POSTERIOR AGREEMENT FOR 1D CONNECTIVITY

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Implementation of " **Pipeline Validation for Connectivity-based Cortex Parcellation** " by Nico S. Gorbach, Marc Tittgemeyer and Joachim M. Buhmann

Contents


```
clear all; close all; clc
```

Introduction

This code documentation demonstrates that seed clusters become indistinguishable with increasing noise in the target connectivity scores. Ornstein-Uhlenbeck (OU) processes with different initial conditions were used to emulate fiber tracking between seed and target objects.Seed objects are grouped based upon their connectivity scores to target objects which were obtained by sampling from the OU-process 200 times. The means of the OU processes were selected such that, at low and medium SDE diffusion coefficients, three clusters of seed objects can be statistically distinguished from each other based soley on the connectivity scores of the seed objects. Contrastingly, at a high SDE diffusion coefficient the overlap in connectivity scores attributed to different seed objects become so great such that only two (and not three) clusters of seed objects can be statistically distinguished from each other.

Input

Set the number of potential clusters, the number of Ornstein-Uhlenbeck samples per seed coordinate and the diffusion term.

```
K = 3;                          % number of potential clusters
ntrials = 1000;                 % number of Ornstein-Uhlenbeck trials
diffusion = [0.1,3,10];          % diffusion in Ornstein-Uhlenbeck process
final_time = 10;                % final time in Ornstein-Uhlenbeck process
seed_coords = 1:60;              % seed coordinates
target_coord = [10,12,20,50];   % target coordinates
```

```
for n = 1:length(diffusion)
```

Generate noisy trajectories

Connectivity matrix is generated by sampling from the Ornstein-Uhlenbeck process

```
    target_coord_assign(:,1) = [ones(20,1);3*ones(20,1),;4*ones(20,1)];
    target_coord_assign(:,2) = [2*ones(40,1);4*ones(20,1)];
    [~,~,true_cluster_labels(:,n)] = unique(target_coord_assign,'rows');
    nSamples = 10;
    edges = 1:1:80;

    for l = 1:ntrials
        for i = 1:length(seed_coords)
            for k = 1:size(target_coord_assign,2)
                [truth(l).trajectory(i,:,k),time] = OU_process(seed_coords(i),target_coord(target_coord_assign(i,k)),final_time,diffusion(n));
            end
        end
    end

    % packing
    trajectory_all{n} = [reshape(target_coord_assign,[],1),[truth(1).trajectory(:,:,1);truth(1).trajectory(:,:,2)]];
```

Connectivity matrices

```
    for m = 1:2
        connectivity_matrix{n}{m} = [];
        for i = 1:length(seed_coords)
            clear trajectory;
            for j = 1:nSamples
                k =randi(2);
```

```
            [trajectory(j,:),time] = OU_process(seed_coords(i),target_coord(target_coord_assign(i,k)),final_time,diffusion(n));
        end
        connectivity_matrix{n}{m}(i,:) = histcounts(trajectory(:,end),edges);
    end
end

% remove columns of zeros
rem_idx(n,:) = sum(connectivity_matrix{n}{1},1) + sum(connectivity_matrix{n}{2},1) == 0;
connectivity_matrix{n}{1}(:,rem_idx(n,:)) = [];
connectivity_matrix{n}{2}(:,rem_idx(n,:)) = [];
```

```
% normalize connectivity matrix

data1 = connectivity_matrix{n}{1};
data2 = connectivity_matrix{n}{2};
```

```
% start timer
tic;
```

Deterministic annealing

Determine global minimizer.

```
% Annealing settings
beta_init = 0.1;                                 % starting inverse temperature
beta_step = 1.02;                                % inverse temperature step
beta_stop = 5;                                  % stopping inverse temperature
perturb_sd = 0.01;                                % centroid perturbation

% Initialization of Gibbs distributions
gibbs_dist1 = ones(size(data1,1),K) ./ K;
gibbs_dist2 = ones(size(data2,1),K) ./ K;

% Initialization of centroids
centroid1 = gibbs_dist1'*data1;
centroid1 = bsxfun(@rdivide,centroid1,sum(centroid1,2));
centroid1(centroid1==0) = eps;
centroid2 = gibbs_dist2'*data2;
centroid2 = bsxfun(@rdivide,centroid2,sum(centroid2,2));
centroid2(centroid2==0) = eps;

j = 0; beta = beta_init;
while beta < beta_stop
```

