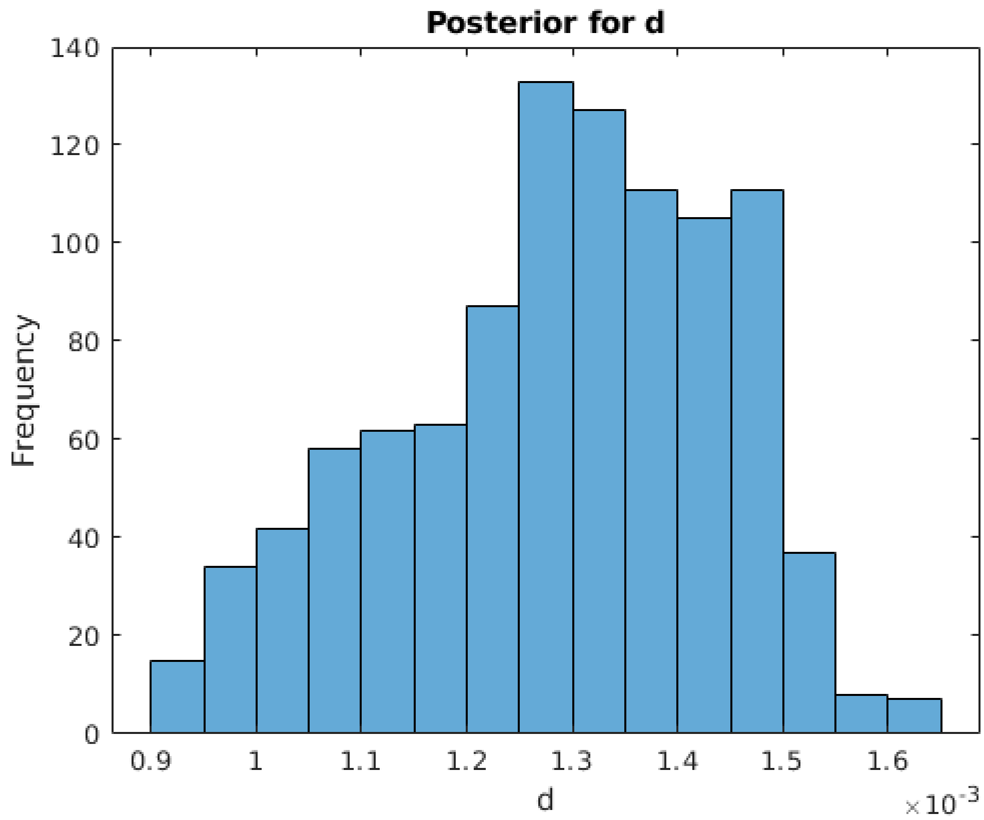
```
ninety_five_percent_range_S0_high = mcmc_samples_sorted(ceil(length(mcmc_samples)*(1-0.
```

```
ninety_five_percent_range_S0_high =
   4.2817e+03
```

```
ninety_five_percent_range_S0_low = mcmc_samples_sorted(ceil(length(mcmc_samples)*0.025)
```

```
ninety_five_percent_range_S0_low =
   4.2330e+03
```

```
figure
histogram(mcmc_samples(:, 2))
xlabel('d');
ylabel('Frequency');
title('Posterior for d');
```




```
two_sigma_range_S0_high = mean(mcmc_samples(:, 2)) + 2*std(mcmc_samples(:, 2))
```

```
two_sigma_range_S0_high =
   1.5969e-03
```

```
two_sigma_range_S0_low = mean(mcmc_samples(:, 2)) - 2*std(mcmc_samples(:, 2))
```

```
two_sigma_range_S0_low =
   9.7803e-04
```

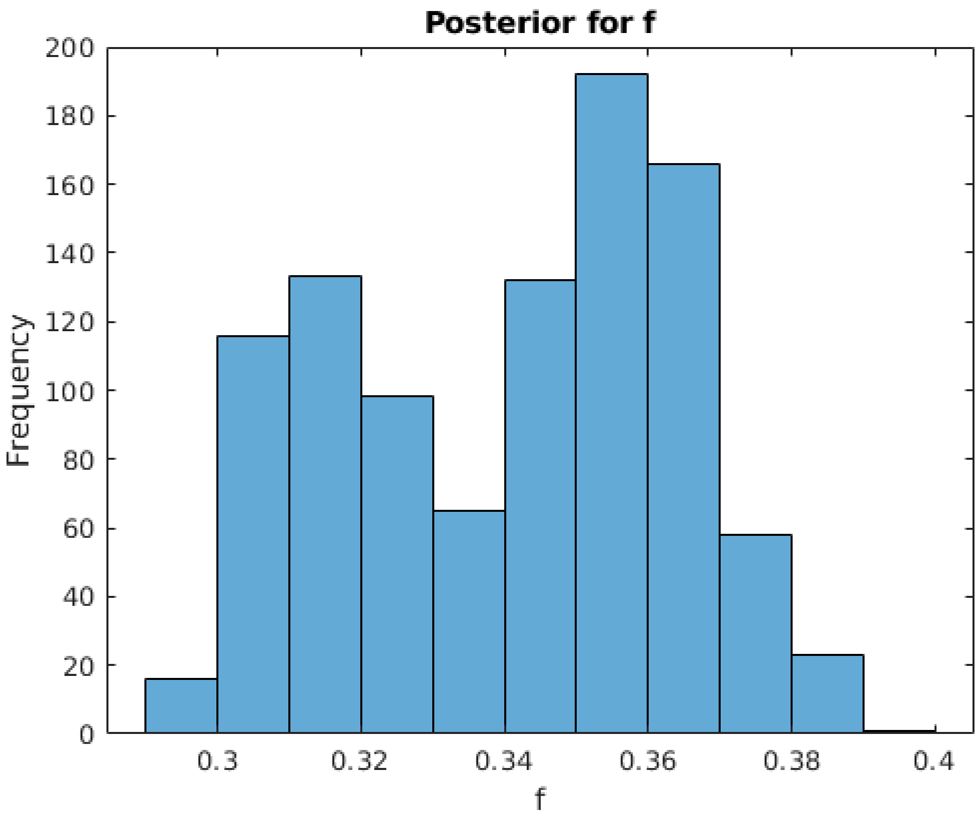
```
ninety_five_percent_range_S0_high = mcmc_samples_sorted(ceil(length(mcmc_samples)*(1-0.
```

```
ninety_five_percent_range_S0_high =
   1.5231e-03
```

```
ninety_five_percent_range_S0_low = mcmc_samples_sorted(ceil(length(mcmc_samples)*0.025)
```

```
ninety_five_percent_range_S0_low =
   9.6327e-04
```

```
figure
histogram(mcmc_samples(:, 3))
xlabel('f');
ylabel('Frequency');
title('Posterior for f');
```




```
two_sigma_range_S0_high = mean(mcmc_samples(:, 3)) + 2*std(mcmc_samples(:, 3))
