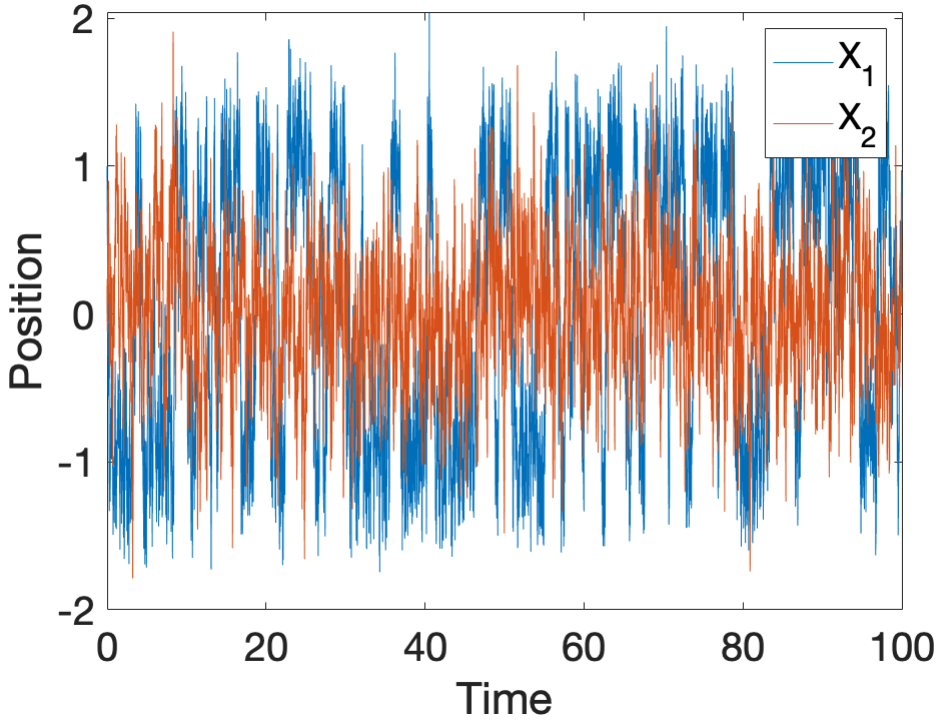
Analysis of the Simulation Data from Double-Well Potential

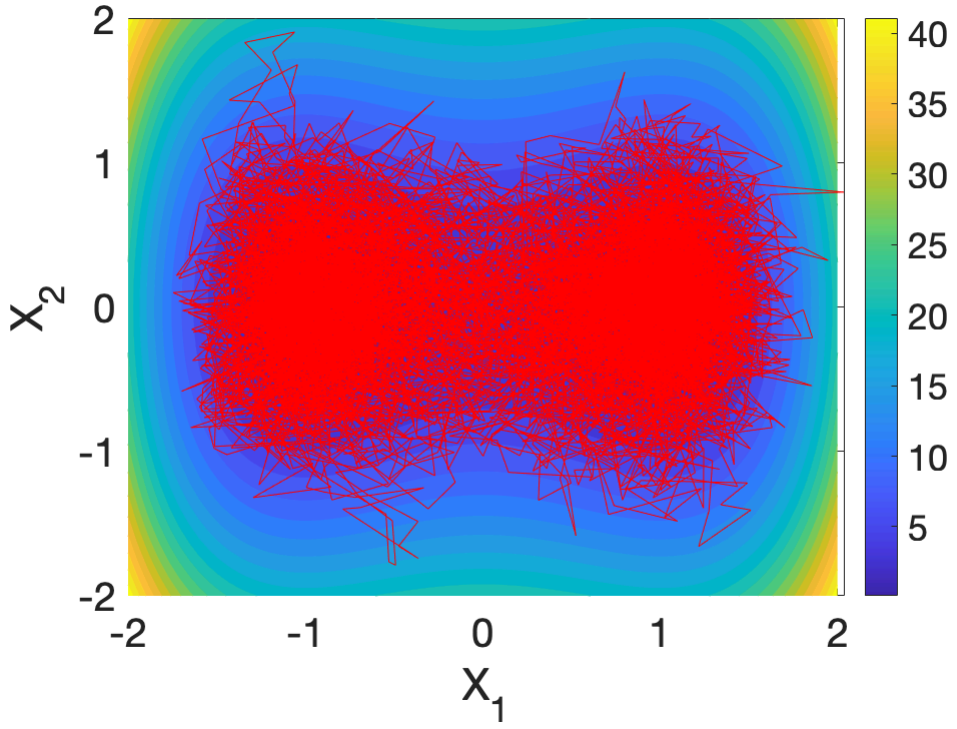
```
clearvars;
addpath(genpath('../'))
```

