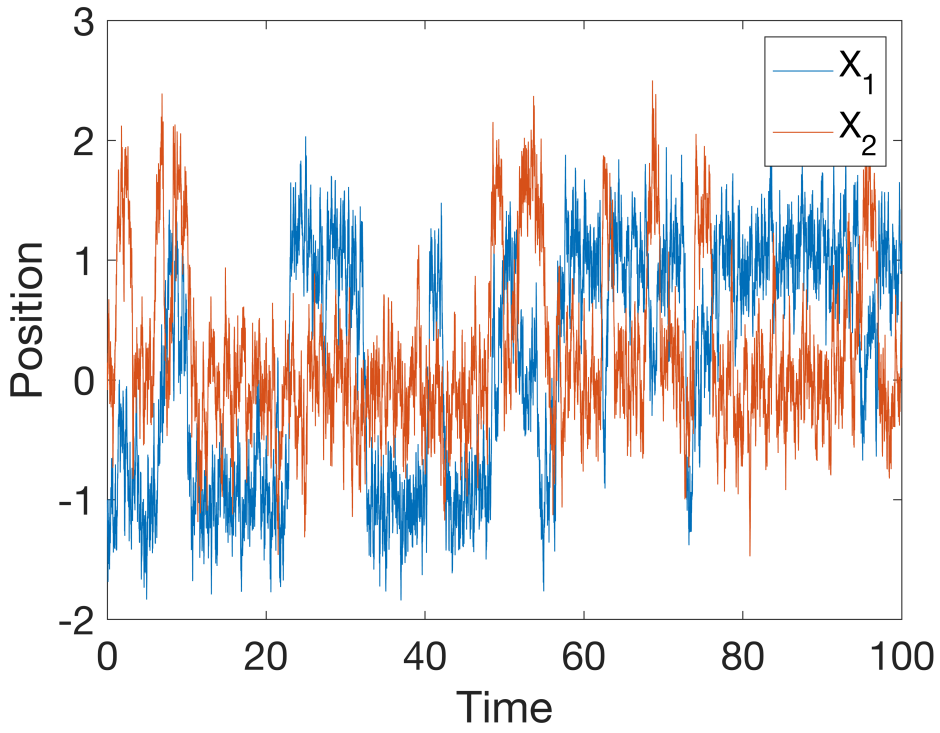
Analysis of the Simulation Data from Triple-Well Potential

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

Generating simulation data

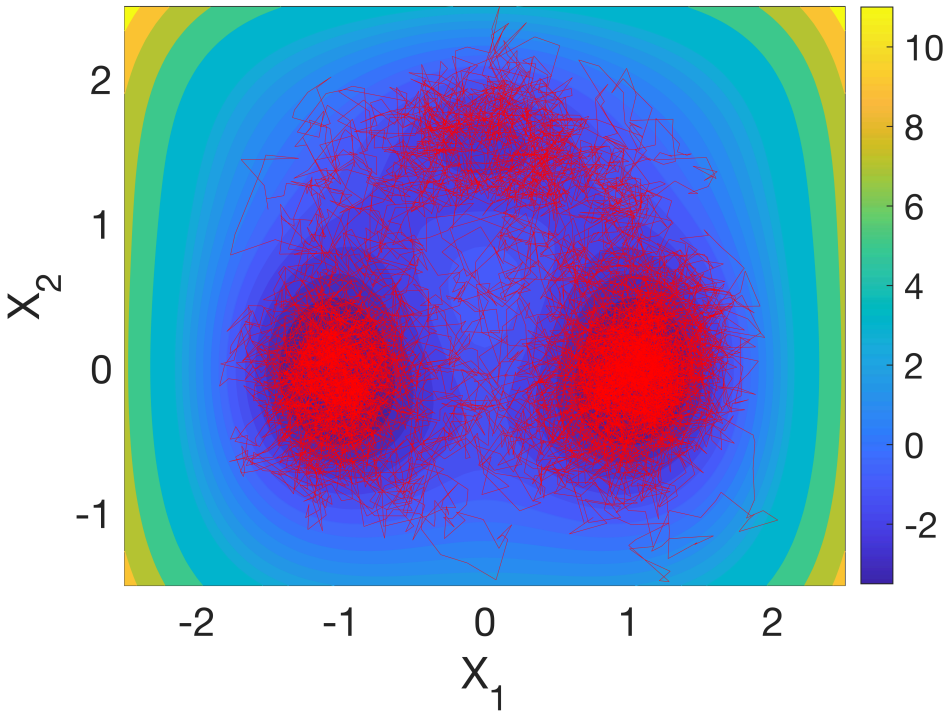
```
rng(1)
x_0 = [-1,0]';
par.T_max = 100;
par.dt = 1e-2;
sigma = 0.8; % 1.2,1.5
[x_out, t_out] = generating_simulation_data (@triple_well_gradient_neg, sigma, x_0, par);
```

```
figure;
plot(t_out,x_out)
set(gca,'FontSize',20)
legend('X_{1}','X_{2}')
xlabel('Time')
ylabel('Position')
```




```
figure;
fc = fcontour(@triple_well_potential,[-2.5 2.5 -1.5 2.5],'Fill',"on" );
fc.LevelList = [-10:0.5:3,3:2:50];
colorbar
hold on
plot(x_out(1,:),x_out(2,:),"Color",'r','LineWidth',0.2)
```