```

```
two_sigma_range_S0_high =
   3.8749e-01
```

```
two_sigma_range_S0_low = mean(mcmc_samples(:, 3)) - 2*std(mcmc_samples(:, 3))
```

```
two_sigma_range_S0_low =
   2.9450e-01
```

```
ninety_five_percent_range_S0_high = mcmc_samples_sorted(ceil(length(mcmc_samples)*(1-0.
```

```
ninety_five_percent_range_S0_high =
   3.7950e-01
```

```
ninety_five_percent_range_S0_low = mcmc_samples_sorted(ceil(length(mcmc_samples)*0.025)
```

```
ninety_five_percent_range_S0_low =
   3.0168e-01
```

1.3 Model Selection

Loading Data

```
% Load the diffusion signal
```

```
fid = fopen('data_p1.3-1.4/isbi2015_data_normalised.txt', 'r', 'b');
fgetl(fid); % Read in the header
D = fscanf(fid, '%f', [6, inf])'; % Read in the data
fclose(fid);

% Select the first of the 6 voxels
meas = D(:,1);

% Load the protocol
fid = fopen('data_p1.3-1.4/isbi2015_protocol.txt', 'r', 'b');
fgetl(fid);
A = fscanf(fid, '%f', [7, inf]);
fclose(fid);

% Create the protocol
grad_dirs = A(1:3,:);
G = A(4,:);
delta = A(5,:);
smalldel = A(6,:);
TE = A(7,:);

GAMMA = 2.675987E8;
bvals = ((GAMMA*smalldel.*G).^2).*(delta-smalldel/3);
% convert bvals units from s/m^2 to s/mm^2
bvals = bvals/10^6;
```

Core Questions:

Q1.3.1 - Fit Ball-&-Stick model from 1.1.3 to the new data.