Generating simulation data

```
rng(1)
x_0 = [1,0]';
par.T_max = 100;
par.dt = 1e-2;
sigma = 2;
[x_out, t_out] = generating_simulation_
figure;
plot(t_out,x_out)
set(gca,'FontSize',20)
legend('X_{1}','X_{2}')
xlabel('Time')
ylabel('Position')
```




```
figure;
fc = fcontour(@double_well_potential,[-
fc.LevelList = [-10:0.1:3,3:2:50];
set(gca,'FontSize',20)
colorbar
hold on
plot(x_out(1,:),x_out(2,:),"Color",'r',
xlabel('X_{1}')
ylabel('X_{2}')
```




```
data = x_out(:,1:5:end)';
%save
%{
save('../Data/double_well.mat','x_out',
%}
```

Load the Data and Estimate Number of Clusters by EPI

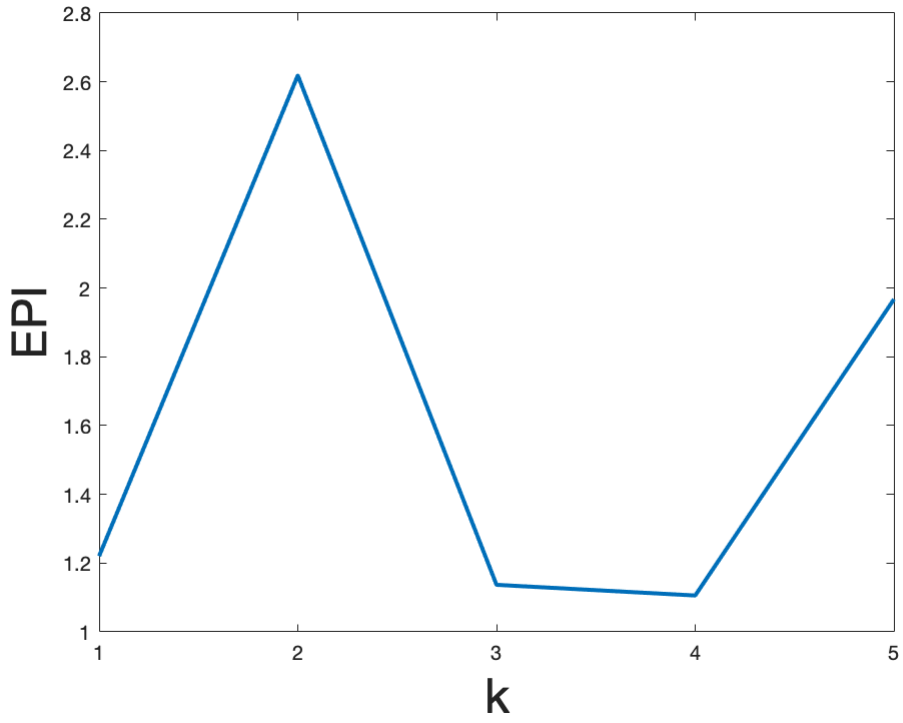
From EPI plot, we intend to seek for the index where peak occurs, which serves

as the candidate for the choice of cluster numbers

```
out = EstClusterNum(data,[]);
```

```
Computed P-values 500 of 2001 datapoint
Computed P-values 1000 of 2001 datapoir
Computed P-values 1500 of 2001 datapoir
Computed P-values 2000 of 2001 datapoir
Mean value of sigma: 0.56525
Minimum value of sigma: 0.49359
Maximum value of sigma: 0.67268
```

```
figure;
plot(out.ratio(1:5), 'linewidth',2.0)
xlabel('k', 'FontSize', 24);
ylabel('EPI', 'FontSize', 24);
xticks(0:30);
```



