# Analysis of the Simulation Data from Saddle-Node Bifurcation

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

## Generating simulation data

```
rng(1)
%{
lambda_0 = -3;
x_0 = 2.1038;
par.T_max = 6;
par.dt = 1e-5;
sigma = 40;
[x_out, t_out, lambda_out] = generating_simulation_data (@V_potential, sigma, x_0, lambda_0, pa
figure;
plot(t_out,x_out)


sample_id = abs(t_out-3.257)<0.02;
x_out_sample = x_out(sample_id);
t_out_sample = t_out(sample_id);

figure;
plot(t_out_sample,x_out_sample)

N_cell = length(x_out_sample);
sub_sample_id = 1:2:N_cell;
N_cell = length(sub_sample_id);
data = x_out_sample(sub_sample_id )';
true_labs = t_out_sample (sub_sample_id );


%save

save('../Data/saddlenode_new.mat','x_out_sample','t_out_sample','sample_id','x_out','t_out','la
%}
```

## Load the Data and Estimate Number of Clusters by EPI

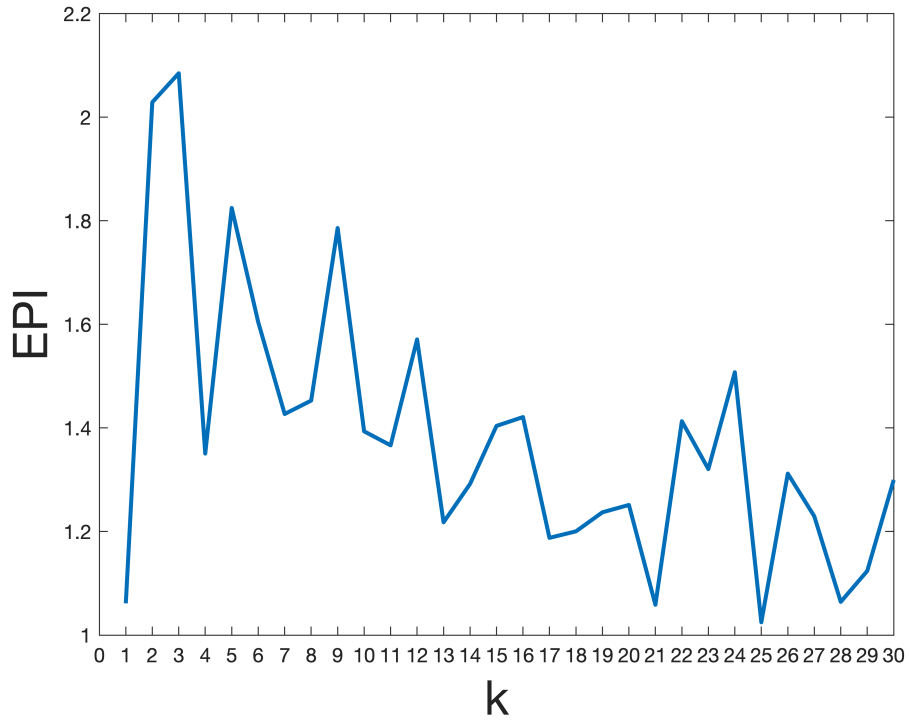
From EPI plot, we intend to seek for the index where peak occurs, which serves as the candidate for the choice of cluster numbers

```
load saddlenode.mat
% parameter and option settings
par.choice_distance = 'euclid';
out = EstClusterNum(data,par);
```

```
Computed P-values 500 of 2000 datapoints...
Computed P-values 1000 of 2000 datapoints...
Computed P-values 1500 of 2000 datapoints...
Computed P-values 2000 of 2000 datapoints...
Mean value of sigma: 0.62417
```

```
Minimum value of sigma: 0.54639
Maximum value of sigma: 0.75299
```

```
plot(out.ratio(1:30), '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 = 20; % number of random trails in MuTrans, increase this to guaratee more robustnes
% the main function of MuTrans
Output = DynamicalAnalysis (data, par);
```

```
Computed P-values 500 of 2000 datapoints...
Computed P-values 1000 of 2000 datapoints...
Computed P-values 1500 of 2000 datapoints...
Computed P-values 2000 of 2000 datapoints...
Mean value of sigma: 0.62417
Minimum value of sigma: 0.54639
Maximum value of sigma: 0.75299
J_new = 2.0186
J_new = 1.9458
J_new = 1.7978
J_new = 1.2289
J_new = 1.2248
J_new = 1.2228
J_new = 1.2227
J_new = 1.2227
J_new = 1.2726
```

```
J_new = 1.2064
J_new = 1.2029
J_new = 1.2022
J_new = 1.2014
J_new = 1.2012
J_new = 1.2012
J_new = 1.2039
J_new = 1.2013
J_new = 1.2012
J_new = 1.2012
J_new = 1.9314
J_new = 1.3082
J_new = 1.2736
J_new = 1.2414
J_new = 1.2271
J_new = 1.2238
