2 Appendix B: Code

```
# %% [markdown]
    # # Q1.1.1
    # %%
    # Import the necessary libraries
    import numpy as np
    import matplotlib.pyplot as plt
    import matplotlib.patches as patches
    from matplotlib.ticker import FormatStrFormatter
10
12
    import scipy.stats as stats
    from scipy.io import loadmat
    from scipy.optimize import minimize
    from scipy.special import expit, logit
17
    # set hyperparameters for common voxels and slices we will be using
18
    im\_slice = 71
    vox_i = 91
20
    vox_j = 64
21
    dim_i = 145
22
    dim_j = 174
23
24
    # %%
25
    # Load in the diffusion MRI data set and calculate settings for each component image
26
    dwis = loadmat('data.mat')['dwis']
    dwis = np.double(dwis)
    dwis = dwis.transpose((3, 0, 1, 2))
    [Dc, Dx, Dy, Dz] = dwis.shape
    qhat = np.loadtxt("bvecs", delimiter = " ").T
    bvals = 1000 * np.sum(qhat * qhat, axis=1)
    # %%
    \# Solve for x in log(A) = Gx - where x has all unknowns
    x = np.zeros((dim_i, dim_j, 7))
    quadratic_matrix = -bvals * np.array([qhat[:,0]**2, 2*qhat[:,0]*qhat[:,1], 2*qhat[:,0]*qhat[:,1], qhat[:,1]**2, 2*qhat[:,1]**2
    G = np.concatenate([np.ones((108,1)), quadratic_matrix.T], axis=1)
    # for each voxel calculate the solution
41
    for i in range(dim_i):
42
        for j in range(dim_j):
43
            A = dwis[:,i,j,im_slice]
44
            if np.min(A) > 0:
45
                W = np.diag(A**2)
46
                invmap = np.linalg.pinv(G.T @ W @ G) @ G.T @ W
47
                x[i,j,:] = invmap @ np.log(A)
48
49
    # calculate the DT for each voxel
50
    D = np.zeros((dim_i,dim_j,3,3))
51
    for i in range(dim_i):
        for j in range(dim_j):
            Dxx = x[i,j,1]
            Dxy = x[i,j,2]
            Dxz = x[i,j,3]
            Dyy = x[i,j,4]
57
            Dyz = x[i,j,5]
58
            Dzz = x[i,j,6]
59
            D[i,j] = np.array(
```

```
[[Dxx, Dxy, Dxz],
61
                  [Dxy, Dyy, Dyz],
62
                  [Dxz, Dyz, Dzz]]
63
64
65
66
67
68
     # Plot the model estimate against the measure signal at voxel 92x65
69
70
     A_est = np.exp(G @ np.squeeze(x[vox_i,vox_j,:]).reshape((-1,1)))
71
     A_exact = np.squeeze(dwis[:,vox_i,vox_j,im_slice])
72
     # Create grid of subplots
73
     plt.scatter(np.arange(108), A_exact, marker='o', color='b', label='Observations')
74
     plt.scatter(np.arange(108), A_est, marker='x', color='r', label='Model Estimate')
     plt.title(f'DT Model - at voxel {vox_i+1}x{vox_j+1}')
     plt.show()
79
     # %%
80
     # Calculate mean diffusivity across the image
     mean_D = np.zeros((dim_i,dim_j))
82
83
     for i in range(dim_i):
84
        for j in range(dim_j):
85
            mean_D[i,j] = np.trace(D[i,j]) / 3
86
87
     # Calculate FA
88
    FA = np.zeros((dim_i,dim_j))
89
     eig_val_D = np.zeros(((dim_i,dim_j,3)))
90
     eig_vec_D = np.zeros((dim_i,dim_j,3,3))
91
92
    for i in range(dim_i):
93
        for j in range(dim_j):
94
             eig_val, eig_vec = np.linalg.eig(np.squeeze(D[i,j]))
95
             eig_vec_D[i,j,:,:] = eig_vec
             eig_val_D[i,j,:] = eig_val
             if eig_val.sum() > 0:
                # %%
102
     # plot Mean Diffusivity
103
     fig, axs = plt.subplots(1, figsize=(5, 5))
104
105
     axs.imshow(np.flipud(mean_D.T), cmap='gray')
     axs.set_title('DT Model - Mean Diffusivity')
106
107
     # Show the plot
108
     plt.show()
109
110
111
     # %%
112
     # Plot the FA weighted with eigenvalues on RBG spectrum
113
    FA_RGB = np.zeros((dim_i,dim_j,3))
114
115
    for i in range(dim_i):
116
        for j in range(dim_j):
117
             principal_eig_idx = np.argmax(np.abs(eig_val_D[i,j]))
118
             if eig_val_D[i,j,principal_eig_idx] > 0:
119
                 eig_vec = eig_vec_D[i,j,:,principal_eig_idx]
                FA_RGB[i,j,:] = FA[i,j] * np.abs(np.array([eig_vec[0], eig_vec[1], eig_vec[2]]))
     # normalise RGB values
```

```
FA_RGB = FA_RGB / np.max(FA_RGB)
124
125
     # print to screen FA_RGB
126
     fig, axs = plt.subplots(1, 2)
127
     fig.suptitle('DT Model\nFractional Anisotropy')
128
129
     axs[0].imshow(np.flipud(FA.T), cmap='gray')
130
131
     axs[1].imshow(np.flipud(np.transpose(FA_RGB, (1,0,2))))
132
133
     plt.tight_layout()
134
     np.transpose
135
136
137
     # %% [markdown]
138
139
     # # Q1.1.2
     # ### Ball and Stick Model
141
     # %%
     def ball_stick(x):
143
144
         # Extract the parameters
145
         # diff: diffusion
146
         # f: fraction of signal contributed by diffusion tensor along fiber direction theta, phi
147
         S0, diff, f, theta, phi = x
148
149
         # Fiber direction
150
         fibdir = np.array([
151
             np.cos(phi) * np.sin(theta),
152
             np.sin(phi) * np.sin(theta),
153
             np.cos(theta),
154
         1)
155
156
         # creates a 2D array of fibdir stacked ontop of each other len(bvals) times
157
         # so now has the dimensions [len(bvals)x3]
158
         tile = np.tile(fibdir, (len(bvals), 1))
159
         fibdotgrad = np.sum(qhat * tile, axis=1)
         S = S0 * (f * np.exp(-bvals * diff * (fibdotgrad**2)) + (1-f) * np.exp(-bvals * diff))
         return S
163
164
165
166
     def BallStickSSD(x, voxel):
167
         S = ball_stick(x)
         # Compute sum of square differences
168
         return np.sum((voxel - S) ** 2)
169
170
171
     \# Use minimize for non-linear estimation of the ball-and-stick parameters
172
     # The first starting point finds a spurious local min; the second
173
     # a more reasonable min.
174
     avox = dwis[:,vox_i,vox_j,im_slice]
175
     \#startx = np.array([3500, -5e-6, 120, 0, 0])
176
     #startx = np.array([4200, 4e-4, 0.25, 0, 0])
177
     # start given by moodle note:
178
     startx = np.array([3300, 1.0e-03, 4.5e-01, 1.0, 1.0])
179
     results = minimize(
180
         fun=BallStickSSD,
181
182
         x0=startx.