Dynamical Analysis and Output

```
tic;
par.choice_distance = 'euclid';
par.K_cluster = 2; %selected based on E
par.trials = 2; % number of random trai
% the main function of MuTrans
Output = DynamicalAnalysis (data, par);
```

```
Computed P-values 500 of 2001 datapoint
Computed P-values 1000 of 2001 datapoir
Computed P-values 1500 of 2001 datapoir
Computed P-values 2000 of 2001 datapoir
```

```
Mean value of sigma: 0.56525
Minimum value of sigma: 0.49359
Maximum value of sigma: 0.67268
Computed P-values 500 of 2001 datapoint
Computed P-values 1000 of 2001 datapoir
Computed P-values 1500 of 2001 datapoir
Computed P-values 2000 of 2001 datapoir
Mean value of sigma: 0.024841
Minimum value of sigma: 0.011406
Maximum value of sigma: 0.11343
Iteration 10: error is 49.7663
Iteration 20: error is 44.793
Iteration 30: error is 42.3252
Iteration 40: error is 41.6031
Iteration 50: error is 41.1513
Iteration 60: error is 40.9008
Iteration 70: error is 40.7205
Iteration 80: error is 40.5912
Iteration 90: error is 40.4917
Iteration 100: error is 1.8194
Iteration 110: error is 1.5155
```

```
Iteration 120: error is 1.2301
Iteration 130: error is 1.0449
Iteration 140: error is 0.92788
Iteration 150: error is 0.85732
Iteration 160: error is 0.80968
Iteration 170: error is 0.77235
Iteration 180: error is 0.744
Iteration 190: error is 0.72155
Iteration 200: error is 0.70321
Iteration 210: error is 0.68823
Iteration 220: error is 0.67563
Iteration 230: error is 0.66508
Iteration 240: error is 0.65607
Iteration 250: error is 0.64829
Iteration 260: error is 0.63619
Iteration 270: error is 0.623
Iteration 280: error is 0.61251
Iteration 290: error is 0.60468
Iteration 300: error is 0.5986
Iteration 310: error is 0.59368
Iteration 320: error is 0.5897
```

```
Iteration 330: error is 0.58638
Iteration 340: error is 0.58355
Iteration 350: error is 0.58113
Iteration 360: error is 0.57903
Iteration 370: error is 0.57719
Iteration 380: error is 0.57554
Iteration 390: error is 0.57406
Iteration 400: error is 0.5727
Iteration 410: error is 0.57148
Iteration 420: error is 0.5703
Iteration 430: error is 0.5692
Iteration 440: error is 0.56827
Iteration 450: error is 0.56739
Iteration 460: error is 0.5666
Iteration 470: error is 0.56589
Iteration 480: error is 0.56523
Iteration 490: error is 0.56461
Iteration 500: error is 0.56404
Iteration 510: error is 0.5635
Iteration 520: error is 0.563
Iteration 530: error is 0.56253
```

```
Iteration 540: error is 0.56209
Iteration 550: error is 0.56167
Iteration 560: error is 0.56128
Iteration 570: error is 0.56092
Iteration 580: error is 0.56057
Iteration 590: error is 0.56024
Iteration 600: error is 0.55992
Iteration 610: error is 0.55962
Iteration 620: error is 0.55934
Iteration 630: error is 0.55907
Iteration 640: error is 0.55881
Iteration 650: error is 0.55856
Iteration 660: error is 0.55833
Iteration 670: error is 0.5581
Iteration 680: error is 0.55788
Iteration 690: error is 0.55768
Iteration 700: error is 0.55747
Iteration 710: error is 0.55728
Iteration 720: error is 0.5571
Iteration 730: error is 0.55692
Iteration 740: error is 0.55675
```

```
Iteration 750: error is 0.55658
Iteration 760: error is 0.55642
Iteration 770: error is 0.55627
Iteration 780: error is 0.55612
Iteration 790: error is 0.55598
Iteration 800: error is 0.55584
Iteration 810: error is 0.5557
Iteration 820: error is 0.55557
Iteration 830: error is 0.55545
Iteration 840: error is 0.55532
Iteration 850: error is 0.55521
Iteration 860: error is 0.55509
Iteration 870: error is 0.55498
Iteration 880: error is 0.55487
Iteration 890: error is 0.55476
Iteration 900: error is 0.55466
Iteration 910: error is 0.55456
Iteration 920: error is 0.55446
Iteration 930: error is 0.55437
Iteration 940: error is 0.55428
Iteration 950: error is 0.55419
```

```