J_new = 1.2228
J_new = 1.2227
J_new = 1.2227
J_new = 1.7034
J_new = 1.5456
J_new = 1.3847
J_new = 1.2039
J_new = 1.2013
J_new = 1.2012
J_new = 1.2012
J_new = 2.0398
J_new = 1.9975
J_new = 1.9374
J_new = 1.8711
J_new = 1.8338
J_new = 1.7806
J_new = 1.7073
J_new = 1.6795
J_new = 1.6351
J_new = 1.5776
J_new = 1.4679
J_new = 1.2018
J_new = 1.2013
J_new = 1.2012
J_new = 1.2012
J_new = 1.7439
J_new = 1.2251
J_new = 1.2064
J_new = 1.2029
J_new = 1.2022
J_new = 1.2014
J_new = 1.2012
J_new = 1.2012
J_new = 1.4074
J_new = 1.2198
J_new = 1.2118
J_new = 1.2047
J_new = 1.2022
J_new = 1.2012
J_new = 1.2012
J_new = 1.2566
J_new = 1.2138
J_new = 1.2031
J_new = 1.2022
J_new = 1.2014
J_new = 1.2012
J_new = 1.2012
J_new = 1.9787
J_new = 1.9039
```

```
J_new = 1.8986
J_new = 1.8913
J_new = 1.8793
J_new = 1.8363
J_new = 1.6907
J_new = 1.6654
J_new = 1.6276
J_new = 1.5695
J_new = 1.4416
J_new = 1.2014
J_new = 1.2012
J_new = 1.2012
J_new = 1.4496
J_new = 1.2050
J_new = 1.2024
J_new = 1.2016
J_new = 1.2012
J_new = 1.2012
J_new = 1.9824
J_new = 1.9375
J_new = 1.9336
J_new = 1.9305
J_new = 1.9276
J_new = 1.9196
J_new = 1.9075
J_new = 1.8997
J_new = 1.8934
J_new = 1.8835
J_new = 1.8584
J_new = 1.6937
J_new = 1.6728
J_new = 1.6341
J_new = 1.5790
J_new = 1.4702
J_new = 1.2014
J_new = 1.2012
J_new = 1.2012
J_new = 1.6831
J_new = 1.2031
J_new = 1.2022
J_new = 1.2014
J_new = 1.2012
J_new = 1.2012
J_new = 1.2270
J_new = 1.2235
J_new = 1.2227
J_new = 1.2227
J_new = 1.7183
J_new = 1.2072
J_new = 1.2031
J_new = 1.2022
J_new = 1.2014
J_new = 1.2012
J_new = 1.2012
J_new = 1.2220
J_new = 1.2057
J_new = 1.2024
J_new = 1.2016
J_new = 1.2012
J_new = 1.2012
J_new = 1.9753
J_new = 1.9521
J_new = 1.9035
J_new = 1.8986
J_new = 1.8833
```

```
J_new = 1.8606
J_new = 1.8512
J_new = 1.8470
J_new = 1.8458
J_new = 1.8448
J_new = 1.8441
J_new = 1.8414
J_new = 1.8297
J_new = 1.7931
J_new = 1.6386
J_new = 1.2334
J_new = 1.2262
J_new = 1.2235
J_new = 1.2227
J_new = 1.2227
J_new = 1.7555
J_new = 1.2307
J_new = 1.2275
J_new = 1.2241
J_new = 1.2234
J_new = 1.2209
J_new = 1.2157
J_new = 1.2083
J_new = 1.2039
J_new = 1.2013
J_new = 1.2012
J_new = 1.2012
J_new = 1.2070
J_new = 1.2026
J_new = 1.2021
J_new = 1.2014
J_new = 1.2012
J_new = 1.2012
J_new = 1.2866
J_new = 1.2247
J_new = 1.2232
J_new = 1.2227
J_new = 1.2227
J_new = 1.2227
E_best = 0.0375
```