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




```
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

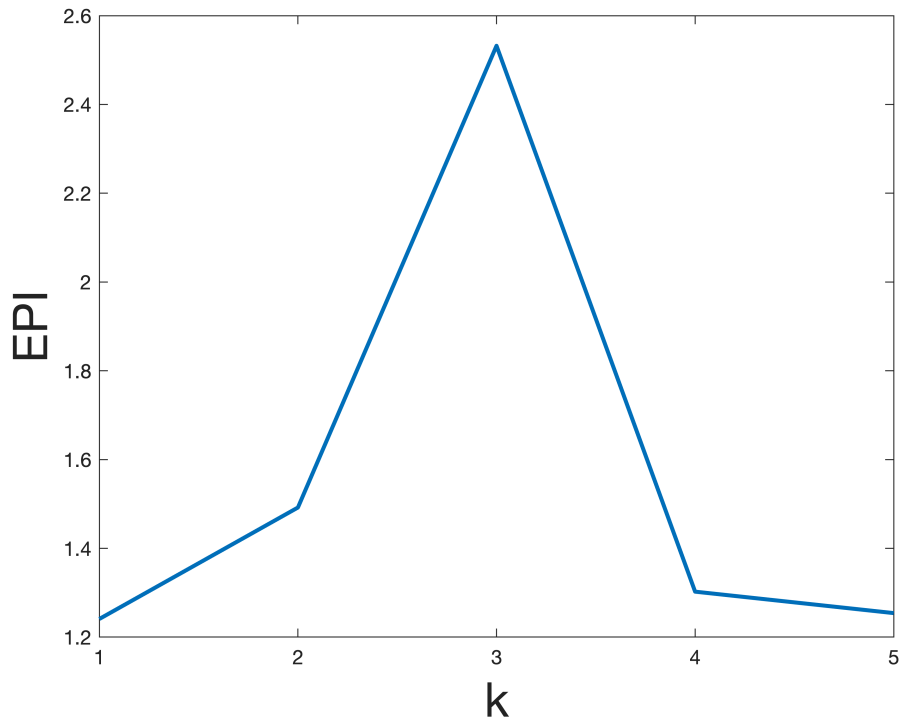
From EPI plot, we intend to seek for the index where peak occurs, which serves as the candidate for the choice of cluster numbers

```
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: 0.61654
Minimum value of sigma: 0.4928
Maximum value of sigma: 0.78183
```