Iteration 960: error is 0.5541
Iteration 970: error is 0.55402
Iteration 980: error is 0.55393
Iteration 990: error is 0.55385
Iteration 1000: error is 0.55377
J_new = 1.8448
J_new = 1.8440
J_new = 1.8435
J_new = 1.8432
J_new = 1.8431
J_new = 1.8430
J_new = 1.8430
Computed P-values 500 of 2001 datapoint
Computed P-values 1000 of 2001 datapoir
Computed P-values 1500 of 2001 datapoir
Computed P-values 2000 of 2001 datapoir
Mean value of sigma: 0.024841
Minimum value of sigma: 0.011406
Maximum value of sigma: 0.11343
Iteration 10: error is 49.7659
Iteration 20: error is 44.7401
```

```
Iteration 30: error is 42.4186
Iteration 40: error is 41.805
Iteration 50: error is 41.4433
Iteration 60: error is 41.0955
Iteration 70: error is 40.8841
Iteration 80: error is 40.7423
Iteration 90: error is 40.629
Iteration 100: error is 1.8534
Iteration 110: error is 1.5425
Iteration 120: error is 1.2628
Iteration 130: error is 1.0745
Iteration 140: error is 0.95517
Iteration 150: error is 0.88338
Iteration 160: error is 0.83358
Iteration 170: error is 0.79519
Iteration 180: error is 0.76592
Iteration 190: error is 0.74267
Iteration 200: error is 0.72378
Iteration 210: error is 0.70833
Iteration 220: error is 0.69542
Iteration 230: error is 0.6845
```

```
Iteration 240: error is 0.67515
Iteration 250: error is 0.66708
Iteration 260: error is 0.65452
Iteration 270: error is 0.64075
Iteration 280: error is 0.62976
Iteration 290: error is 0.62142
Iteration 300: error is 0.61487
Iteration 310: error is 0.60958
Iteration 320: error is 0.60522
Iteration 330: error is 0.60154
Iteration 340: error is 0.59837
Iteration 350: error is 0.59564
Iteration 360: error is 0.59324
Iteration 370: error is 0.59111
Iteration 380: error is 0.58921
Iteration 390: error is 0.5875
Iteration 400: error is 0.58594
Iteration 410: error is 0.58453
Iteration 420: error is 0.58323
Iteration 430: error is 0.58203
Iteration 440: error is 0.58092
```

```
Iteration 450: error is 0.57989
Iteration 460: error is 0.57893
Iteration 470: error is 0.57802
Iteration 480: error is 0.57717
Iteration 490: error is 0.57638
Iteration 500: error is 0.57561
Iteration 510: error is 0.57489
Iteration 520: error is 0.5742
Iteration 530: error is 0.57355
Iteration 540: error is 0.57292
Iteration 550: error is 0.57232
Iteration 560: error is 0.57176
Iteration 570: error is 0.5712
Iteration 580: error is 0.57067
Iteration 590: error is 0.57016
Iteration 600: error is 0.56967
Iteration 610: error is 0.5692
Iteration 620: error is 0.56874
Iteration 630: error is 0.5683
Iteration 640: error is 0.56786
Iteration 650: error is 0.56745
```

```
Iteration 660: error is 0.56704
Iteration 670: error is 0.56665
Iteration 680: error is 0.56626
Iteration 690: error is 0.56589
Iteration 700: error is 0.56552
Iteration 710: error is 0.56517
Iteration 720: error is 0.56482
Iteration 730: error is 0.56448
Iteration 740: error is 0.56415
Iteration 750: error is 0.56383
Iteration 760: error is 0.56351
Iteration 770: error is 0.5632
Iteration 780: error is 0.5629
Iteration 790: error is 0.56261
Iteration 800: error is 0.56231
Iteration 810: error is 0.56203
Iteration 820: error is 0.56175
Iteration 830: error is 0.56148
Iteration 840: error is 0.56121
Iteration 850: error is 0.56095
Iteration 860: error is 0.56069
```

```
Iteration 870: error is 0.56043
Iteration 880: error is 0.56018
Iteration 890: error is 0.55994
Iteration 900: error is 0.5597
Iteration 910: error is 0.55946
Iteration 920: error is 0.55923
Iteration 930: error is 0.559
Iteration 940: error is 0.55877
Iteration 950: error is 0.55855
Iteration 960: error is 0.55833
Iteration 970: error is 0.55811
Iteration 980: error is 0.5579
Iteration 990: error is 0.55769
Iteration 1000: error is 0.55748
J_new = 1.8440
J_new = 1.8432
J_new = 1.8431
J_new = 1.8430
J_new = 1.8430
E_best = 0.1465
```