Perturb centroids

Avoid local minimum by perturbing centroids: $\phi_{kj}^{(\cdot)} = \phi_{kj}^{(\cdot)} + \epsilon$

```
    %r = perturb_sd * rand(size(centroid1));
    centroid1 = centroid1 + perturb_sd * rand(size(centroid1));
    centroid1 = bsxfun(@rdivide,centroid1,sum(centroid1,2)); % normalize
    centroid2 = centroid2 + perturb_sd * rand(size(centroid1));
    centroid2 = bsxfun(@rdivide,centroid2,sum(centroid2,2)); % normalize
```

Expectation maximization

Iterate between determining Gibbs distributions and maximzing variational lower bound w.r.t. centroids.

```
    for iter = 1:80
```

Costs for histogram clustering given instance 1

KL divergence between empirical probabilities (data) and centroid probabilities (up to proportionality constant): $R_{ik}^{(1)} = -\sum_j x_{ij}^{(1)} \log(\phi_{kj}^{(1)})$

```
        potential1 = -data1 * log(centroid1)';
```

Costs for histogram clustering given instance 2

KL divergence between empirical probabilities (data) and centroid probabilities (up to proportionality constant): $R_{ik}^{(2)} = -\sum_j x_{ij}^{(2)} \log(\phi_{kj}^{(2)})$

```
        potential2 = -data2 * log(centroid2)';
```

Gibbs distribution 1

Maximum entropy distribution: $p_{ik}^{(1)} = \exp\left(-\beta R_{ik}^{(1)}\right)/Z$

```
        gibbs_dist1 = exp(-beta * potential1);
        partition_sum1 = sum(gibbs_dist1,2);
        gibbs_dist1 = bsxfun(@rdivide,gibbs_dist1,partition_sum1);

        % avoid underflow
        idx = find(partition_sum1==0);
        if ~isempty(idx)
            [~,min_cost_idx] = min(potential1(idx,:),[],2);
            max_ind = sub2ind(size(gibbs_dist1),idx,min_cost_idx);
            gibbs_dist1(idx,:) = zeros(length(idx),K);
            gibbs_dist1(max_ind) = 1;
```

```
            end
```

Gibbs distribution 2

Maximum entropy distribution: $p_{ik}^{(2)} = \exp\left(-\beta R_{ik}^{(2)}\right)/Z$

```
            gibbs_dist2 = exp(-beta * potential2);
            partition_sum2 = sum(gibbs_dist2,2);
            gibbs_dist2 = bsxfun(@rdivide,gibbs_dist2,partition_sum2);

            % avoid underflow
            idx = find(partition_sum2==0);
            if ~isempty(idx)
                [~,min_cost_idx] = min(potential2(idx,:),[],2);
                max_ind = sub2ind(size(gibbs_dist2),idx,min_cost_idx);
                gibbs_dist2(idx,:) = zeros(length(idx),K);
                gibbs_dist2(max_ind) = 1;
            end
```

Joint Gibbs distribution

Maximum entropy distribution: $p_{ik}^{(1,2)} = \exp\left(-\beta(R_{ik}^{(1)} + R_{ik}^{(2)})\right)/Z$

```
            dist_joint = exp(-beta * (potential1 + potential2));
            joint_partition_sum = sum(dist_joint,2);
```

Centroids for instance 1

Probability prototype: $\phi_{kj}^{(1)} = \frac{\sum_i p_{ik}^{(1)} x_{ij}^{(1)}}{\sum_j \sum_{i'} p_{i'k}^{(1)} x_{i'j}^{(1)}}$

```
            centroid1 = gibbs_dist1'*data1;
            centroid1 = bsxfun(@rdivide,centroid1,sum(centroid1,2));
            centroid1(centroid1==0) = eps;
```

Centroids for instance 2

Probability prototype: $\phi_{kj}^{(2)} = \frac{\sum_i p_{ik}^{(2)} x_{ij}^{(2)}}{\sum_j \sum_{i'} p_{i'k}^{(2)} x_{i'j}^{(2)}}$

```
            centroid2 = gibbs_dist2'*data2;
            centroid2 = bsxfun(@rdivide,centroid2,sum(centroid2,2));
            centroid2(centroid2==0) = eps;
        end
```

```
        beta = beta * beta_step;    % increase inverse temperature (complexity)
```

Match clusters across data instances

Use Hungarian algorithm to match clusters.

```
        %if beta < 10
        match_clusters_idx = munkres(pdist2(centroid1,centroid2));
        potential2=potential2(:,match_clusters_idx);
        %end
```

Log partition sum for instance 1

Determine log partition sum while avoiding underflow: $\log Z_1 = \sum_i \log \sum_k \exp\left(-\beta R_{ik}^{(1)}\right)$

```
        scaled_cost1 = -beta * potential1;
        % log-sum-exp trick to prevent underflow
        max_scaled_cost1 = max(scaled_cost1,[],2);
        log_partition_sum1 = max_scaled_cost1 + log(sum(exp(scaled_cost1-max_scaled_cost1),2));
```