| Iteration | Func-count | f(x) | Step-size | First-order optimality |
|---|---|---|---|---|
| 0 | 1 | 1.20181 | | 1.83e-05 |
| 1 | 11 | 1.17728 | 168199 | 0.00031 |
| 2 | 13 | 1.17708 | 0.1 | 0.000334 |
| 3 | 14 | 1.17143 | 1 | 0.00031 |
| 4 | 15 | 1.16935 | 1 | 0.000237 |
| 5 | 16 | 1.16811 | 1 | 0.000192 |
| 6 | 17 | 1.16574 | 1 | 0.000122 |
| 7 | 18 | 1.16484 | 1 | 0.000138 |
| 8 | 19 | 1.16393 | 1 | 6.32e-05 |
| 9 | 20 | 1.16347 | 1 | 6.29e-05 |
| 10 | 21 | 1.16293 | 1 | 0.000139 |
| 11 | 22 | 1.16238 | 1 | 0.000276 |
| 12 | 23 | 1.16147 | 1 | 0.000109 |
| 13 | 24 | 1.16084 | 1 | 5.13e-05 |
| 14 | 25 | 1.16049 | 1 | 9.18e-05 |
| 15 | 26 | 1.16029 | 1 | 9.94e-05 |
| 16 | 27 | 1.15977 | 1 | 4.86e-05 |
| 17 | 28 | 1.15947 | 1 | 4.86e-05 |
| 18 | 29 | 1.1593 | 1 | 4.19e-05 |
| 19 | 31 | 1.15915 | 0.487773 | 8.1e-05 |

| Iteration | Func-count | f(x) | Step-size | First-order optimality |
|---|---|---|---|---|
| 20 | 32 | 1.15903 | 1 | 7.84e-05 |

```
    21          33          1.15891              1       3.4e-05
    22          34          1.15881              1      9.82e-05
    23          35          1.15873              1      3.35e-05
    24          36          1.15864              1      3.12e-05
    25          38          1.15857       0.444354      0.000106
    26          39          1.15848              1      8.83e-05
    27          41          1.15832        0.47393      0.000129
    28          42          1.15818              1      0.000118
    29          43          1.15804              1      6.79e-05
    30          44          1.15792              1      6.74e-05
    31          45          1.15782              1      9.52e-05
    32          46          1.15773              1      3.66e-05
    33          47          1.15767              1      0.000128
    34          48          1.15757              1      3.84e-05
    35          49          1.15751              1       2.4e-05
    36          50          1.15743              1      0.000149
    37          51          1.15735              1      3.36e-05
    38          52          1.15729              1      3.15e-05
    39          53          1.15722              1      6.24e-05
                                                     First-order
Iteration  Func-count       f(x)        Step-size       optimality
    40          54          1.15718              1      3.82e-05
    41          55           1.1571              1      5.86e-05
    42          56          1.15704              1      6.87e-05
    43          57          1.15698              1      4.89e-05
    44          58          1.15688              1      5.25e-05
    45          59           1.1568              1       3.5e-05
    46          60          1.15674              1      7.43e-05
    47          61          1.15666              1      5.69e-05
    48          62           1.1566              1      3.66e-05
    49          63          1.15657              1      2.86e-05
    50          64          1.15655              1       2.3e-05
    51          65          1.15654              1      2.43e-05
    52          66          1.15652              1       1.6e-05
    53          67          1.15652              1      9.58e-06
    54          68          1.15651              1      7.84e-06
    55          69          1.15651              1      6.93e-06
    56          70           1.1565              1         6e-06
    57          71           1.1565              1      6.79e-06
    58          72           1.1565              1      6.78e-06
    59          73           1.1565              1         7e-06
                                                     First-order
Iteration  Func-count       f(x)        Step-size       optimality
    60          74          1.15649              1      6.09e-06
    61          75          1.15649              1      5.87e-06
    62          76          1.15649              1      5.49e-06
    63          77          1.15649              1      5.67e-06
    64          78          1.15649              1      6.04e-06
    65          79          1.15648              1      5.02e-06
    66          80          1.15648              1      4.98e-06
    67          81          1.15648              1      4.55e-06
    68          82          1.15648              1         5e-06
    69          83          1.15648              1       3.7e-06
    70          84          1.15648              1      3.09e-06
    71          85          1.15648              1      3.56e-06
    72          86          1.15647              1      3.76e-06
    73          87          1.15647              1      4.83e-06
    74          88          1.15647              1      4.57e-06
    75          89          1.15647              1      2.92e-06
    76          90          1.15647              1      2.76e-06
    77          91          1.15647              1      2.82e-06
    78          92          1.15647              1         3e-06
    79          93          1.15647              1      3.07e-06
                                                     First-order
Iteration  Func-count       f(x)        Step-size       optimality
```

```
    80          94          1.15647              1       3.96e-06
    81          95          1.15647              1       4.51e-06
    82          96          1.15647              1       4.26e-06
    83          97          1.15647              1        2.2e-06
    84          98          1.15647              1       1.86e-06
    85          99          1.15647              1       2.09e-06
    86         100          1.15647              1       2.75e-06
    87         101          1.15646              1       2.81e-06
    88         102          1.15646              1       3.33e-06
    89         103          1.15646              1       2.27e-06
    90         104          1.15646              1       1.58e-06
    91         105          1.15646              1       1.71e-06
    92         106          1.15646              1       1.87e-06
    93         107          1.15646              1       2.18e-06
    94         108          1.15646              1       3.47e-06
    95         109          1.15646              1       4.49e-06
    96         110          1.15646              1       4.47e-06
    97         111          1.15646              1       2.79e-06
    98         112          1.15646              1       1.68e-06
    99         113          1.15646              1       1.73e-06
                                                        First-order
 Iteration  Func-count       f(x)        Step-size       optimality
   100         114          1.15646              1        2.1e-06
   101         115          1.15646              1       2.18e-06
   102         116          1.15646              1       2.08e-06
   103         117          1.15646              1       1.82e-06
   104         118          1.15646              1       1.22e-06
   105         119          1.15646              1        1.4e-06
   106         120          1.15646              1       1.19e-06
   107         121          1.15646              1       1.12e-06
   108         122          1.15646              1       1.07e-06
   109         123          1.15646              1       1.08e-06
   110         124          1.15645              1       1.32e-06
   111         125          1.15645              1       1.27e-06
   112         126          1.15645              1       1.58e-06
   113         127          1.15645              1       1.71e-06
   114         128          1.15645              1       1.15e-06
   115         129          1.15645              1       9.26e-07

Optimization completed: The first-order optimality measure, 9.256173e-07, is less
than options.OptimalityTolerance = 1.000000e-06.

Elapsed time is 77.902009 seconds.
```

```
toc;
```

