Analysis of the Simulation Data from Double-Well Potential
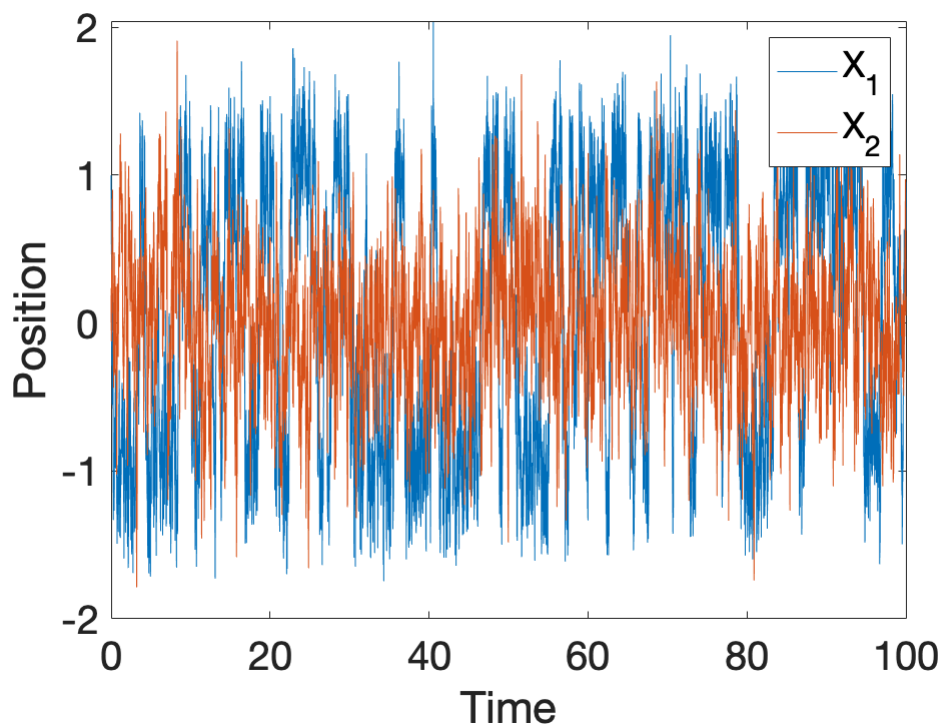
```matlab
clearvars;
addpath(genpath('../'))
```

Generating simulation data

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



```matlab
figure;
fc = fcontour(@double_well_potential,[-2 2 -2 2],'Fill',"on");
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','LineWidth',0.1)
xlabel('X_{1}')
```

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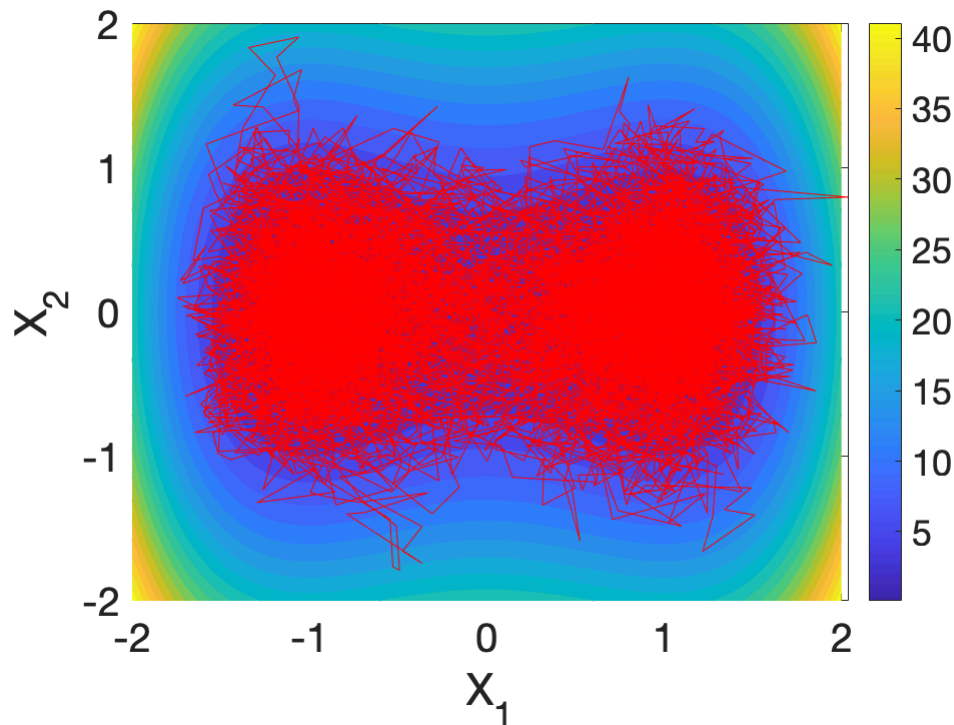


```
data = x_out(:,1:5:end)';
%save
%{
save('../Data/double_well.mat','x_out','t_out');
%}
```