```
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 = 3; %selected based on EPI
par.trials = 2; % number of random trails in MuTrans, increase this to guaratee more robustness
par.initial = 'random';
% 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: 0.61654
Minimum value of sigma: 0.4928
Maximum value of sigma: 0.78183
J_new = 1.8788
J_new = 1.5264
J_new = 1.4310
J_new = 1.3600
J_new = 1.3389
J_new = 1.3370
J_new = 1.3361
J_new = 1.3356
J_new = 1.3350
J_new = 1.3344
J_new = 1.3344
J_new = 2.1691
J_new = 1.7141
J_new = 1.6497
J_new = 1.6321
```

```
J_new = 1.6197
J_new = 1.6060
J_new = 1.5878
J_new = 1.5664
J_new = 1.5358
J_new = 1.4971
J_new = 1.4413
J_new = 1.3711
J_new = 1.3485
J_new = 1.3424
J_new = 1.3387
J_new = 1.3374
J_new = 1.3361
J_new = 1.3352
J_new = 1.3350
J_new = 1.3348
J_new = 1.3344
J_new = 1.3344
E_best = 0.1221
```

Iteration	Func-count	f(x)	Step-size	First-order optimality
0	1	1.33688		4.32e-05
1	10	1.27642	104888	0.000344
2	12	1.27471	0.120435	0.000344
3	14	1.2667	0.261503	0.000296
4	16	1.26264	0.57029	0.00023
5	17	1.26189	1	0.000347
6	18	1.25815	1	0.000326
7	20	1.25667	0.40636	0.000178
8	21	1.25579	1	0.000242
9	22	1.25547	1	0.000313
10	23	1.25414	1	0.000161
11	25	1.25349	0.507507	0.000113
12	26	1.25284	1	0.000176
13	27	1.25228	1	0.00021
14	28	1.25154	1	0.00017
15	29	1.25109	1	0.000152
16	30	1.25065	1	0.000147
17	31	1.25026	1	0.000106
18	32	1.24992	1	0.000107
19	33	1.24958	1	9.97e-05

Iteration	Func-count	f(x)	Step-size	First-order optimality
20	34	1.24936	1	0.000154
21	35	1.24908	1	0.000102
22	36	1.24893	1	9.31e-05
23	37	1.24869	1	7.07e-05
24	38	1.24855	1	0.000109
25	39	1.24842	1	0.000116
26	40	1.24827	1	6.78e-05
27	41	1.2482	1	0.000103
28	42	1.24806	1	6.79e-05
29	43	1.24804	1	0.000108
30	44	1.24794	1	8.03e-05
31	46	1.24788	0.524903	2.55e-05
32	47	1.24784	1	4.58e-05
33	48	1.24779	1	5.62e-05
34	49	1.24777	1	6.02e-05
35	50	1.24773	1	3.54e-05
36	51	1.24772	1	4.78e-05
37	52	1.2477	1	2.79e-05
38	53	1.24769	1	2.7e-05
39	54	1.24766	1	3.42e-05

Iteration	Func-count	f(x)	Step-size	First-order optimality