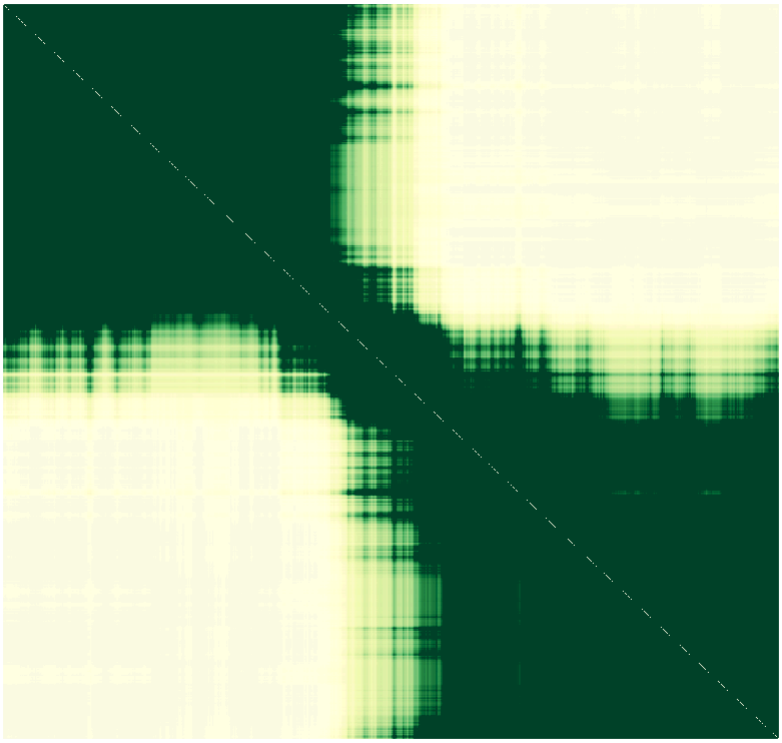
```
Elapsed time is 77.917476 seconds.
```

```
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)
```



```
%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)
```