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

```
par.choice_distance = 'euclid';
out = EstClusterNum(data,par);
```

```
Computed P-values 500 of 2001 datapoints...
Computed P-values 1000 of 2001 datapoints...
Computed P-values 1500 of 2001 datapoints...
Computed P-values 2000 of 2001 datapoints...
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);
```
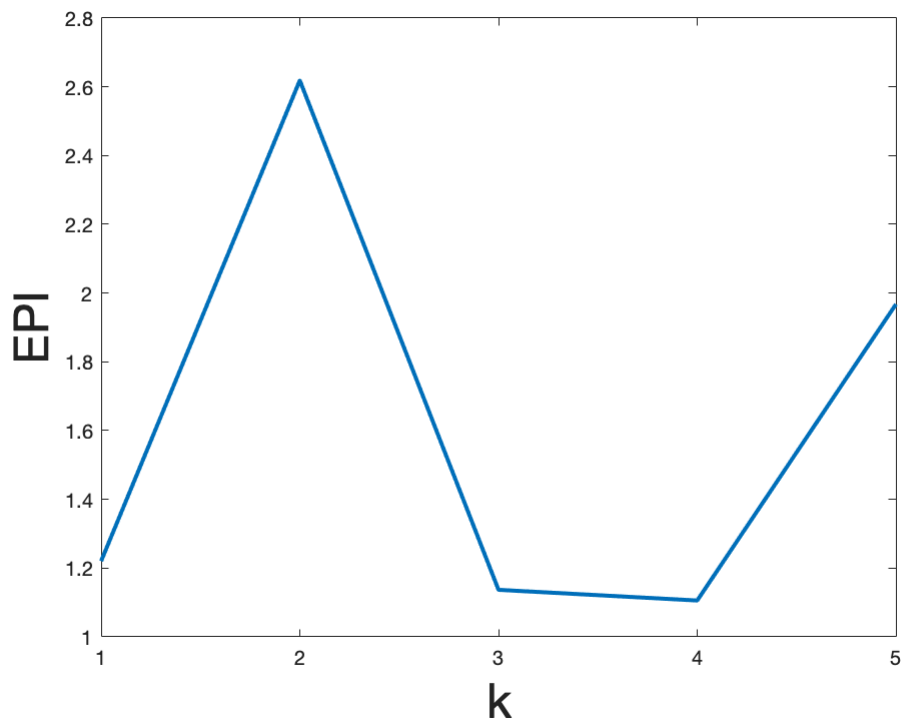
Dynamical Analysis and Output

```
tic;
par.choice_distance = 'euclid';
par.K_cluster = 2; %selected based on EPI
par.trials = 2; % number of random trails in MuTrans, increase this to guaratee more robustness
% the main function of MuTrans
Output = DynamicalAnalysis (data, par);
```