         args=(avox,),
183
     )
184
185
     results
```

```
187
     # %%
188
     # Use the fitted parameters to get estimated values
189
     A_est = ball_stick(results['x'])
190
     A_exact = np.squeeze(dwis[:,vox_i,vox_j,im_slice])
191
192
     # Find the mean and std of the errors
193
     error dist = stats.describe(A est - A exact)
194
     error_mean = error_dist[2]
195
     error_var = error_dist[3]
196
     print(f"error mean: {error_mean:.1f}")
197
     print(f"error std: {np.sqrt(error_var):.1f}")
198
199
     # Use the given noise std to calculate the expected SSD
200
     ss\_expected = 108 * 200**2
201
202
     ss_exact = results['fun']
203
     print(f"expected SS: {ss_expected:.1f}, calculated SS: {ss_exact:.1f}, diff: {(ss_expected - ss_exact):.1f}")
204
     # Create grid of subplots to compare
205
     plt.scatter(np.arange(108), A_exact, marker='o', color='b', label='Observations')
206
     plt.scatter(np.arange(108), A_est, marker='x', color='r', label='Model Estimate')
207
208
     plt.title(f'Ball and Stick at {vox_i+1}x{vox_j+1}\noptimize without contstraints')
209
     plt.show()
210
211
     # %% [markdown]
212
     # # Q1.1.3
213
214
     # %%
215
     # We are now constraining the parameters (S0, diff >0, f in (0,1), theta, phi in (0,2pi))
216
     # We do this by transforming x to be squared, or expit() and scaled to ensure they are in the
217
     # correct domain. Because the transformation happens after the optimizer quesses x_{-}t+1 we
218
     # have to transform the optimized solution to get the correct fitted parameters
219
220
     \# Given S0**0.5, diff**0.5, logit(f), logit(theta/pi) and logit(phi/2*pi) - we transform back to domain we want it
221
222
     def transform(x):
         return [x[0]**2, x[1]**2, expit(x[2]), expit(x[3])*np.pi, expit(x[4])*2*np.pi]
223
     # Given SO, diff, f, theta, and phi, we inverse transform it to the unconstrained domain
225
226
     def transform_inv(x):
         return [x[0]**0.5, x[1]**0.5, logit(x[2]), logit(x[3]/(np.pi)), logit(x[4]/(2*np.pi))]
227
228
229
     def BallStickSSD_constrained(x, voxel):
         # given x that is unconstrained, we transform it to our wanted domain
230
         S = ball_stick(transform(x))
231
         # Compute sum of square differences
232
         return np.sum((voxel - S) ** 2)
233
234
235
     # %%
236
     # Use the transform to find the parameters constrained
237
     # note: stratx is in our constrained domain, so we have to inverse transform it to be in
238
     # the unconstrained domain
239
     results = minimize(
240
         fun=BallStickSSD_constrained,
241
         x0=transform inv(startx).
242
         args=(avox,),
243
     )
244
245
     results
     \# With constraints the fitting works and we get sensible results (S0, diff >0, etc.)
     # and plotting against observed values we get much better results
```

```
250
          # %%
251
          # Use the fitted parameters to get estimated values
252
          print(f"found fitted x = {transform(results['x'])}")
253
          #A_est = ball_stick(transform(results['x']))
254
          #A_exact = np.squeeze(dwis[:,91,64,71])
255
          A_est = ball_stick(transform(results['x']))
256
          A_exact = np.squeeze(dwis[:,vox_i,vox_j,im_slice])
257
258
          # Find the mean and std of the errors
259
          error_dist = stats.describe(A_est - A_exact)
260
          error_mean = error_dist[2]
261
          error_var = error_dist[3]
262
          print(f"error mean: {error_mean}")
263
          print(f"error std: {np.sqrt(error_var)}")
264
265
266
          # Use the standard deviation to calculate the estimated Sum of Squares diff
267
          ss_expected = 108 * 200*200
          ss_exact = results['fun']
          print(f"estimated SS: {ss_expected}, calculated SS: {ss_exact}, diff: {ss_expected - ss_exact}")
269
270
          # Create grid of subplots to compare
271
          plt.scatter(np.arange(108), A_exact, marker='o', color='b', label='Observations')
272
         plt.scatter(np.arange(108), A_est, marker='x', color='r', label='Model Estimate')
273
         plt.legend()
274
         plt.title(f'Observations \ vs \ Ball \ and \ Stick \ Model \ at \ voxel \ \{vox\_i+1\} \\ x\{vox\_j+1\} \\ \ noptimized \ with \ constraints'\} \\ \ noptimized \ with \ constraints' \} \\ \ noptimized \ with \ constraints' \} \\ \ noptimized \ with \ noptimized \ noptimized \ with \ noptimized \ with \ noptimized \
275
         plt.show()
276
277
          # %% [markdown]
278
          # Sum of squres has significantly reduced because now the model is fitting the observed data much better
279
280
          # %% [markdown]
281
          # # 01.1.4
282
283
          # %%
284
          # for the same voxel run multiple times to try and find the best minimum
285
          def BallStickSSD_constrained_findSSDmin(max_iter, startx, avox):
                  # given parameters of a single avox, run max_iter times and find converged SSD each time
                  # return all found solutions and SSD values
                 noise_std = startx / 5
                 num_parameters = startx.size
                 X_single_voxel = np.zeros((max_iter, num_parameters))
                 X_SSD = np.zeros(max_iter)
293
294
                 for i in range(max_iter):
295
                         # find some noise, add to the start, and transform and inverse it to make sure the
296
                         # peturbed start is a realistic start
297
                         noise = np.random.normal(loc=np.zeros(num_parameters), scale=noise_std)
298
                         x_i = startx + noise
299
                         x_i = transform_inv(transform(x_i))
300
                         results = minimize(
301
                                 fun=BallStickSSD_constrained,
302
                                x0=transform_inv(x_i),
303
304