```
    40          55          1.24766              1       3.62e-05
    41          56          1.24764              1       2.67e-05
    42          57          1.24764              1       2.86e-05
    43          58          1.24762              1       2.26e-05
    44          59          1.24762              1       1.69e-05
    45          60          1.24761              1       1.97e-05
    46          61           1.2476              1       1.69e-05
    47          62           1.2476              1       1.96e-05
    48          63          1.24759              1       1.74e-05
    49          64          1.24759              1       1.82e-05
    50          65          1.24758              1       1.26e-05
    51          66          1.24758              1       1.52e-05
    52          67          1.24758              1       1.15e-05
    53          68          1.24758              1       1.34e-05
    54          69          1.24757              1       7.61e-06
    55          70          1.24757              1       1.08e-05
    56          71          1.24757              1       9.83e-06
    57          72          1.24757              1       5.99e-06
    58          73          1.24757              1       6.69e-06
    59          74          1.24756              1       4.97e-06
                                                        First-order
Iteration  Func-count       f(x)        Step-size       optimality
    60          75          1.24756              1       8.66e-06
    61          76          1.24756              1       6.05e-06
    62          77          1.24756              1       6.45e-06
    63          78          1.24756              1       5.41e-06
    64          79          1.24756              1       4.74e-06
    65          80          1.24756              1       5.74e-06
    66          81          1.24756              1       4.45e-06
    67          82          1.24755              1       5.61e-06
    68          83          1.24755              1       6.87e-06
    69          84          1.24755              1       5.88e-06
    70          85          1.24755              1       5.25e-06
    71          86          1.24755              1        3.7e-06
    72          87          1.24755              1       3.57e-06
    73          88          1.24755              1       2.81e-06
    74          89          1.24755              1       2.58e-06
    75          90          1.24755              1        4.5e-06
    76          91          1.24755              1       5.51e-06
    77          92          1.24755              1       3.69e-06
    78          93          1.24755              1       3.86e-06
    79          94          1.24754              1       4.23e-06
                                                        First-order
Iteration  Func-count       f(x)        Step-size       optimality
    80          95          1.24754              1       6.98e-06
    81          96          1.24754              1       3.95e-06
    82          97          1.24754              1       4.24e-06
    83          98          1.24754              1       4.52e-06
    84          99          1.24754              1       4.06e-06
    85         100          1.24754              1       4.82e-06
    86         101          1.24754              1       3.61e-06
    87         102          1.24754              1          4e-06
    88         103          1.24754              1       2.21e-06
    89         104          1.24754              1       3.87e-06
    90         105          1.24754              1       1.56e-06
    91         106          1.24754              1       2.37e-06
    92         107          1.24754              1       1.88e-06
    93         108          1.24754              1       2.05e-06
    94         109          1.24754              1       2.54e-06
    95         110          1.24754              1       4.59e-06
    96         111          1.24754              1       3.77e-06
    97         112          1.24754              1       6.53e-06
    98         113          1.24754              1       1.87e-06
    99         114          1.24754              1       3.49e-06
                                                        First-order
```

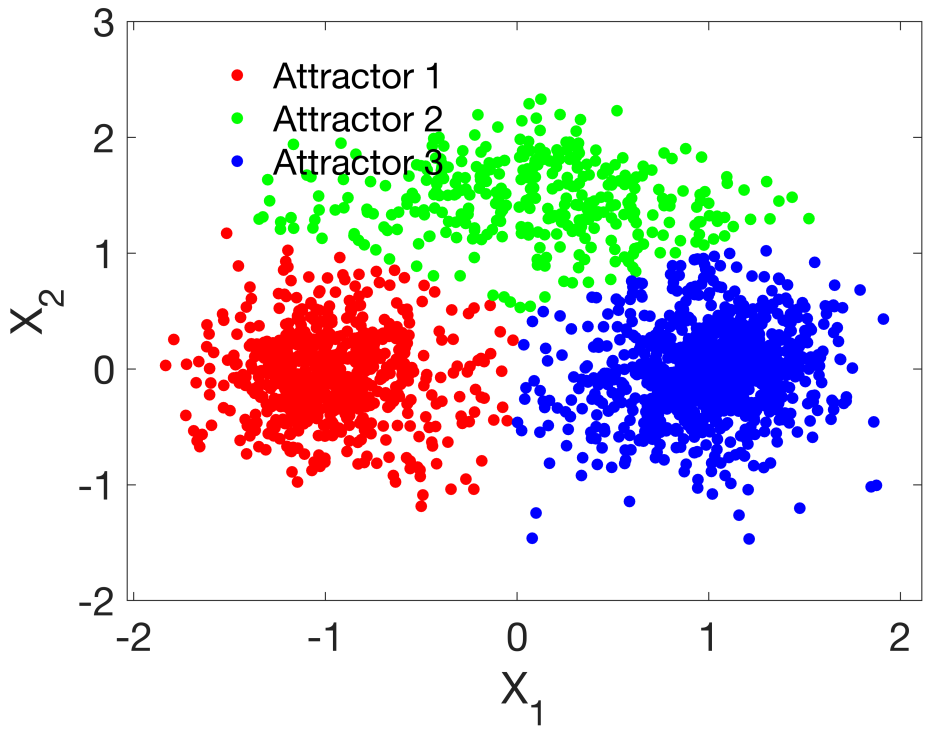
```
 Iteration  Func-count       f(x)        Step-size       optimality
   100         115          1.24754              1       2.14e-06
   101         116          1.24754              1       2.18e-06
   102         117          1.24753              1       3.18e-06
   103         118          1.24753              1       4.61e-06
   104         119          1.24753              1       2.81e-06
   105         120          1.24753              1       4.47e-06
   106         121          1.24753              1       3.09e-06
   107         122          1.24753              1       3.18e-06
   108         123          1.24753              1       2.49e-06
   109         124          1.24753              1       2.42e-06
   110         125          1.24753              1       1.71e-06
   111         126          1.24753              1       1.84e-06
   112         127          1.24753              1       2.07e-06
   113         128          1.24753              1       2.17e-06
   114         129          1.24753              1       3.12e-06
   115         130          1.24753              1       5.22e-06
   116         131          1.24753              1       2.24e-06
   117         132          1.24753              1        3.4e-06
   118         133          1.24753              1       3.92e-06
   119         134          1.24753              1       3.34e-06
                                                     First-order
 Iteration  Func-count       f(x)        Step-size       optimality
   120         135          1.24753              1       2.16e-06
   121         136          1.24753              1        3.8e-06
   122         137          1.24753              1       1.84e-06
   123         138          1.24753              1       2.78e-06
   124         139          1.24753              1          2e-06
   125         140          1.24753              1       2.58e-06
   126         141          1.24753              1       2.48e-06
   127         142          1.24753              1       1.57e-06
   128         143          1.24753              1       2.26e-06
   129         144          1.24753              1       1.91e-06
   130         145          1.24753              1       1.86e-06
   131         146          1.24753              1       1.61e-06
   132         147          1.24753              1       1.58e-06
   133         148          1.24752              1       1.19e-06
   134         149          1.24752              1       1.67e-06
   135         150          1.24752              1       1.39e-06
   136         151          1.24752              1       1.64e-06
   137         152          1.24752              1       1.79e-06
   138         153          1.24752              1       2.23e-06
   139         154          1.24752              1       1.61e-06
                                                     First-order
 Iteration  Func-count       f(x)        Step-size       optimality
   140         155          1.24752              1        2.2e-06
   141         156          1.24752              1       2.48e-06
   142         157          1.24752              1       1.61e-06
   143         158          1.24752              1       2.43e-06
   144         159          1.24752              1       3.16e-06
   145         160          1.24752              1       2.46e-06
   146         161          1.24752              1       1.23e-06
   147         162          1.24752              1       1.28e-06
   148         163          1.24752              1       9.17e-07