Log partition sum for instance 2

Determine log partition sum while avoiding underflow: $\log Z_2 = \sum_i \log \sum_k \exp\left(-\beta R_{ik}^{(2)}\right)$

```
        scaled_cost2 = -beta * potential2;
        % log-sum-exp trick to prevent underflow
        max_scaled_cost2 = max(scaled_cost2,[],2);
        log_partition_sum2 = max_scaled_cost2 + log(sum(exp(scaled_cost2-max_scaled_cost2),2));
```

Joint log partition sum

Determine joint log partition sum while avoiding underflow: $\log Z_{12} = \sum_i \log \sum_k \exp\left(-\beta(R_{ik}^{(1)} + R_{ik}^{(2)})\right)$

```
        joint_scaled_cost = -beta * (potential1 + potential2);
        % log-sum-exp trick to prevent underflow
        max_scaled_cost3 = max(joint_scaled_cost,[],2);
        log_joint_partition_sum = max_scaled_cost3 + log(sum(exp(joint_scaled_cost-max_scaled_cost3),2));
```

```
        j = j+1;
```

Generalization capacity

Resolution of the hypothesis space: $GC(\beta) = \log(k) + \frac{1}{n}(\log Z_{12} - \log Z_1 - \log Z_2)$

```
        gc{n}(j) = log(K) + sum(log_joint_partition_sum - log_partition_sum1 ...
            - log_partition_sum2) ./ size(partition_sum1,1);

        % pack
        inv_temp(j) = beta;
        gibbs_dist_packed1{n}(:,:,j) = gibbs_dist1;
        gibbs_dist_packed2{n}(:,:,j) = gibbs_dist2;
```

```
    end
```

Number of equivariant transformations

Richness of the hypothesis space: $\frac{1}{n}\log|\{\tau\}| = H(n_1/n, \ldots, n_k/n)$

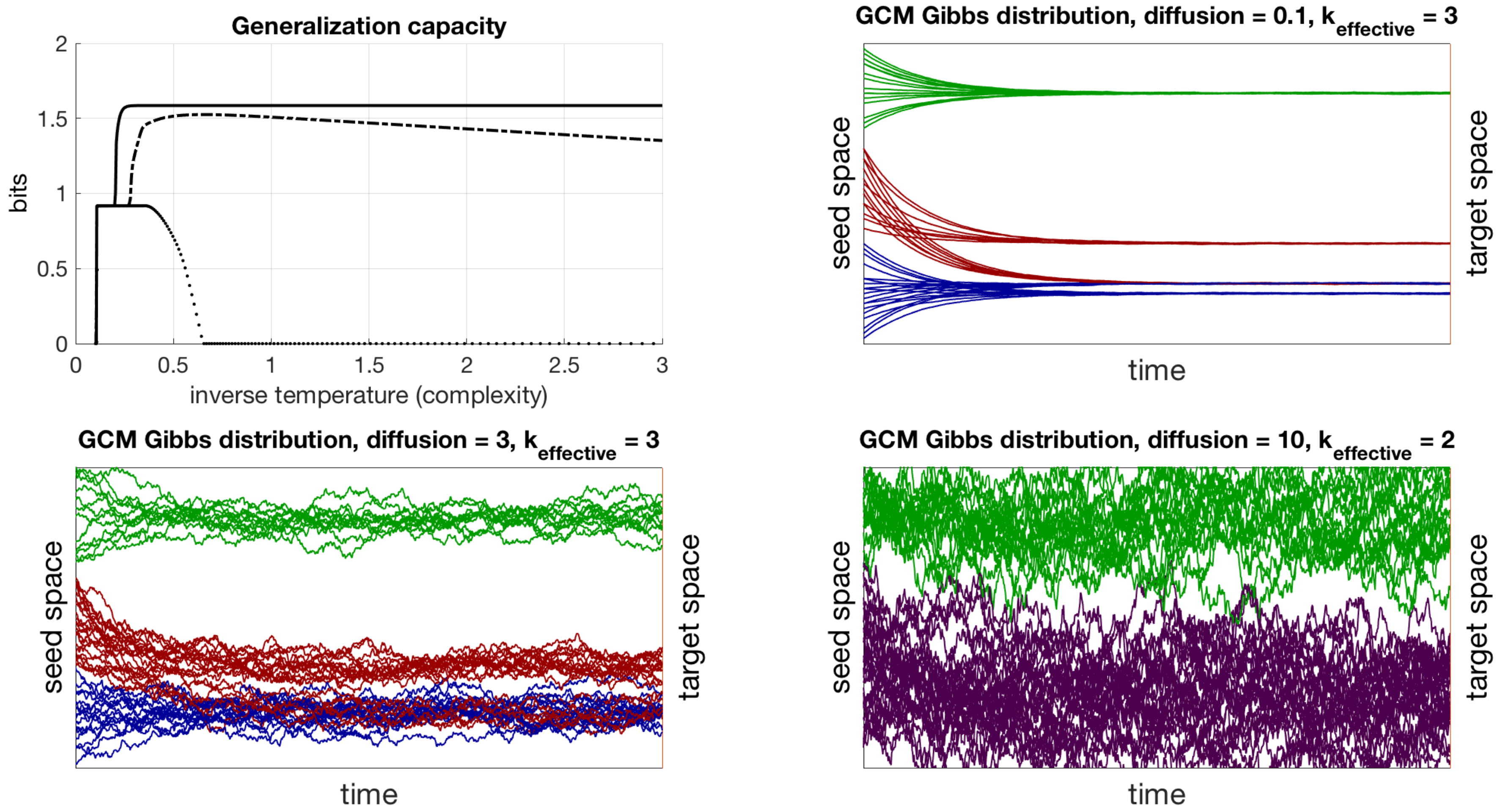
```
    d = sum(round(gibbs_dist1),1); d = d./sum(d); d(d==0) = 1;
    nTransformations = -d * log(d)';

    % correct generalization capacity
    gc{n} = gc{n} - log(K) + nTransformations;
```