Iteration	Func-count	f(x)
0	1	1.84352
1	11	1.79746
2	14	1.7973
3	15	1.79128
4	16	1.78939
5	17	1.78791
6	18	1.78707
7	19	1.78657
8	20	1.78628
9	21	1.7859
10	22	1.78563
11	23	1.78544
12	24	1.78529
13	25	1.78512
14	26	1.78498
15	27	1.78487
16	28	1.78477
17	29	1.78469
18	30	1.78459
19	31	1.78452

Iteration	Func-count	f(x)
20	32	1.78439
21	33	1.78431
22	34	1.78419
23	35	1.7841
24	36	1.78399
25	37	1.78388
26	38	1.7838
27	39	1.78371
28	40	1.78363
29	41	1.78355
30	42	1.78349
31	43	1.78344
32	44	1.78339
33	45	1.78335
34	46	1.78332
35	47	1.78329
36	48	1.78327
37	49	1.78325
38	50	1.78323

39	51	1.78322

Iteration	Func-count	f(x)
40	52	1.7832
41	53	1.7832
42	54	1.78319
43	55	1.78318
44	56	1.78318
45	57	1.78317
46	58	1.78317
47	59	1.78316
48	60	1.78316
49	61	1.78316
50	62	1.78316
51	63	1.78316
52	64	1.78316
53	65	1.78315
54	66	1.78315
55	67	1.78315
56	68	1.78315
57	69	1.78315

```
    58            70           1.78315
    59            71           1.78315

 Iteration  Func-count        f(x)
    60            72           1.78315
    61            73           1.78315
    62            74           1.78315
    63            75           1.78315

Optimization completed: The first-order
than options.OptimalityTolerance = 1.00

Elapsed time is 38.325406 seconds.
```

```
toc;
```

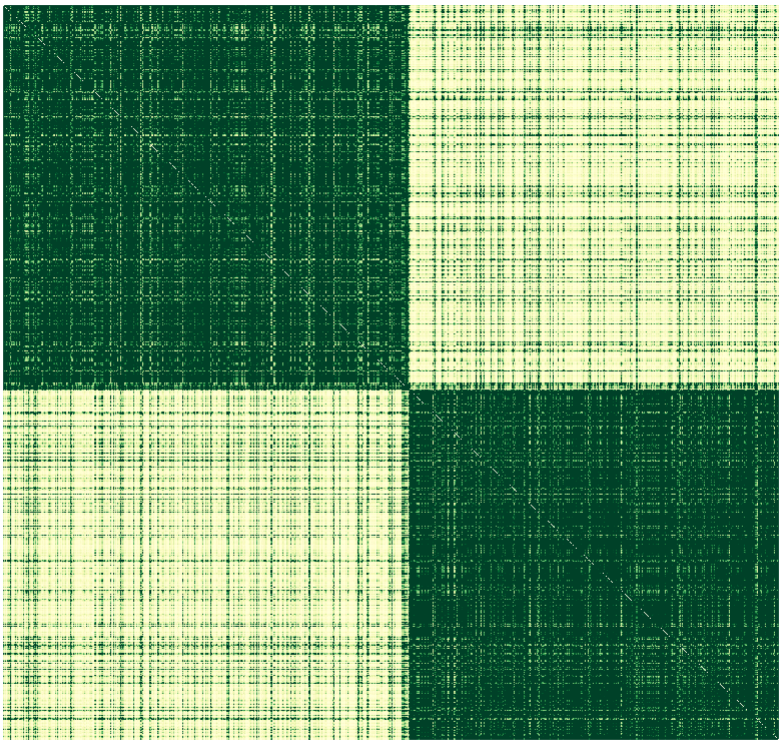
```
Elapsed time is 38.340527 seconds.
```

```
class_order = Output.class_order;
rho_class = Output.rho_class;
perm_class = Output.perm_class;
P_perm = Output.P_perm;
```

```
P_hat = Output.P_hat;
P_appr_perm = Output.P_appr_perm;
P_rho = Output.P_rho;
labs_perm = Output.labs_perm;
data_perm = Output.data_perm;
mu_hat = Output.mu_hat;
k = Output.k;
H = Output.H;
```