Optimization completed: The first-order optimality measure, 9.173883e-07, is less
than options.OptimalityTolerance = 1.000000e-06.

Elapsed time is 144.648490 seconds.
```

```
toc;
```

```
Elapsed time is 144.666496 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;
```

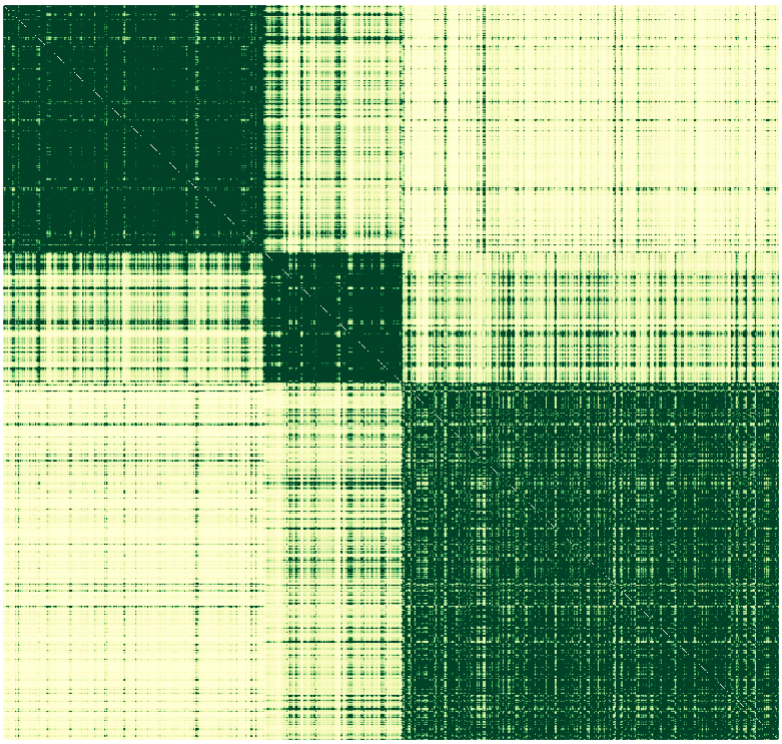
```
figure;
gscatter(data_perm(:,1),data_perm(:,2),class_order,[],[],20)
legend('Attractor 1','Attractor 2','Attractor 3')
xlabel('X_{1}')
ylabel('X_{2}')
set(gca,'FontSize',20)
legend boxoff
```



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])
```