                                args=(avox,),
305
                         X_single_voxel[i,:] = results['x']
                         SSD_result = results['fun']
                         if np.isnan(SSD_result):
                                 SSD_result = np.inf
                         X_SSD[i] = SSD_result
310
311
                 return X_single_voxel, X_SSD
312
```

```
313
314
     def find_prob_finding_SSD_globalmin(startx, avox, max_iter=100, eps=1e-1):
315
         # given a voxex, and a starting position. Optimize to solve for x with 95% confidence the global minima has been found
316
317
         X_single_voxel, X_SSD = BallStickSSD_constrained_findSSDmin(max_iter, startx=startx, avox=avox)
318
319
         min SSD = np.min(X SSD)
320
         min_SSD_count = np.isclose(X_SSD, min_SSD, eps).sum()
321
         p = min_SSD_count / X_SSD.shape[0]
322
         print(f"min_SSD: {min_SSD}, found min {min_SSD_count} times, prob_global_min = {p}")
323
324
         return p
325
     # given prob of finding global min, return how many times we have to run optimisation
326
     # to have 95% chance of finding it
327
328
     def find_N_for_95percent_global_min(p):
         return int(np.ceil(np.log(0.05) / np.log(1-p)))
     # %%
331
     # Check a number of different voxels for the number of times we have to run optimisation
332
     # to have a 95% prob of finding the global min
333
     voxel_idxs = np.array([[vox_i,vox_j], [60,60], [55,55], [80,60], [85,55], [85, 72], [70, 70]])
334
     N_array = np.zeros(shape=voxel_idxs.shape[0])
335
336
     for i, voxel_idx in enumerate(voxel_idxs):
337
         p = find_prob_finding_SSD_globalmin(startx, dwis[:, voxel_idx[0], voxel_idx[1], im_slice], max_iter=100)
338
         N_array[i] = find_N_for_95percent_global_min(p)
339
340
     print(f"Found Ns: {N_array}")
341
     N_global_min = int(N_array.max())
342
     print(f"Will use the max N found in our small sample: max_N = {N_global_min}")
343
344
     # %% [markdown]
345
346
     # # 01.1.5
347
348
     # %%
     # use the found max N found across checked voxels to find the global min at each voxel in image slice
     # Note: this function takes a while so the solution has been run once and saved down
     # change is_skip to FALSE to re-calculate from scratch
352
     is_skip = True
353
354
     file_path = "X_optimize_each_voxel_with_same_N.npy"
355
     if not is_skip:
356
         X = np.zeros((dim_i, dim_j, startx.size))
357
         X = np.load(file_path)
358
359
         for i in range(dim_i):
360
             for j in range(dim_j):
361
                 A = dwis[:,i,j,im_slice]
362
                 if np.min(A) > 0:
363
                      x_single_voxel, x_SSD = BallStickSSD_constrained_findSSDmin(N_global_min, startx, dwis[:,i,j,im_slice])
364
                      min_idx = np.argmin(x_SSD)
365
                      X[i,j,:] = transform(x_single_voxel[min_idx,:])
366
367
              # save each row to a file
             np.save(file_path, X)
368
             print(f"row {i} complete")
369
     else:
370
         X = np.load(file_path)
371
372
373
     # %%
```

```
# Calculate RESNORM across the image slice
376
377
     RESNORM = np.zeros(shape=(dim_i, dim_j))
378
379
     for i in range(dim_i):
380
         for j in range(dim_j):
381
              RESNORM[i,j] = BallStickSSD(X[i,j,:], voxel=dwis[:,i,j, im_slice])
382
383
     # %%
384
     (RESNORM > 4e7).sum()
385
386
387
     \# plot the SO, d, f, and the RESNORM, and fibre direction of n
388
389
     SO = X[:,:,0]
390
391
     d_raw = X[:,:,1]
     d_processed = np.where(d_raw > 3, 0, d_raw)
     f = X[:,:,2]
     theta = X[:,:,3]
     phi = X[:,:,4]
395
396
     n_zplane_x = np.sin(theta) * np.cos(phi) * f
397
     n_zplane_y = - np.sin(theta) * np.sin(phi) * f
398
399
     n_yplane_x = np.sin(theta) * np.sin(phi) * f
400
     n_yplane_y = np.cos(theta) * f
401
402
403
     # plot FA
404
     # Create a 2x2 grid of subplots
405
     fig, axs = plt.subplots(2,2, figsize=(10, 10))
406
     fig.suptitle('Mapped parameters\nUsing Transform Optimised method with Ball & Stick')
407
408
     axs[0,0].imshow(np.flipud(S0.T), cmap='gray')
409
     axs[0,0].set_title('S0')
410
411
     axs[0,1].imshow(np.flipud(f.T), cmap='gray')
412
413
     axs[0,1].set_title('f')
415
     axs[1,0].imshow(np.flipud(d_raw.T), cmap='gray', vmax=0.004)
     axs[1,0].set_title('diffusivity\nmapped between (0, 0.004)')
416
418
     axs[1,1].imshow(np.flipud(RESNORM.T), cmap='gray', vmax=1.5e7)
     axs[1,1].set_title('RESNORM\nmapped between (0, 1.5e7)')
419
420
     # Show the plot
421
     plt.tight_layout()
422
     plt.show()
423
424
     # %%
425
426
     fig, axs = plt.subplots(1, figsize=(8, 8))
427
428
     axs.quiver(n_zplane_x.T, n_zplane_y.T)
429
     axs.set_title('n\nprojected onto the x-z plane')
430
     axs.set_aspect('equal')
431
432
433
     plt.show()
434
     # %% [markdown]
     # There are many outliers in the found parameters so there are some found parameters that don't have found solutions. This can
437
     # %% [markdown]
```

```
# # Q1.2.1
439
440
         # %%
441
442
443
444
         # Classical Bootstrapping method
445
         \# Sample with replacement T times to get A_t sampled data set. Each data set solve for parameters
446
         # Plot the found parameters on a histogram and keep the middle 95%. Calculate sigma for the estimate
447
         def calssical_bootstrap_find_parameters(vox_i, vox_j, im_slice, T=300):
448
                N_data = dwis.shape[0]
449
                \hbox{\it\# create indexes for $T$ different iteration, each iteration have $N$ samples indexes}
450
                sampled_idxs = np.random.randint(N_data, size=(T,N_data))
451
                bootstrap_parameters = np.zeros(shape=(T, 5))
452
453
454
                for t in range(T):
                        A_t = dwis[sampled_idxs[t], vox_i, vox_j, im_slice]