Plot the Cell-Cell Scale rwTPM

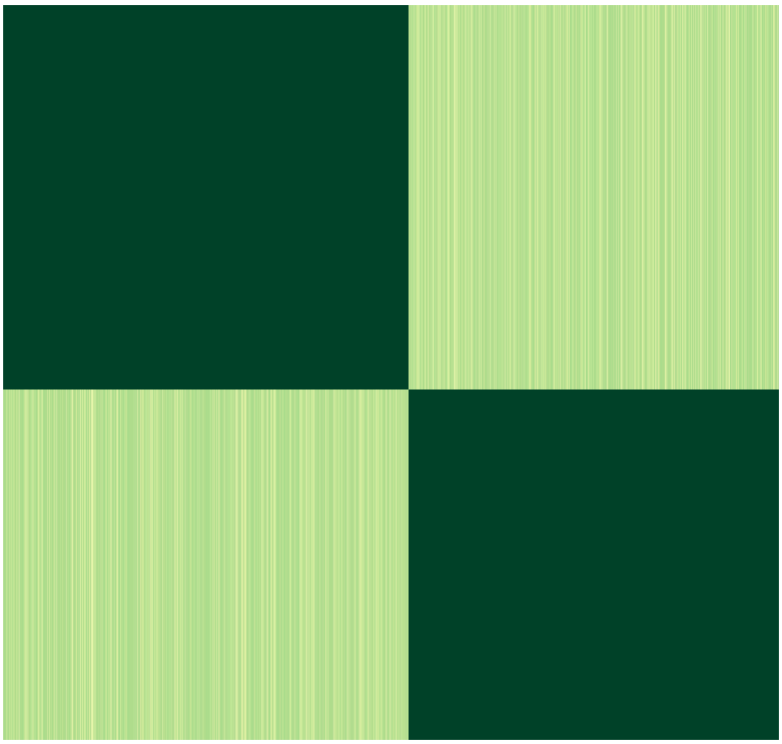
```
max_P = 0.2* max(max(P_rho));
c_lim = [0 max_P];
cmp = 'ylgn';

figure('rend','painters','pos',[10 10 5
colormap(brewermap([],cmp))
imagesc(P_perm);
axis off
set(gca,'xtick',[],'ytick',[]);
caxis(c_lim)
```



```
%colorbar;
```

Plot the Cluster-Cluster Scale rwTPM

```
figure('rend','painters','pos',[10 10 5
colormap(brewermap([],cmp))
imagesc(P_appr_perm);
axis off
set(gca,'xtick',[],'ytick',[]);
caxis(c_lim)
```