```
n_runs = 100;
% Store errors per run here
errors_per_run = zeros(1, n_runs);
min_error = 1e+10;

n = 1;
while n <= n_runs
    % Select a single voxel
    Avox = D(:,1);

    % Define a starting point for the non-linear fit
    startx = [3.5e+00 3e-03 2.5e-01 0 0];

    % Add gaussian noise to each of parameters
    startx_noisy(:, 1) = startx(:, 1) + 1e+03*randn;
    startx_noisy(:, 2) = startx(:, 2) + 1e-03*randn;
    % Repeat if the noisy start value isnt within the constraints
    while any(startx_noisy(:, 1:2) < 0)
        startx_noisy(:, 1) = startx(:, 1) + 1e+03*randn;
        startx_noisy(:, 2) = startx(:, 2) + 1e-03*randn;
    end
```

```
    startx_noisy(:, 3) = startx(:, 3) + 1e-01*randn;
    % Repeat if the noisy start value isnt within the constraints
    while startx_noisy(:, 3) > 1 || startx_noisy(:, 3) < 0
        startx_noisy(:, 3) = startx(:, 3) + 1e-01*randn;
    end
    startx_noisy(:, 4) = startx(:, 4) + 1e-01*randn;
    startx_noisy(:, 5) = startx(:, 5) + 1e-01*randn;

    % Perform inverse transform
    startx_noisy(:, 1:2) = sqrt(startx_noisy(:, 1:2));
    startx_noisy(:, 3) = sqrt(-log(startx_noisy(:, 3)));

    % Define various options for the non-linear fitting
    % algorithm.
    h=optimset('MaxFunEvals',20000,...
     'Algorithm','quasi-newton',...
     'TolX',1e-10,...
     'TolFun',1e-10, 'Display', 'off');

    % Now run the fitting
    try
        [parameter_hat,RESNORM,EXITFLAG,OUTPUT]=fminunc('BallStickSSD_transformation',s
    catch
        continue
    end

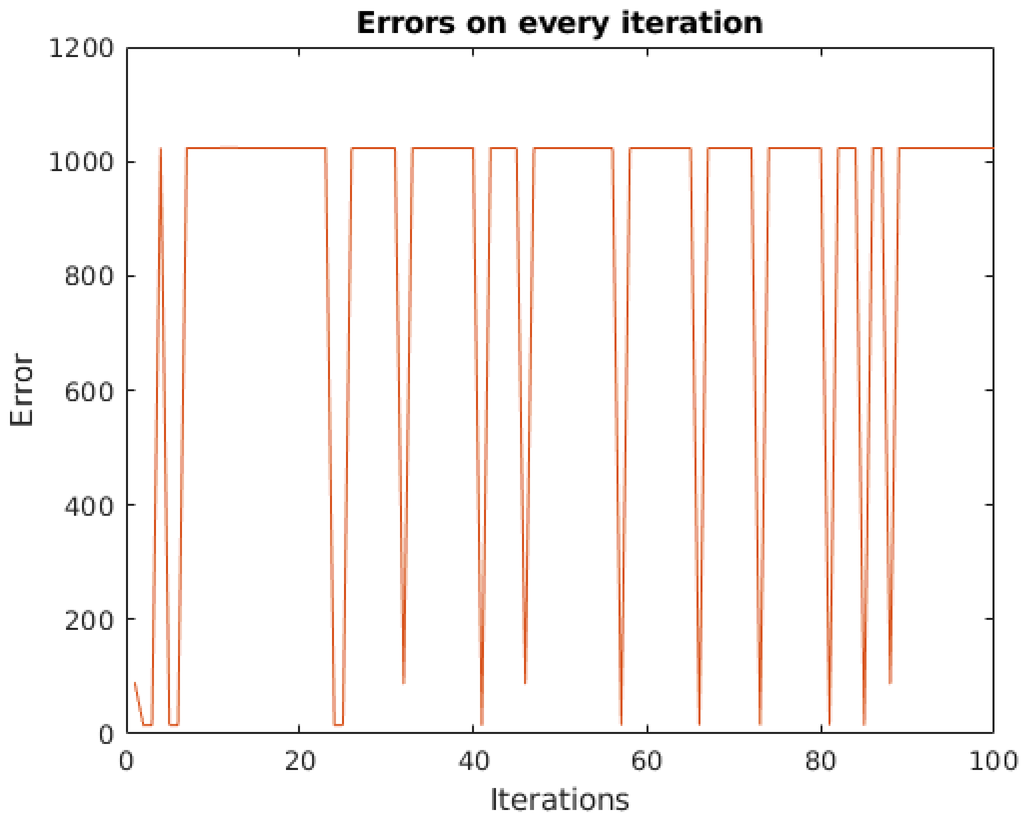
%     parameter_hat(:, 1) = parameter_hat(:, 1)^2;
%     parameter_hat(:, 2) = parameter_hat(:, 2)^2;
%     parameter_hat(:, 3) = exp(-parameter_hat(:, 3)^2);

    % Store
    errors_per_run(:, n) = RESNORM;

    % Save parameters if they have the smallest minimum
    if RESNORM < min_error
        min_error = RESNORM;
        best_params_BS = parameter_hat;
    end

    n = n + 1;
end
```

```
figure
plot(n_runs)
hold on;
plot(errors_per_run)
xlabel('Iterations')
ylabel('Error')
title('Errors on every iteration')
```




```
% Find proportion of trials with smallest value of RESNORM
min_error
```

```
min_error =
   1.5106e+01
```

```
count = 0;
tolerance = 0.1;
for n=1:n_runs
    if (errors_per_run(n) - min_error <= tolerance)