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

| | | | | First-order |
Iteration	Func-count	f(x)	Step-size	optimality
0	1	1.84352		1.94e-05
1	11	1.79746	158511	0.000297
2	14	1.7973	0.0231234	0.000316
3	15	1.79128	1	0.000133
4	16	1.78939	1	0.000184
5	17	1.78791	1	9.97e-05
6	18	1.78707	1	5.03e-05
7	19	1.78657	1	9.08e-05
8	20	1.78628	1	7.29e-05
9	21	1.7859	1	2.43e-05
10	22	1.78563	1	2.96e-05
11	23	1.78544	1	3.21e-05
12	24	1.78529	1	3.12e-05
13	25	1.78512	1	3.24e-05
14	26	1.78498	1	2.74e-05
15	27	1.78487	1	2.96e-05
16	28	1.78477	1	1.71e-05
17	29	1.78469	1	1.9e-05
18	30	1.78459	1	1.96e-05
19	31	1.78452	1	2.24e-05

| | | | | First-order |
Iteration	Func-count	f(x)	Step-size	optimality
20	32	1.78439	1	2.36e-05
21	33	1.78431	1	2.08e-05
22	34	1.78419	1	2.44e-05
23	35	1.7841	1	2.45e-05
24	36	1.78399	1	2.97e-05
25	37	1.78388	1	1.85e-05
26	38	1.7838	1	1.95e-05
27	39	1.78371	1	1.69e-05
28	40	1.78363	1	1.64e-05
29	41	1.78355	1	1.43e-05
30	42	1.78349	1	1.45e-05
31	43	1.78344	1	1.15e-05
32	44	1.78339	1	1.06e-05
33	45	1.78335	1	1.1e-05
34	46	1.78332	1	1.3e-05
35	47	1.78329	1	9.36e-06
36	48	1.78327	1	9.4e-06
37	49	1.78325	1	6.75e-06
38	50	1.78323	1	8.19e-06
39	51	1.78322	1	6.12e-06

| | | | | First-order |
Iteration	Func-count	f(x)	Step-size	optimality
40	52	1.7832	1	7.86e-06
41	53	1.7832	1	7.24e-06
42	54	1.78319	1	6.14e-06
43	55	1.78318	1	4.4e-06

				First-order
44	56	1.78318	1	5.21e-06
45	57	1.78317	1	3.46e-06
46	58	1.78317	1	3.56e-06
47	59	1.78316	1	3.02e-06
48	60	1.78316	1	3.6e-06
49	61	1.78316	1	2.89e-06
50	62	1.78316	1	2.77e-06
51	63	1.78316	1	2.3e-06
52	64	1.78316	1	2.69e-06
53	65	1.78315	1	2.18e-06
54	66	1.78315	1	1.93e-06
55	67	1.78315	1	1.46e-06
56	68	1.78315	1	1.63e-06
57	69	1.78315	1	1.52e-06
58	70	1.78315	1	1.61e-06
59	71	1.78315	1	1.28e-06