                        if np.min(A_t > 0):
                               x_single_voxel, x_SSD = BallStickSSD_constrained_findSSDmin(N_global_min, startx, A_t)
                               min_idx = np.argmin(x_SSD)
458
                               bootstrap_parameters[t,:] = transform(x_single_voxel[min_idx,:])
459
460
                return bootstrap_parameters
461
462
463
464
         # method to plot the histogram of bootstrap parameters given data and axes
465
         def plot_histogram_sigma_95percent(axs, data, title, shade_colour='grey', shade_alpha=0.4, sigma_line_colour='red', mean_colour='red', mean_colour
466
                T = data.size
467
                data_std = np.std(data)
468
                data_sorted_idx = np.argsort(data)
469
                data_95_idx = [data_sorted_idx[int(T * 0.025)], data_sorted_idx[int(T * 0.975)]]
470
                data_95_range = [data[data_95_idx[0]], data[data_95_idx[1]]]
471
                data_2sigma_range = [data.mean() - 2*data_std, data.mean() + 2*data_std]
474
                 # plot histograms of data with shaded 95% region, and line showing 2 sigma range
                height_values, _, _ = axs.hist(data)
                axs.axvspan(xmin=data_95_range[0], xmax=data_95_range[1], facecolor=shade_colour, alpha=shade_alpha, label='95% confidence
                axs.plot(data_2sigma_range, [height_values.max()/2,height_values.max()/2], marker='|', c=sigma_line_colour, label='2 sigma
                axs.scatter(data.mean(), height_values.max()/2, marker='x', c=mean_colour, label='parameter mean')
                if is_legend:
479
                        axs.legend()
480
                axs.set_title(title)
481
482
                return data_95_range, data_2sigma_range
483
484
485
         # use classical bootstrapping method to find a range of parameters and plot on a histogram
486
487
         vox_is = np.array([vox_i, 80, 60, 85])
488
         vox_js = np.array([vox_j, 60, 60, 72])
489
490
         num_vox = vox_is.size
491
492
         bootstrap_2sigma_range = np.zeros(shape=(num_vox,2))
493
494
         bootstrap_95_range = np.zeros(shape=(num_vox,2))
495
         fig, axs = plt.subplots(num_vox,3, figsize=(10, 10))
496
         fig.suptitle(f'Classical Bootstrap')
497
498
         print('Bootstrap parameter ranges\n')
499
         for vox in range(vox_is.size):
500
                if vox==0:
501
```

```
is_legend=True
502
503
                       is_legend=False
504
                bootstrap_parameters = calssical_bootstrap_find_parameters(vox_is[vox], vox_js[vox], im_slice=im_slice, T=200)
505
                bootstrap_95_range[0,:], bootstrap_2sigma_range[0,:] = plot_histogram_sigma_95percent(axs[vox, 0], bootstrap_parameters[:,
506
                bootstrap_95_range[1,:], bootstrap_2sigma_range[1,:] = plot_histogram_sigma_95percent(axs[vox, 1], bootstrap_parameters[:,
507
                bootstrap_95_range[2,:], bootstrap_2sigma_range[2,:] = plot_histogram_sigma_95percent(axs[vox, 2], bootstrap_parameters[:,
508
509
                # print the ranges for each parameter:
510
                print(f'Voxel: {vox_is[vox]+1}x{vox_js[vox]+1}')
511
                print(f"S0: mean = {bootstrap_parameters.mean(axis=0)[0]}, 95% confidence = {bootstrap_95_range[0]}, 2sigma range = {bootstrap_solutions.mean(axis=0)[0]}
512
513
                print(f"Diffusivity: mean = {bootstrap_parameters.mean(axis=0)[1]}, 95% confidence = {bootstrap_95_range[1]}, 2sigma range
                print(f"f: mean = {bootstrap_parameters.mean(axis=0)[2]}, 95% confidence = {bootstrap_95_range[2]}, 2sigma range = {bootstrap_
514
515
        plt.tight_layout()
516
517
518
         # %% [markdown]
519
         # The first two plots for SO and d match fairly well between 2 sigma range and the diffusivity which gives evidence that the di
520
         # %% [markdown]
521
         # # Q1.2.2
522
         # MCMC
523
524
         # for t in range(T):
525
                  y is sampled from dist Q
526
                   calculate alpha(x_t-1, y)
527
                   if alpha > U(0,1):
528
                          x_t = y
529
                   else
530
                          x \cdot t = x \cdot t - 1
531
                   remove burn in
532
                   take every stride-th element as sample
533
         #
                   return\ sample\_dist
534
535
         # %%
536
         # given a ndarray of points, and a ndarray of standard deviations for each dimension
537
         # return a point sampled from a gaussian located at the point with std
         def q_sample_from_dist(x, param_std):
                # add noise, then transform and inverse then inverse to ensure we remain within our domain
                return transform(transform_inv(x + np.random.randn(x.size) * param_std))
541
542
543
         # given parameters x and y, calculate the probability of p(A|y) \ / \ p(A|x)
544
         \# ie. how likely are we to sample y relative to x
         # note: this is assuming the q distribution is symmetrical
545
         def alpha_prob_ratio(y, x, data, noise_std):
546
                x_SSD = BallStickSSD(x, data)
547
                y_SSD = BallStickSSD(y, data)
548
                return np.exp((1 / (2 * noise_std**2)) * (x_SSD - y_SSD)) * (np.sin(y[3]) / np.sin(x[3]))
549
550
         # given burn_in, number of samples to throw away after burn (stride), and other parameters
551
         # return the samples sequence from the distribution p(x|A)
552
         def MCMC(data, x0=startx, burn_in=100, stride=10, sample_length=100, param_std=startx/5, noise_std=200):
553
                param_num = 5
554
                raw_sequence_length = burn_in + stride * sample_length
555
                raw_sequence = np.zeros(shape=(raw_sequence_length, param_num))
556
                accepted = np.zeros(raw_sequence_length)
557
558
                # initialise parameters