        count = count + 1;
    end
end

best_params_BS
```

```
best_params_BS = 1×6
   1.0099e+00   1.4321e-03   5.7493e-01  -1.5447e+00  -8.2863e-02   1.0832e-01
```

```
proportion = count / n_runs
```

```
proportion =
   1.2000e-01
```

```
% proportion = p(the run will find a global min) = p
% p(atleast 1 global min in n runs) = 1 - p(no global min in N runs)
```

```
% 0.95 = 1 - nC0*p^0*(1-p)^n
n_runs = log(0.05)/log(1-proportion)
```

```
n_runs =
   2.3435e+01
```

Q1.3.2 - Adapt code further to fit various different models.

Implement Diffusion Tensor Model

```
% Select a single voxel
Avox = D(:, 1);

% Create the design matrix
G = [ones(1, length(Avox)); -bvals.*grad_dirs(1, :).^2; -2*bvals.*grad_dirs(1,:).*grad_

% Compute parameter vector x
x = G\log(Avox);

% Compute error
S = G*x;
error = sum((Avox - S).^2)
```

```
error =
   1.0507e+04
```

Implement zeppelin-and-stick model

```
n_runs = 10;
% Store errors per run here
errors_per_run = zeros(1, n_runs);
min_error = 1e+10;

n = 1;
while n <= n_runs
    % Select a single voxel
    Avox = D(:,1);

    % Define a starting point for the non-linear fit
    startx = [3.5e+00 3e-03 2.5e-01 3e-03 0 0];

    % Add gaussian noise to each of parameters
    startx_noisy(:, 1) = startx(:, 1) + 1e+03*randn;
    startx_noisy(:, 2) = startx(:, 2) + 1e-03*randn;
    startx_noisy(:, 4) = startx(:, 4) + randn;
    % Repeat if the noisy start value isnt within the constraints
    while any(startx_noisy(:, [1:2, 4]) < 0)
        startx_noisy(:, 1) = startx(:, 1) + 1e+03*randn;
        startx_noisy(:, 2) = startx(:, 2) + 1e-03*randn;
        startx_noisy(:, 4) = startx(:, 4) + randn;
```

```
    end
    startx_noisy(:, 3) = startx(:, 3) + 1e-01*randn;
    % Repeat if the noisy start value isnt within the constraints
    while startx_noisy(:, 3) > 1 || startx_noisy(:, 3) < 0
        startx_noisy(:, 3) = startx(:, 3) + 1e-01*randn;
    end
    startx_noisy(:, 5) = startx(:, 5) + 1e-01*randn;
    startx_noisy(:, 6) = startx(:, 6) + 1e-01*randn;

    % Perform inverse transformation on first three parameters
    startx_noisy(:, [1:2]) = sqrt(startx_noisy(:, [1:2]));
    startx_noisy(:, 3) = sqrt(-log(startx_noisy(:, 3)));
    startx_noisy(:, 4) = sqrt(startx_noisy(:, 4)/2);

    % Define various options for the non-linear fitting
    % algorithm.