				First-order
Iteration	Func-count	f(x)	Step-size	optimality
60	72	1.78315	1	1.45e-06
61	73	1.78315	1	1.22e-06
62	74	1.78315	1	1.08e-06
63	75	1.78315	1	9.19e-07

```
Optimization completed: The first-order optimality measure, 9.186200e-07, is less
than options.OptimalityTolerance = 1.000000e-06.

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 10 500  450])
colormap(brewermap([],cmp))
imagesc(P_perm);
axis off
set(gca,'xtick',[],'ytick',[]);
caxis(c_lim)
```
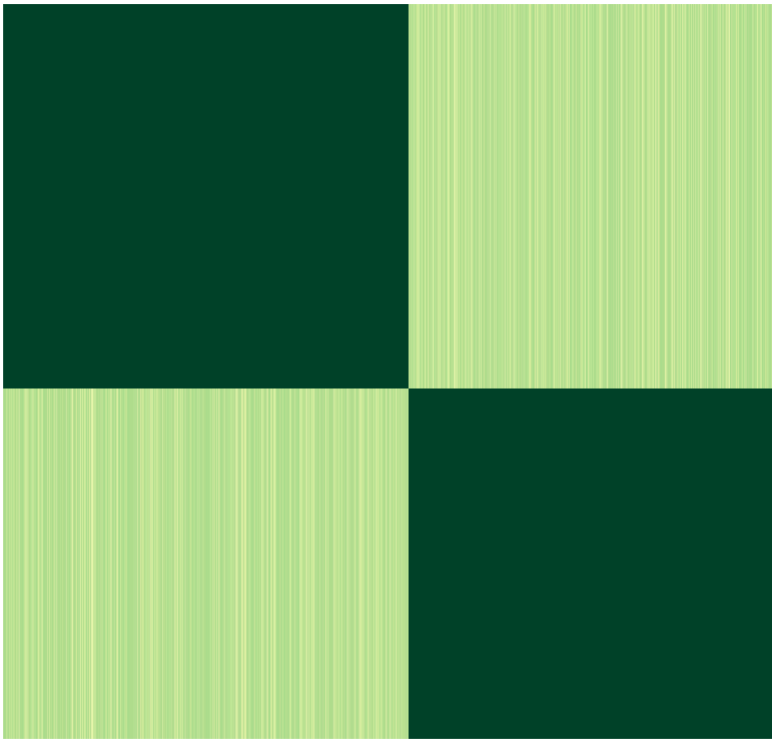
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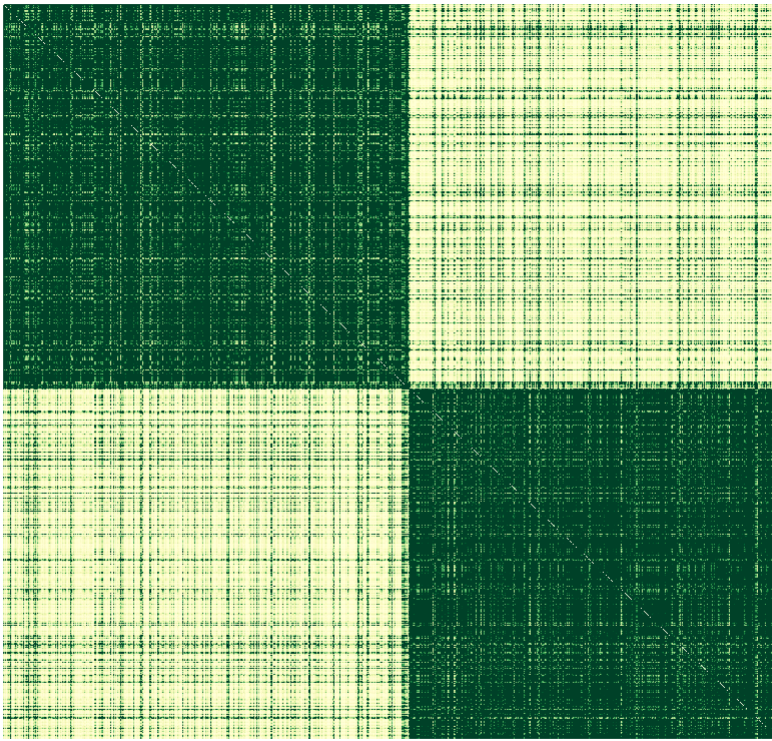
```
%colorbar;
```
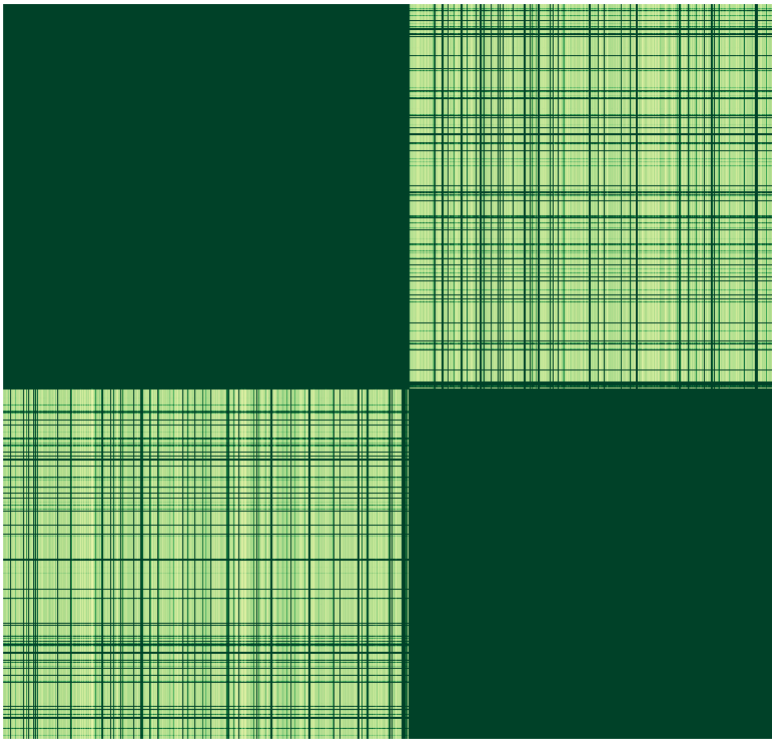
Plot the Cluster-Cluster Scale rwTPM

```
figure('rend','painters','pos',[10 10 500  450])
colormap(brewermap([],cmp))
imagesc(P_appr_perm);
axis off
set(gca,'xtick',[],'ytick',[]);
caxis(c_lim)
```
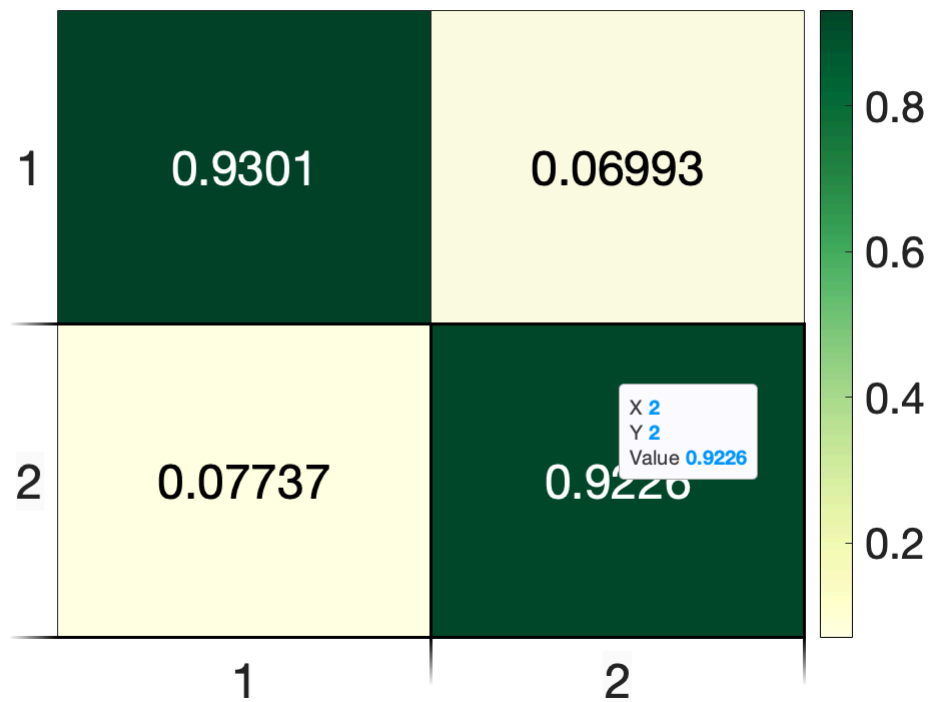
```
%colorbar;
```