               raw_sequence[0,:] = x0
560
561
                for t in range(1, raw_sequence_length):
562
                       x = raw_sequence[t-1,:]
563
                       y = q_sample_from_dist(x, param_std)
564
```

```
alpha = alpha_prob_ratio(y, x, data, noise_std=noise_std)
565
              if alpha > np.random.rand():
566
                  raw_sequence[t] = y
567
                  accepted[t] = 1
568
             else:
569
                 raw_sequence[t] = x
570
571
         acceptance_after_burn = accepted[burn_in:].sum()/(raw_sequence_length-burn_in)
572
         print(f"MCMC Complete: Total sequence length {raw_sequence_length}\nraw acceptance rate of {100*accepted.sum()/raw_sequence_length}
573
574
         print(f"after burn in acceptance rate of {100*acceptance_after_burn:.0f}%")
575
         after_burn_sequence = raw_sequence[burn_in:]
576
         final_sequence_idxs = np.arange(sample_length) * stride
577
         return after_burn_sequence[final_sequence_idxs], acceptance_after_burn
578
579
580
     # %%
     burn_in = 2000
     stride = 5
     sample_length = 2000
584
585
     # 82% total
586
     #param_std=np.array([1e1, 1e-6, 1e-3, 1e-2, 1e-2])
587
     # 50% individual
588
     #param_std=np.array([5e1, 4e-5, 2e-2, 6e-2, 8e-2])
589
     # 70% individual
590
     param_std=np.array([3e1, 1.5e-5, 1e-2, 2e-2, 3e-2])
591
592
     data = dwis[:, vox_i, vox_j, im_slice]
593
     MCMC_sequence, acceptance_rate = MCMC(data, startx, burn_in=burn_in, stride=stride, sample_length=sample_length, param_std=par
594
595
596
     fig, axs = plt.subplots(3, 2, figsize=(10, 10))
597
     fig.suptitle(f'MCMC - at vox:{vox_i+1}x{vox_j+1}\nburn in: {burn_in}, keep every {stride}th sample, kept sequence {sample_leng
598
     MCMC_S0 = MCMC_sequence[:,0]
     MCMC_d = MCMC_sequence[:,1]
     MCMC_f = MCMC_sequence[:,2]
     burn_in_colour = 'grey'
604
     shade_alpha = 0.4
605
606
607
     axs[0,0].plot(MCMC_S0)
     axs[0,0].set_title('MCMC SO')
608
     axs[1,0].plot(MCMC_d)
609
     axs[1,0].set_title('MCMC d')
610
     axs[2,0].plot(MCMC_f)
611
     axs[2,0].set_title('MCMC f')
612
613
     MCMC_SO_95_range, MCMC_SO_2sigma_range = plot_histogram_sigma_95percent(axs[0, 1], MCMC_SO, 'SO', is_legend=True)
614
     MCMC_d_95_range, MCMC_d_2sigma_range = plot_histogram_sigma_95percent(axs[1, 1], MCMC_d, 'Diffusivity')
615
     MCMC_f_95_range, MCMC_f_2sigma_range = plot_histogram_sigma_95percent(axs[2, 1], MCMC_f, 'f')
616
617
618
     axs[1,1].xaxis.set_major_formatter(FormatStrFormatter('%.2e'))
     axs[1,1].tick_params(axis='x', labelsize=7)
619
620
     print('MCMC parameter ranges\n')
621
     print(f'Voxel: {vox_i+1}x{vox_j+1}')
622
     print(f"S0: mean = {MCMC_S0.mean()}, 95% confidence = {MCMC_S0_95_range}, 2sigma range = {MCMC_S0_2sigma_range}")
     print(f"Diffusivity: mean = {MCMC_d.mean()}, 95% confidence = {MCMC_d_95_range}, 2sigma range = {MCMC_d_2sigma_range}")
     print(f"f: mean = {MCMC_f.mean()}, 95% confidence = {MCMC_f_95_range}, 2sigma range = {MCMC_f_2sigma_range}\n")
625
626
     plt.tight_layout()
627
```

```
628
     # %%
629
     # Compare the Boostrap output to MCMC output
630
     MCMC_x = np.array([MCMC_S0.mean(),
631
                         MCMC_d.mean(),
632
                         MCMC_f.mean(),
633
                         MCMC_sequence[:,3].mean(),
634
                         MCMC_sequence[:,4].mean()])
635
     bootstrap_x = np.array([bootstrap_parameters.mean(axis=0)[0],
636
                              bootstrap_parameters.mean(axis=0)[1],
637
                              bootstrap_parameters.mean(axis=0)[2],
638
                              bootstrap_parameters.mean(axis=0)[3],
639
640
                              bootstrap_parameters.mean(axis=0)[4]])
641
     MCMC_est = ball_stick(MCMC_x)
642
643
     bootstrap_est = ball_stick(bootstrap_x)
     A_exact = np.squeeze(dwis[:,vox_i,vox_j,im_slice])
     MCMC_SSD = BallStickSSD(MCMC_x, dwis[:,vox_i,vox_j,im_slice])
     bootstrap_SSD = BallStickSSD(bootstrap_x, dwis[:,vox_i,vox_j,im_slice])
647
648
     # Create grid of subplots to compare
649
     plt.scatter(np.arange(108), A_exact, marker='o', color='b', label='Observations')
650
     plt.scatter(np.arange(108), MCMC_est, marker='x', color='r', label='MCMC')
651
     plt.scatter(np.arange(108), bootstrap_est, marker='x', color='g', label='Bootstrap')
652
     plt.legend()
653
     plt.title(f'MCMC vs Bootstrap fit at voxel {vox_i+1}x{vox_j+1}')
654
     plt.show()
655
656
657
658
     # %% [markdown]
659
     # # 01.3.1
660
661
     # %%
662
     # load in normalised data
663
     \# D.shape = 3612x6
     # D has headers: vox1, vox2, vox3, vox4, vox5, vox6
     D = np.genfromtxt('isbi2015_data_normalised.txt', skip_header=1, dtype=float, encoding='utf-8')
     # load in protocol
668
     # A.shape = 3612x7
     # A has headers: dir-x, dir-y, dir-z, |G|, DELTA, delta, TE
671
     A = np.genfromtxt('isbi2015_protocol.txt', skip_header=1, dtype=float, encoding='utf-8')
672
673
     # dir-x, dir-y, dir-z
     grad_dirs = A[:,0:3]
                              # mT/mm
674
     G = A[:,3]
                              # mT/mm
675
     delta = A[:,4]
676
     smalldel = A[:,5]
                              # ms (10x-3)
677
     TE = A[:,6]
                              # s x10-6
678
679
     GAMMA = 2.675987e8
680
681
     bvals = ((GAMMA * smalldel * G)**2) * (delta - (smalldel / 3))
682
     # convert bvals to s/mm^2 from s/m^2
683
     bvals = bvals / (10**6)
684
685
     qhat = grad_dirs
     num_vox = D.shape[1]
     noise\_std = 0.04
688
     # %%
690
```

```
# given a model find the min SSD
691
     def model_SSD_constrained_findSSDmin(model_constrained_SSD, transform, transform_inv, max_iter, startx, avox, method='BFGS'):
692
          # given parameters of a single avox, run max_iter times and find converged SSD each time