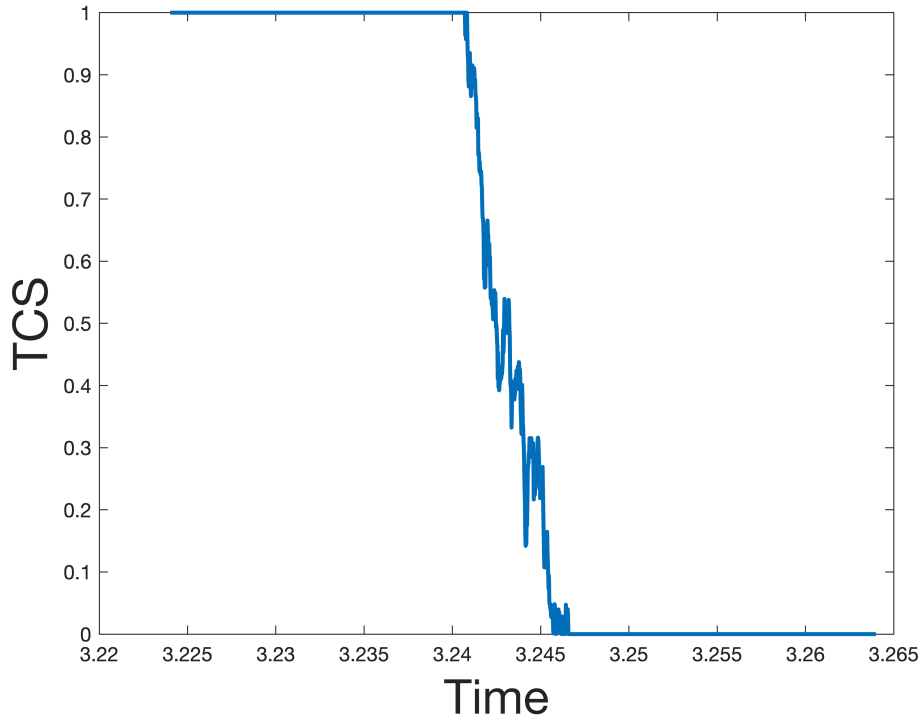
```
%colorbar;
```

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
```

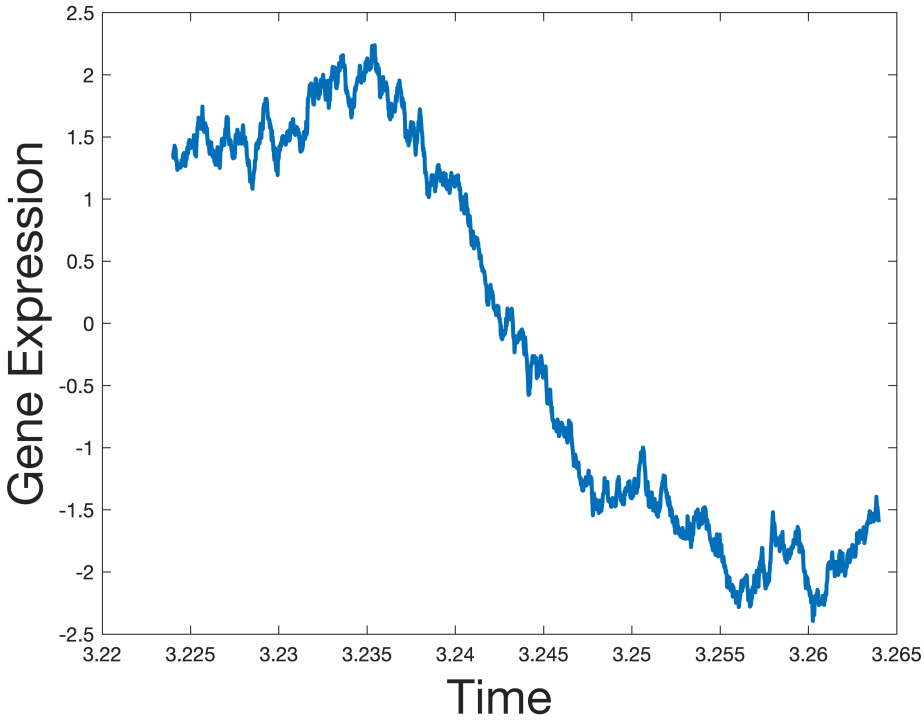
Plot Transition Cell Score (TCS)

```
figure;
plot(labs_perm, rho_class(:,1),'LineWidth',2)
xlabel('Time', 'FontSize', 24);
ylabel('TCS', 'FontSize', 24);
```




Plot Actual Simulation Trajectory (Gene Expression)

```
figure;
plot(labs_perm, data_perm,'LineWidth',2)
xlabel('Time', 'FontSize', 24);
ylabel('Gene Expression', 'FontSize', 24);
```


Gene Expression
Time
2.5
2
1.5
1
0.5
0
-0.5
-1
-1.5
-2
-2.5
3.22
3.225
3.23
3.235
3.24
3.245
3.25
3.255
3.26
3.265