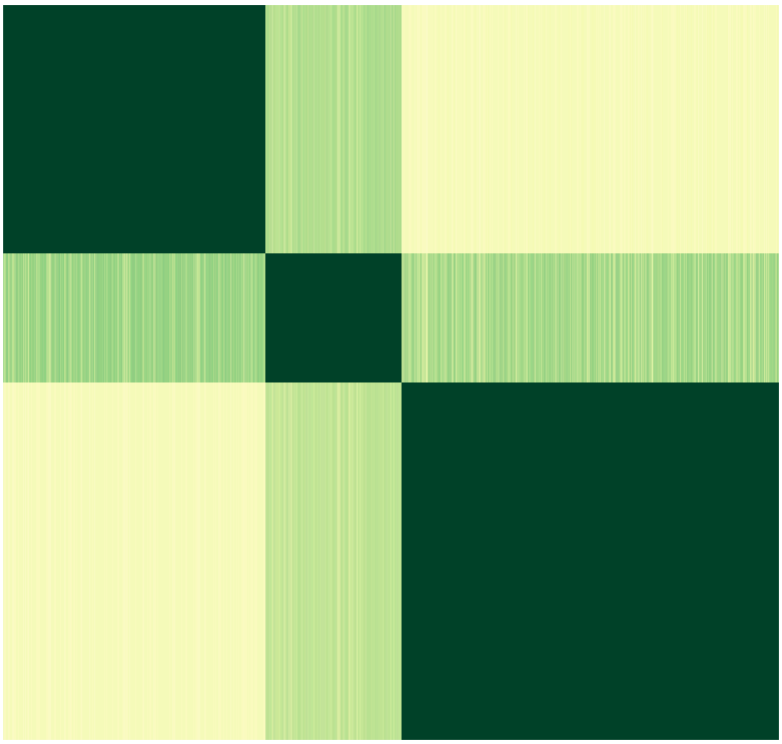
```
colormap(brewermap([],cmp))
imagesc(P_perm);
axis off
set(gca,'xtick',[],'ytick',[]);
caxis(c_lim)
```



```
%colorbar;
```