693
          # return best found solution and SSD value
694
695
         noise_std = np.abs(startx / 5)
696
         num_parameters = startx.size
697
         X_single_voxel = np.zeros((max_iter, num_parameters))
698
         X_SSD = np.zeros(max_iter)
699
700
         for i in range(max_iter):
701
              # find some noise, add to the start, and transform and inverse it to make sure the
702
              # peturbed start is a realistic start
703
             noise = np.random.normal(loc=np.zeros(num_parameters), scale=noise_std)
704
             x_i = startx + noise
705
706
             x_i = transform_inv(transform(x_i))
             results = minimize(
                  fun=model_constrained_SSD,
                  x0=transform_inv(x_i),
                  method=method,
710
                  args=(avox,),
711
712
             X_single_voxel[i,:] = results['x']
713
             SSD_result = results['fun']
714
             if np.isnan(SSD_result):
715
                  SSD_result = np.inf
716
             X_SSD[i] = SSD_result
717
718
         min_idx = np.argmin(X_SSD)
719
         x = X_single_voxel[min_idx]
720
         min_SSD = X_SSD[min_idx]
721
         min_SSD_count = np.isclose(X_SSD, min_SSD, 1e-1).sum()
722
723
         return x, min_SSD, min_SSD_count
724
725
726
727
     # given a model plot the results against observed signal
     def model_plot_results(model, X, voxels, RESNORMs, model_name):
          # plot the results
730
         col_num = 2
731
732
         row_num = 3
         data_num = voxels.shape[0]
733
734
         fig, axs = plt.subplots(col_num, row_num, figsize=(10, 10))
735
         fig.suptitle(model_name)
736
737
         vox = 0
738
         for col in range(2):
739
             for row in range(3):
740
                  A_est = model(X[vox])
741
                  A_exact = np.squeeze(voxels[:,vox])
742
743
744
                  # Create grid of subplots to compare
                  axs[col, row].scatter(np.arange(data_num), A_exact, marker='o', color='b', label='Observations')
745
746
                  axs[col,row].scatter(np.arange(data_num), A_est, marker='x', color='r', label='Model Estimate')
                  axs[col, row].set_title(f'Voxel {vox + 1}\nRESNORM: {RESNORMs[vox]:.1f}')
747
                  axs[col,row].legend()
749
                  vox = vox+1
750
751
         plt.show()
752
```

```
# %% [markdown]
754
     # Find solution for Ball & Stick model and plot for each voxel
755
756
757
     D.shape
758
759
     # %%
760
     # solve for x in each voxel
761
     num_param = 5
762
     max iter = 100
763
     BS_startx = np.array([1, 5.0e-03, 8e-01, 1.0e+00, 1.0e+00])
764
765
     BS_results = np.zeros(shape=(num_vox, num_param))
766
767
     BS_SSD_results = np.zeros(shape=(num_vox))
768
769
     for vox in range(num_vox):
770
         x, min_SSD, min_SSD_count = model_SSD_constrained_findSSDmin(BallStickSSD_constrained, transform, transform_inv, max_iter,
771
         BS_results[vox] = transform(x)
         BS_SSD_results[vox] = min_SSD
772
         print(f'N = {find_N_for_95percent_global_min(min_SSD_count / max_iter)}, p = {min_SSD_count / max_iter}, RESNORM = {min_SSD_count / max_iter}
773
774
775
     model_plot_results(ball_stick, BS_results, D, BS_SSD_results, 'Ball & Stick')
776
777
     # %% [markdown]
778
     # # Q1.3.2
779
780
     # %%
781
     # Define the different models
782
     # NOTE: ghat and buals have to be globally set before calling any of these models
783
784
     # Diffusion Tensor
785
     def DT_model(x):
786
         SO, Dxx, Dxy, Dxz, Dyy, Dyz, Dzz = x
787
788
         Diff = np.array(
789
                  [[Dxx, Dxy, Dxz],
                   [Dxy, Dyy, Dyz],
                   [Dxz, Dyz, Dzz]])
793
         S = S0 * np.exp(-bvals * (qhat @ Diff @ qhat.T).diagonal())
794
795
         return S
796
797
     def zeppelin_stick_model(x):
798
          # eig_val_1 >= eig_val_2 > 0
799
          # eig_val_1 is assumed to be the same size as diffusivity
800
          # eig_val_1 is in the same direction as the fibre direction (n_hat)
801
          \# eig\_val\_1 = eig\_val\_2 + eig\_val\_diff
802
          # eigenvalues are setup this way so we can easily constrain the inputs
803
         SO, eig_val_2, eig_val_diff, f, theta, phi = x
804
805
         eig_val_1 = eig_val_2 + eig_val_diff
806
807
         fibdir = np.array([
808
             np.cos(phi) * np.sin(theta),
809
              np.sin(phi) * np.sin(theta),
810
811
              np.cos(theta),
         1)
812
          # creates a 2D array of fibdir stacked ontop of each other len(bvals) times
814
          # so now has the dimensions [len(bvals)x3]
815
          tile = np.tile(fibdir, (len(bvals), 1))
816
```

```
fibdotgrad = np.sum(qhat * tile, axis=1)
817
818
         # intra-cellular signal
819
         # note: largest eigen value is assumed to be the same as the diffusivity
820
         # so we can substitue it in here
821
         S_i = np.exp(-bvals * eig_val_1 * (fibdotgrad**2))
822
823
         # extra-cellular signal
824
         S_e = np.exp(-bvals * (eig_val_2 + (eig_val_1 - eig_val_2) * (fibdotgrad**2)))
825
826
         \# total signal S
827
         S = S0 * (f * S_i + (1-f) * S_e)
828
829
         return S
830
831
832
     def zeppelin_stick_tur_model(x):
         \# same as Zeppelin\_stick\_model but with eig\_val\_2 = (1-f)*eig\_val\_1
         S0, eig_val_2, f, theta, phi = x
         eig_val_1 = eig_val_2 / (1-f)
836
837
         y = [S0, eig_val_1, eig_val_2, f, theta, phi]
838
839
         return zeppelin_stick_model(y)
840
841
842
     def model_SSD(model, x, voxel):
843
         # given a model calculate the modelled signals and return the sum of square difference
844
         # compared to the observed signals
845
         S = model(x)
846
         return np.sum((voxel - S) ** 2)
847
848
     # %%
849