    h=optimset('MaxFunEvals',20000,...
     'Algorithm','quasi-newton',...
     'TolX',1e-10,...
     'TolFun',1e-10, 'Display', 'off');

    % Now run the fitting
    [parameter_hat,RESNORM,EXITFLAG,OUTPUT]=fminunc('ZeppelinStickSSD',startx_noisy,h,A

%     parameter_hat(:, 1) = parameter_hat(:, 1)^2;
%     parameter_hat(:, 2) = parameter_hat(:, 2)^2;
%     parameter_hat(:, 3) = exp(-parameter_hat(:, 3)^2);
%     parameter_hat(:, 4) = 2*parameter_hat(:, 4)^2;

    % Store
    errors_per_run(:, n) = RESNORM;

    % Save parameters if they have the smallest minimum
    if RESNORM < min_error
        min_error = RESNORM;
        best_params_ZS = parameter_hat;
    end

    n = n + 1;
end

best_params_ZS
```

```
best_params_ZS = 1×6
   9.9148e-01   4.0135e-02   9.1189e-01   2.1624e-02  -4.6854e+00  -9.2742e-02
```

```

% Find proportion of trials with smallest value of RESNORM
min_error
```

```
min_error =
   1.0817e+01
```

```
count = 0;
tolerance = 0.1;
```

```
for n=1:n_runs
    if (errors_per_run(n) - min_error <= tolerance)
        count = count + 1;
    end
end

proportion = count / n_runs
```

```
proportion =
   5.0000e-01
```

```

% proportion = p(the run will find a global min) = p
% p(atleast 1 global min in n runs) = 1 - p(no global min in N runs)
% 0.95 = 1 - nC0*p^0*(1-p)^n
n_runs = log(0.05)/log(1-proportion)
```

```
n_runs =
   4.3219e+00
```

Implement zeppelin-and-stick with tortuousity

```
n_runs = 100;
% Store errors per run here
errors_per_run = zeros(1, n_runs);
min_error = 1e+10;

n = 1;
while n <= n_runs
    % Select a single voxel
    Avox = D(:,1);

    % Define a starting point for the non-linear fit
    startx = [3.5e+00 3e-03 2.5e-01 0 0];

    % Add gaussian noise to each of parameters
    startx_noisy(:, 1) = startx(:, 1) + 1e+03*randn;
    startx_noisy(:, 2) = startx(:, 2) + 1e-03*randn;
    % Repeat if the noisy start value isnt within the constraints
    while any(startx_noisy(:, 1:2) < 0)
        startx_noisy(:, 1) = startx(:, 1) + 1e+03*randn;
        startx_noisy(:, 2) = startx(:, 2) + 1e-03*randn;
    end
    startx_noisy(:, 3) = startx(:, 3) + 1e-01*randn;
    % Repeat if the noisy start value isnt within the constraints
    while startx_noisy(:, 3) > 1 || startx_noisy(:, 3) < 0
        startx_noisy(:, 3) = startx(:, 3) + 1e-01*randn;
    end
    startx_noisy(:, 4) = startx(:, 4) + 1e-01*randn;
    startx_noisy(:, 5) = startx(:, 5) + 1e-01*randn;

    % Perform inverse transformation on first three parameters
    startx_noisy(:, 1:2) = sqrt(startx_noisy(:, 1:2));
```

```
    startx_noisy(:, 3) = sqrt(-log(startx_noisy(:, 3)));

    % Define various options for the non-linear fitting
    % algorithm.
    h=optimset('MaxFunEvals',20000,...