Plot the Cluster-Cluster Scale rwTPM

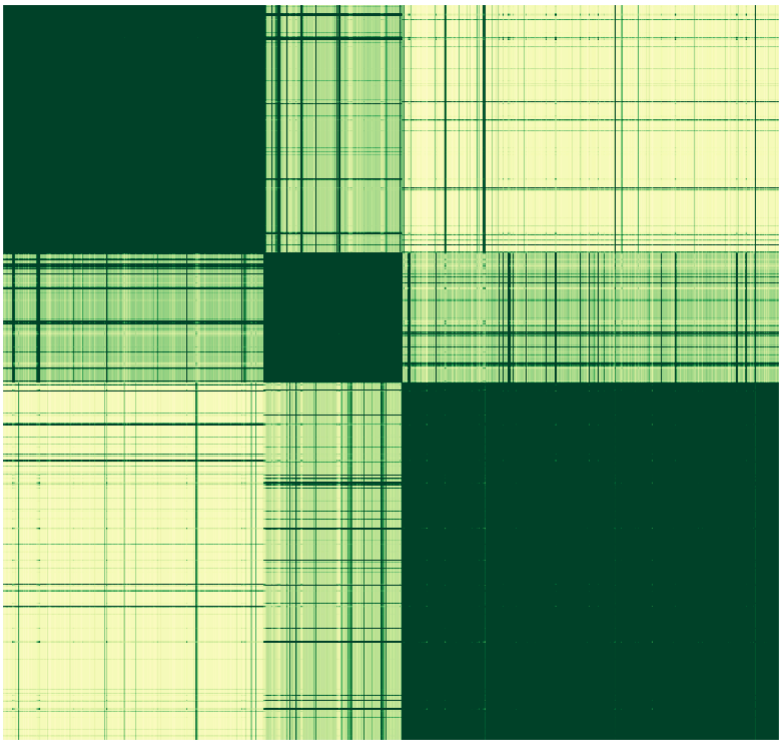
```
figure('rend','painters','pos',[10 10 500  450])
colormap(brewermap([],cmp))
imagesc(P_appr_perm);
axis off
set(gca,'xtick',[],'ytick',[]);
caxis(c_lim)
```