Plot the Cell-Cluster Scale rwTPM

```
figure('rend','painters','pos',[10 10 500  450])
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(brewermap([],cmp)),'FontSize',24)
```

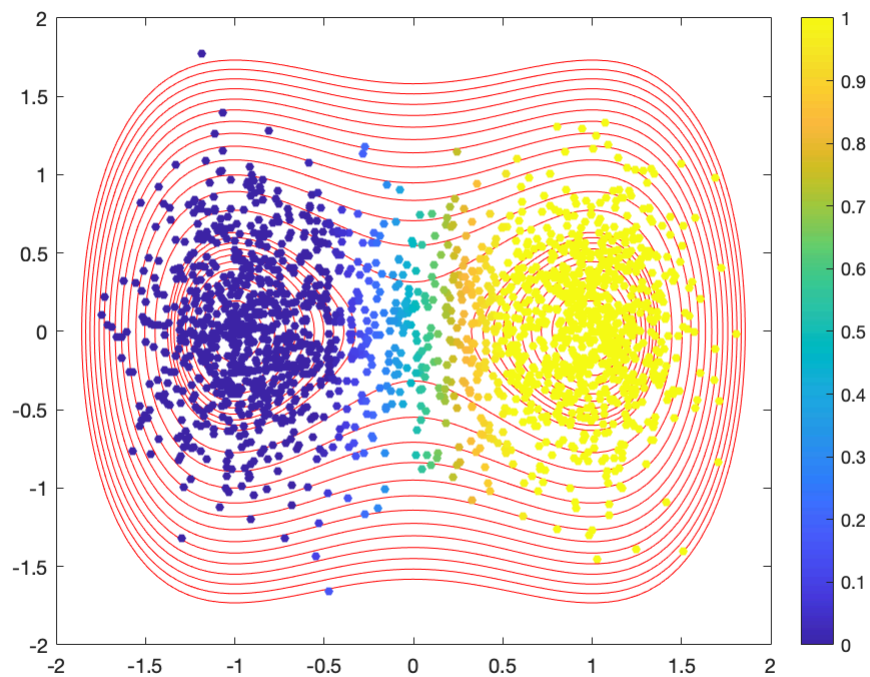|	1	2
1	0.9301	0.06993
2	0.07737	0.9226

```
figure
```

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

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

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

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

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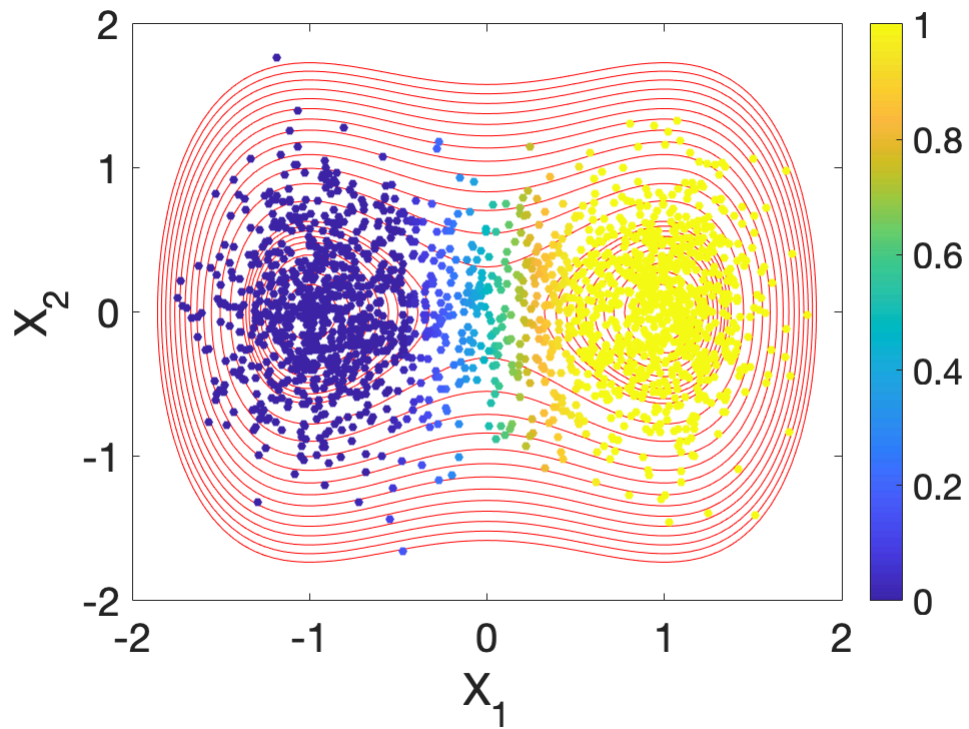
```matlab
function v = double_well_potential(x,y)
    v = 2.5*(x.^2-1).^2+5*y.^2;
end

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