     # We are now constraining the parameters (S0, diff >0, f in (0,1), theta, phi in (0,2pi))
     # We do this by transforming x to be squared, or expit() and scaled to ensure they are in the
     # correct domain. Because the transformation happens after the optimizer guesses x_{-} t + 1 we
     # have to transform the optimized solution to get the correct fitted parameters
     def DT_transform_inv(x):
856
         \# Given x we transform it to what we want to optimize to constrain it
         \# x = SO, Dxx, Dxy, Dxz, Dyy, Dyz, Dzz
858
         Dxx = x[1]
         Dxy = x[2]
860
861
         Dxz = x[3]
         Dyy = x[4]
862
         Dyz = x[5]
863
         Dzz = x[6]
864
865
         # Use the cholesky decomposition to constrain D = L @ L.T
866
         D = np.array(
867
                  [[Dxx, Dxy, Dxz],
868
                   [Dxy, Dyy, Dyz],
869
                   [Dxz, Dyz, Dzz]])
870
871
         L = np.linalg.cholesky(D)
872
         Lxx = L[0,0]
873
         Lxy = L[0,1]
874
875
         Lxz = L[0,2]
         Lyy = L[1,1]
         Lyz = L[1,2]
         Lzz = L[2,2]
878
```

```
return [x[0]**0.5, Lxx, Lxy, Lxz, Lyy, Lyz, Lzz]
880
881
882
      def DT_transform(x):
883
          # Given transformed x return parameters we are looking for
884
          \# x = abs(SO)**0.5, Lxx, Lxy, Lxz, Lyy, Lyz, Lzz
885
          # where L is the cholesky decomposition D = L @ L.T
886
          Lxx = x[1]
887
          Lxy = x[2]
888
          Lxz = x[3]
889
          Lyy = x[4]
890
          Lyz = x[5]
891
          Lzz = x[6]
892
893
          L = np.array(
894
                   [[Lxx, 0, 0],
                    [Lxy, Lyy, 0],
                    [Lxz, Lyz, Lzz]])
          D = L @ L.T
899
          Dxx = D[0,0]
900
          Dxy = D[0,1]
901
          Dxz = D[0,2]
902
          Dyy = D[1,1]
903
          Dyz = D[1,2]
904
          Dzz = D[2,2]
905
906
          return [x[0]**2, Dxx, Dxy, Dxz, Dyy, Dyz, Dzz]
907
908
909
      def DT constrained SSD(x, voxel):
910
          S = DT_model(DT_transform(x))
911
          # Compute sum of square differences
912
          return np.sum((voxel - S) ** 2)
913
914
915
916
      # %%
      # Transformation functions for Zeppelin Stick model
917
      def zeppelin_stick_transform_inv(x):
919
920
          \# Given x we transform it to what we want to optimize to constrain it
          \# x = S0, eig\_val\_2, eig\_val\_diff, f, theta, phi
922
          return [x[0]**0.5, x[1]**0.5, x[2]**0.5, logit(x[3]), logit(x[4]/np.pi), logit(x[5]/(2*np.pi))]
923
924
      def zeppelin_stick_transform(x):
925
          # Given transformed x return parameters we are looking for
926
          \#\ x = abs(SO)**0.5,\ abs(eig\_val\_2)**0.5,\ abs(eig\_val\_diff)**0.5,\ expit(f),\ expit(theta),\ expit(phi)
927
          \texttt{return} \ [\texttt{x}[0] **2, \ \texttt{x}[1] **2, \ \texttt{x}[2] **2, \ \texttt{expit}(\texttt{x}[3]), \ \texttt{expit}(\texttt{x}[4]) **p.p.i, \ \texttt{expit}(\texttt{x}[5]) *2*np.pi]
928
929
930
      def zeppelin_stick_constrained_SSD(x, voxel):
931
          S = zeppelin_stick_model(zeppelin_stick_transform(x))
932
          # Compute sum of square differences
933
          return np.sum((voxel - S) ** 2)
934
935
936
      # %%
937
      # Transformation functions for Zeppelin Stick Turtuosity model
938
      def zeppelin_stick_tur_transform_inv(x):
          \# Given x we transform it to what we want to optimize to constrain it
          \# x = S0, eig\_val\_2, f, theta, phi
942
```

```
return [x[0]**0.5, x[1]**0.5, logit(x[2]), logit(x[3]/np.pi), logit(x[4]/(2*np.pi))]
 943
 944
 945
            def zeppelin_stick_tur_transform(x):
 946
                     # Given transformed x return parameters we are looking for
 947
                     \# x = abs(SO)**0.5, abs(eig\_val\_2)**0.5, expit(f), expit(theta), expit(phi)
 948
                    return [x[0]**2, x[1]**2, expit(x[2]), expit(x[3])*np.pi, expit(x[4])*2*np.pi]
 949
 950
 951
            def zeppelin_stick_tur_constrained_SSD(x, voxel):
 952
                    S = zeppelin_stick_tur_model(zeppelin_stick_tur_transform(x))
 953
                     # Compute sum of square differences
 954
                    return np.sum((voxel - S) ** 2)
 955
 956
 957
 958
            # %%
            # Use least squares to get an estimate on D before using the minimise function
            data_range = [0,1000]
            data_num = data_range[1] - data_range[0]
 962
 963
            # Solve for x in log(A) = Gx - where x has all unknowns
 964
            x = np.zeros(7)
 965
            quadratic_matrix = -bvals[data_range[0]:data_range[0]: ata_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data_range[0]:data
 966
            G = np.concatenate([np.ones((data_range[1] - data_range[0],1)), quadratic_matrix.T], axis=1)
 967
 968
 969
            A = D[data_range[0]:data_range[1],0]
 970
            W = np.diag(A**2)
 971
            invmap = np.linalg.pinv(G.T @ W @ G) @ G.T @ W
 972
            x = invmap @ np.log(A)
 973
 974
            Dxx = x[1]
 975
            Dxy = x[2]
 976
            Dxz = x[3]
 977
 978
            Dyy = x[4]
            Dyz = x[5]
            Dzz = x[6]
            DT = np.array(
 982
                     [[Dxx, Dxy, Dxz],
                             [Dxy, Dyy, Dyz],
 983
 984
                             [Dxz, Dyz, Dzz]]
 985
 986
 987
            y = x.copy()
            y[0] = np.exp(y[0])
 988
            print(f'solution found from MSE: {y}')
 989
 990
 991
            # Use the transform to find the parameters constrained
 992
            DT_startx = y
 993
 994
            # solve for x in each voxel
 995
            num_param = DT_startx.size
 996
            max iter = 10
 997
 998
            DT_results = np.zeros(shape=(num_vox, num_param))
 999
1000
            DT_SSD_results = np.zeros(shape=(num_vox))
1001
            for vox in range(num_vox):
1002