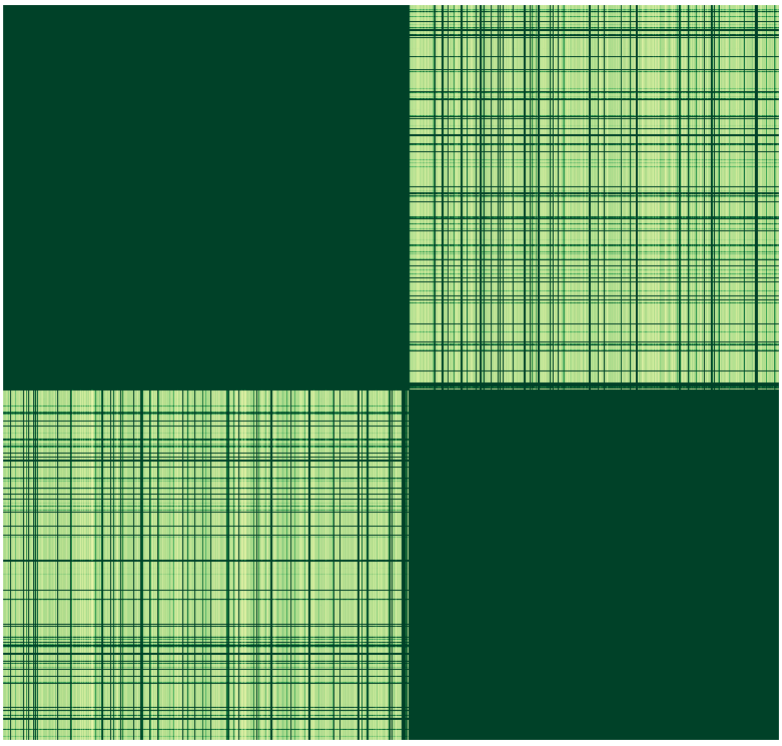


```
%colorbar;
```

Plot the Cell-Cluster Scale rwTPM

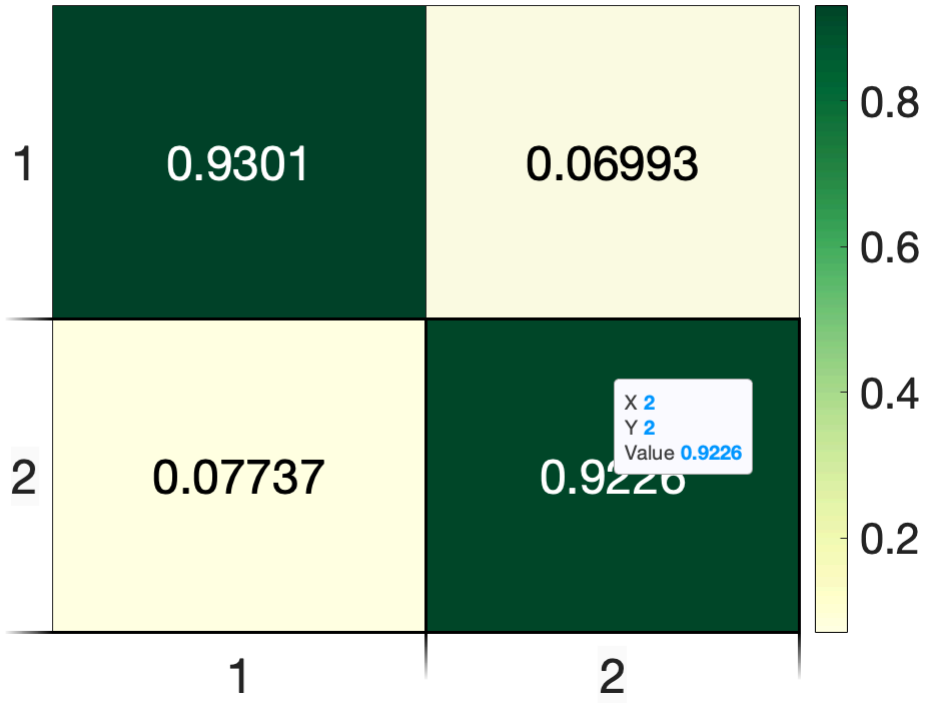
```
figure('rend','painters','pos',[10 10 5
colormap(brewermap([],cmp))
imagesc(P_rho);
axis off
set(gca,'xtick',[],'ytick',[]);
```

```
caxis(c_lim)
%colorbar;
box off
```



Plot Transition Cell Score (TCS)

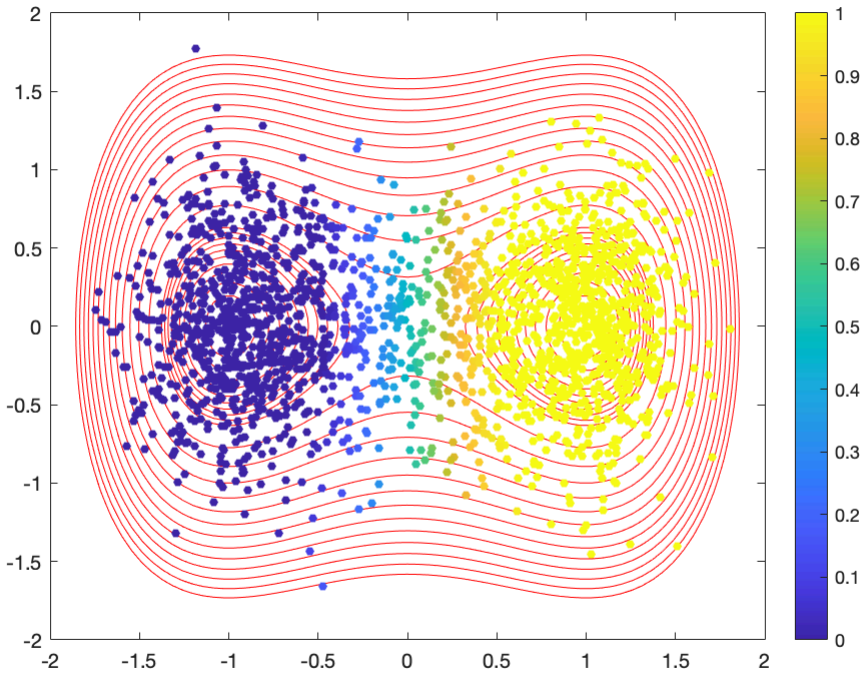
```
figure
heatmap(P_hat,'Colormap',colormap(brewe
```




```
figure
```

```
P_hat = 2×2
    0.9301    0.0699
    0.0774    0.9226
```