     'Algorithm','quasi-newton',...
     'TolX',1e-10,...
     'TolFun',1e-10, 'Display', 'off');

    % Now run the fitting
    try
        [parameter_hat,RESNORM,EXITFLAG,OUTPUT]=fminunc('ZeppelinStickTortuositySSD',st
    catch
        continue
    end

%     parameter_hat(:, 1) = parameter_hat(:, 1)^2;
%     parameter_hat(:, 2) = parameter_hat(:, 2)^2;
%     parameter_hat(:, 3) = exp(-parameter_hat(:, 3)^2);

    % Store
    errors_per_run(:, n) = RESNORM;

    % Save parameters if they have the smallest minimum
    if RESNORM < min_error
        min_error = RESNORM;
        best_params_ZST = parameter_hat;
    end

    n = n + 1;
end

best_params_ZST
```

```
best_params_ZST = 1×6
   9.9566e-01  -3.9116e-02  -8.1203e-01  -1.5442e+00  -8.7052e-02   4.9176e-02
```

```
% Find proportion of trials with smallest value of RESNORM
min_error
```

```
min_error =
   1.1605e+01
```

```
count = 0;
tolerance = 0.1;
for n=1:n_runs
    if (errors_per_run(n) - min_error <= tolerance)
        count = count + 1;
    end
end

proportion = count / n_runs
```

```
proportion =
```

```
   1.3000e-01
```

```
% proportion = p(the run will find a global min) = p
% p(atleast 1 global min in n runs) = 1 - p(no global min in N runs)
% 0.95 = 1 - nC0*p^0*(1-p)^n
n_runs = log(0.05)/log(1-proportion)
```

```
n_runs =
   2.1511e+01
```

Q1.3.3 - Compute AIC and BIC for the 3 models.

```
% Store number of parameters in each model
N_BS = 5;
N_ZS = 6;
N_ZST = 5;

% store number of values in voxel
K = length(Avox);

% compute SSD for each model
SSD_BS = BallStickSSD_transformation(best_params_BS, Avox, bvals, grad_dirs);
SSD_ZS = ZeppelinStickSSD(best_params_ZS, Avox, bvals, grad_dirs);
SSD_ZST = ZeppelinStickTortuositySSD(best_params_ZST, Avox, bvals, grad_dirs);

% compute sigma^2 for each model
sigma_BS = (1/K)*SSD_BS;
sigma_ZS = (1/K)*SSD_ZS;
sigma_ZST = (1/K)*SSD_ZST;

% compute logL for each model
logL_BS = (-K/2)*(log(2*pi) + log(sigma_BS) + 1);
logL_ZS = (-K/2)*(log(2*pi) + log(sigma_ZS) + 1);
logL_ZST = (-K/2)*(log(2*pi) + log(sigma_ZST) + 1);

% Compute AIC score
AIC_BS = 2*(N_BS+1) + K*log((1/K)*SSD_BS)
```

```
AIC_BS =
  -1.9771e+04
```

```
AIC_ZS = 2*(N_ZS+1) + K*log((1/K)*SSD_ZS)
```

```
AIC_ZS =
  -2.0975e+04
```

```
AIC_ZST = 2*(N_ZST+1) + K*log((1/K)*SSD_ZST)
```

```
AIC_ZST =
  -2.0723e+04
```

```
% Compute BIC score
```

```
BIC_BS = N_BS*log(K) - 2*logL_BS
```

```
BIC_BS =
  -9.4831e+03
```

```
BIC_ZS = N_ZS*log(K) - 2*logL_ZS
```

```
BIC_ZS =
  -1.0690e+04
```

```
BIC_ZST = N_ZST*log(K) - 2*logL_ZST
```

```
BIC_ZST =
  -1.0444e+04
```