                    x, min_SSD, min_SSD_count = model_SSD_constrained_findSSDmin(DT_constrained_SSD, DT_transform, DT_transform_inv, max_iter,
1003
                    DT_results[vox] = DT_transform(x)
1004
                    DT_SSD_results[vox] = min_SSD
1005
```

```
print(find_N_for_95percent_global_min(min_SSD_count / max_iter))
1006
1007
      # %%
1008
      model_plot_results(DT_model, DT_results, D, DT_SSD_results, 'Diffusion Tensor')
1009
1010
1011
      # Use the transform to find the parameters constrained
1012
      zep_stick_startx = np.array([1,1e-3,1-3,0.5,1,1])
1013
1014
      # solve for x in each voxel
1015
      num_param = zep_stick_startx.size
1016
      max iter = 60
1017
1018
      zep_stick_results = np.zeros(shape=(num_vox, num_param))
1019
      zep_stick_SSD_results = np.zeros(shape=(num_vox))
1020
1021
1022
      for vox in range(num_vox):
1023
          x, min_SSD, min_SSD_count = model_SSD_constrained_findSSDmin(zeppelin_stick_constrained_SSD, zeppelin_stick_transform, zep
          zep_stick_results[vox] = zeppelin_stick_transform(x)
1024
          zep_stick_SSD_results[vox] = min_SSD
1025
          print(find_N_for_95percent_global_min(min_SSD_count / max_iter))
1026
1027
1028
      model_plot_results(zeppelin_stick_model, zep_stick_results, D, zep_stick_SSD_results, 'Zeppelin & Stick')
1029
1030
1031
      zep_stick_results
1032
1033
      # %%
1034
      # Use the transform to find the parameters constrained
1035
      zep_stick_tur_startx = np.array([1,5e-4,0.5,0.1,1])
1036
1037
      # solve for x in each voxel
1038
1039
      num_param = zep_stick_tur_startx.size
      max_iter = 250
1040
1041
      zep_stick_tur_results = np.zeros(shape=(num_vox, num_param))
      zep_stick_tur_SSD_results = np.zeros(shape=(num_vox))
1045
      for vox in range(num_vox):
1046
1047
          x, min_SSD, min_SSD_count = model_SSD_constrained_findSSDmin(zeppelin_stick_tur_constrained_SSD, zeppelin_stick_tur_transf
1048
          zep_stick_tur_results[vox] = zeppelin_stick_tur_transform(x)
          zep_stick_tur_SSD_results[vox] = min_SSD
1049
          print(find_N_for_95percent_global_min(min_SSD_count / max_iter))
1050
1051
1052
      model_plot_results(zeppelin_stick_tur_model, zep_stick_tur_results, D, zep_stick_tur_SSD_results, 'Zeppelin & Stick with Turtu
1053
1054
      # %% [markdown]
1055
      # # Q1.3.3
1056
1057
1058
      # %%
1059
      def log_like(A_est, A_exact, noise_std):
1060
          var = noise_std**2
1061
          diff_squared_sum = ((A_est - A_exact)**2).sum()
1062
          log_like = (-0.5 * np.log(2*np.pi*var) - (1/(2*var)) * diff_squared_sum )
1063
          return log_like
1064
1065
1066
      def AIC(A_est, A_exact, deg_freedom, noise_std):
1067
          # we are calculating the noise directly so we don't have to increase N by 1
1068
```

```
N = deg_freedom
1069
          K = A_est.shape[0]
1070
1071
          if K/N < 40:
1072
              print('WARNING: K/N > 40 -> should use adjusted AIC')
1073
1074
          LogL = log_like(A_est, A_exact, noise_std)
1075
          AIC = 2*N - 2*LogL
1076
          return AIC
1077
1078
1079
      def BIC(A_est, A_exact, deg_freedom, noise_std):
1080
          # we are calculating the noise directly so we don't have to increase N by 1
1081
          N = deg_freedom
1082
          K = A_est.shape[0]
1083
1084
1085
          LogL = log_like(A_est, A_exact, noise_std)
1086
          BIC = N*np.log(K) - 2*LogL
          return BIC
1087
1088
      # %%
1089
      # calculate the AIC and BIC for each model
1090
      data_num = D.shape[0]
1091
      num_vox = D.shape[1]
1092
1093
      BS_preds = np.zeros(shape=D.shape)
1094
      DT_preds = np.zeros_like(BS_preds)
1095
      zeppelin_stick_preds = np.zeros_like(BS_preds)
1096
      zeppelin_stick_tur_preds = np.zeros_like(BS_preds)
1097
1098
      for vox in range(num_vox):
1099
          start idx = vox*data num
1100
           end_idx = start_idx + data_num
1101
1102
          BS_preds[:, vox] = ball_stick(BS_results[vox])
1103
1104
          DT_preds[:, vox] = DT_model(DT_results[vox])
1105
          zeppelin_stick_preds[:, vox] = zeppelin_stick_model(zep_stick_results[vox])
1106
          zeppelin_stick_tur_preds[:, vox] = zeppelin_stick_tur_model(zep_stick_tur_results[vox])
1107
      AICs = np.zeros(shape=(num_vox, 4))
1108
      BICs = np.zeros(shape=(num_vox, 4))
1109
1110
1111
      for vox in range(num_vox):
1112
          AICs[vox, 0] = AIC(BS_preds[:,vox], D[:,vox], deg_freedom=5, noise_std=0.04)
          AICs[vox, 1] = AIC(DT_preds[:,vox], D[:,vox], deg_freedom=7, noise_std=0.04)
1113
          AICs[vox, 2] = AIC(zeppelin_stick_preds[:,vox], D[:,vox], deg_freedom=6, noise_std=0.04)
1114
          AICs[vox, 3] = AIC(zeppelin_stick_tur_preds[:,vox], D[:,vox], deg_freedom=5, noise_std=0.04)
1115
1116
          BICs[vox, 0] = BIC(BS_preds[:,vox], D[:,vox], deg_freedom=5, noise_std=0.04)
1117
          BICs[vox, 1] = BIC(DT_preds[:,vox], D[:,vox], deg_freedom=7, noise_std=0.04)
1118
          BICs[vox, 2] = BIC(zeppelin_stick_preds[:,vox], D[:,vox], deg_freedom=6, noise_std=0.04)
1119
          BICs[vox, 3] = BIC(zeppelin_stick_tur_preds[:,vox], D[:,vox], deg_freedom=5, noise_std=0.04)
1120
1121
1122
      # %%
      models = {0:'BS', 1:'DT', 2:'zep_stick', 3:'zep_stick_tur'}
1123
1124
1125
      print(f'Model Ranking - Best to worst')
1126
      for vox in range(num_vox):
          print(f'voxel: {vox}')
1127
1128
          AIC_rank = np.argsort(AICs[vox])
1129
          BIC_rank = np.argsort(BICs[vox])
1130
1131
```

```
AIC_text = 'AIC: '
1132
          BIC_text = 'BIC: '
1133
          for rank in range(4):
1134
              str = f'{models[AIC_rank[rank]]}, '
1135
              AIC_text = AIC_text + str
1136
              str = f'{models[BIC_rank[rank]]}, '
1137
              BIC_text = BIC_text + str
1138
          print(AIC_text)
1139
          print(BIC_text + '\n')
1140
```