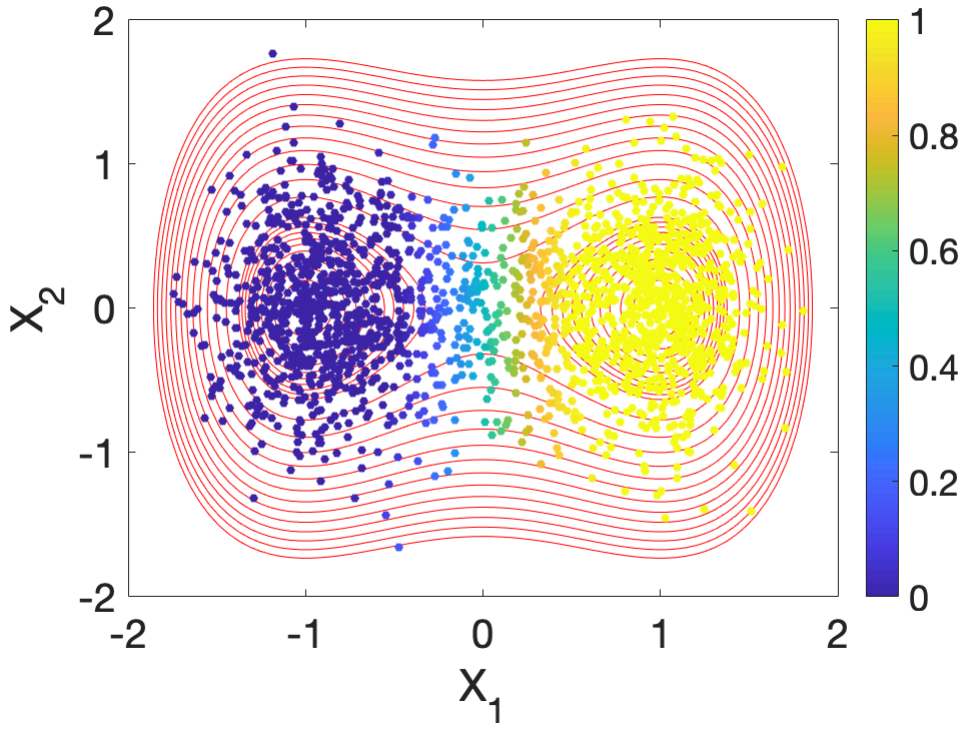
```
fc = fcontour(@double_well_potential,[-
fc.LevelList = [0:0.2:2,3:15];
hold on
scatter(data_perm(:,1),data_perm(:,2),2
colorbar
caxis([0 1])
```




```
set(gca,'FontSize',20)
xlabel('X_{1}')
ylabel('X_{2}')
```

```
figure
fc = fcontour(@double_well_potential,[-
fc.LevelList = [0:0.2:2,3:15];
hold on
scatter(data_perm(:,1),data_perm(:,2),2
colorbar
caxis([0 1])
set(gca,'FontSize',20)
```

```
xlabel('X_{1}')
ylabel('X_{2}')
```




```
function v = double_well_potential(x,y)
    v = 2.5*(x.^2-1).^2+5*y.^2;
end

function dv = double_well_gradient_neg(
    dv = zeros(2,1);
    dv(1) = -10*(x(1)^2-1)*x(1);
    dv(2) = -10*x(2);
end
```