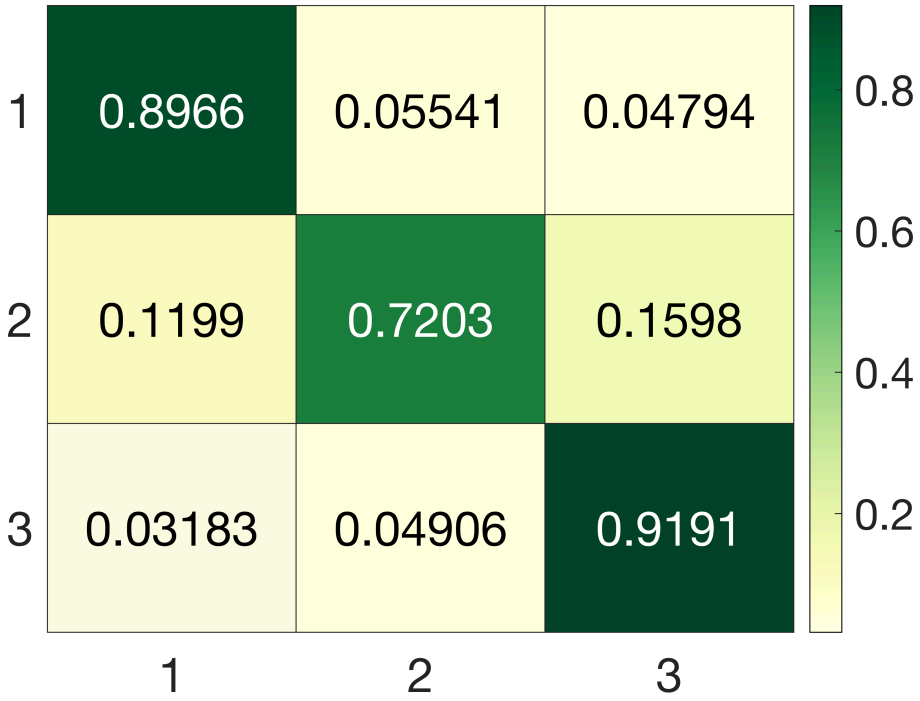
```
%colorbar;
```

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
```

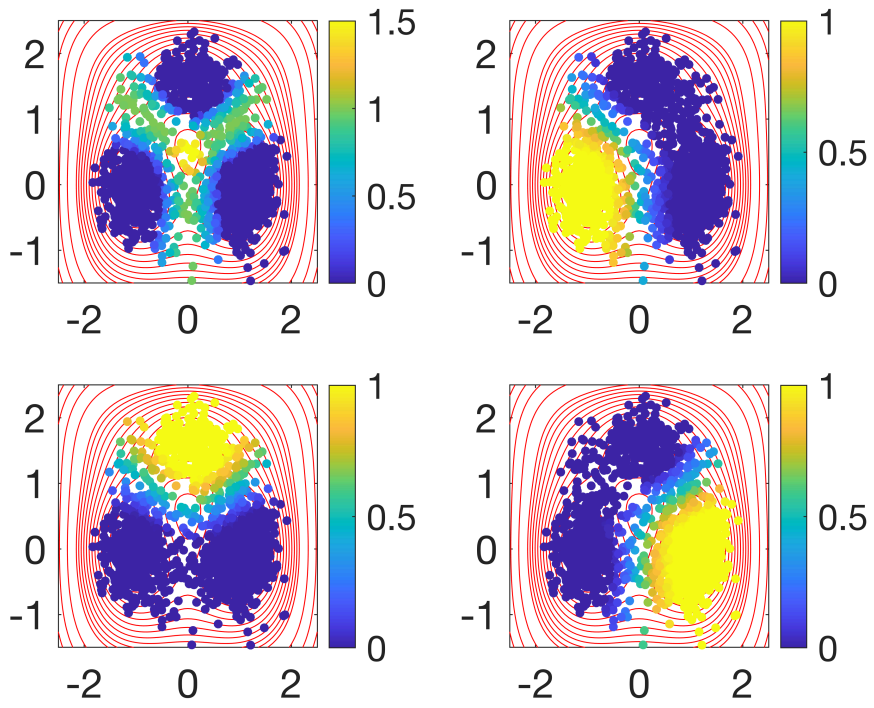


```
figure
heatmap(P_hat,'Colormap',colormap(brewermap([],cmp)),'FontSize',24)
```




```
figure
subplot(2,2,1)
fc = fcontour(@triple_well_potential,[-2.5 2.5 -1.5 2.5],'-r');
fc.LevelList = [-5:0.5:3,3:2:15];
hold on
scatter(data_perm(:,1),data_perm(:,2),20,H,'filled')
colorbar
caxis([0 1.5])
set(gca,'FontSize',20)

subplot(2,2,2)
fc = fcontour(@triple_well_potential,[-2.5 2.5 -1.5 2.5],'-r');
fc.LevelList = [-5:0.5:3,3:2:15];
hold on
scatter(data_perm(:,1),data_perm(:,2),20,rho_class(:,1),'filled')
colorbar
caxis([0 1])
set(gca,'FontSize',20)

subplot(2,2,3)
fc = fcontour(@triple_well_potential,[-2.5 2.5 -1.5 2.5],'-r');
fc.LevelList = [-5:0.5:3,3:2:15];
hold on
scatter(data_perm(:,1),data_perm(:,2),20,rho_class(:,2),'filled')
colorbar
caxis([0 1])
set(gca,'FontSize',20)

subplot(2,2,4)
```

```
fc = fcontour(@triple_well_potential,[-2.5 2.5 -1.5 2.5],'-r');
fc.LevelList = [-5:0.5:3,3:2:15];
hold on
scatter(data_perm(:,1),data_perm(:,2),20,rho_class(:,3),'filled')
colorbar
caxis([0 1])
set(gca,'FontSize',20)
```




```
function v = triple_well_potential(x,y)
    v = 3*exp(-x.^2-(y-1/3).^2)-3*exp(-x.^2-(y-5/3).^2)-5*exp(-(x-1).^2-y.^2)-5*exp(-(x+1).^2-y
end

function dv = triple_well_gradient_neg(x)
    dv = zeros(2,1);
    dv(1) = -6*x(1)*exp(-x(1)^2-(x(2)-1/3)^2)+6*x(1)*exp(-x(1)^2-(x(2)-5/3)^2)+10*(x(1)-1)*exp(
    dv(2) = -6*(x(2)-1/3)*exp(-x(1)^2-(x(2)-1/3)^2)+6*(x(2)-5/3)*exp(-x(1)^2-(x(2)-5/3)^2)+10*x
    dv(1) = -dv(1);
    dv(2) = -dv(2);
end
```