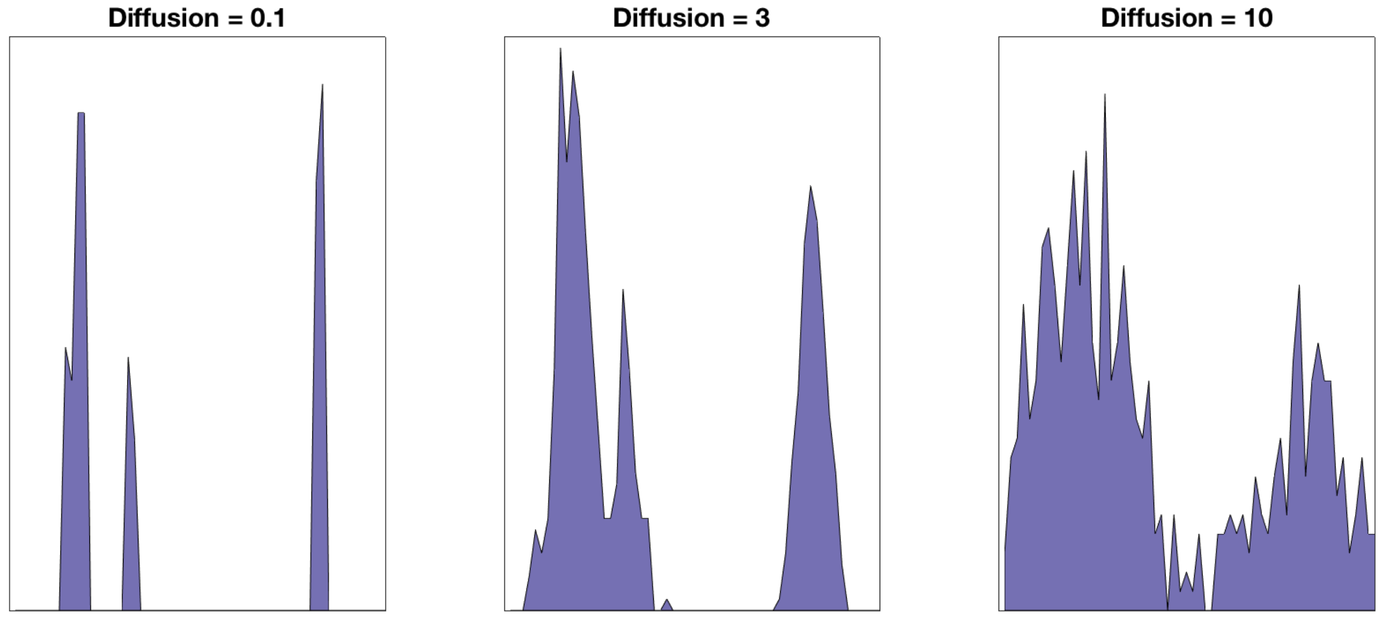
```
    gc{n} = gc{n} * log2(exp(1));       % transforming units from nats to bits
```

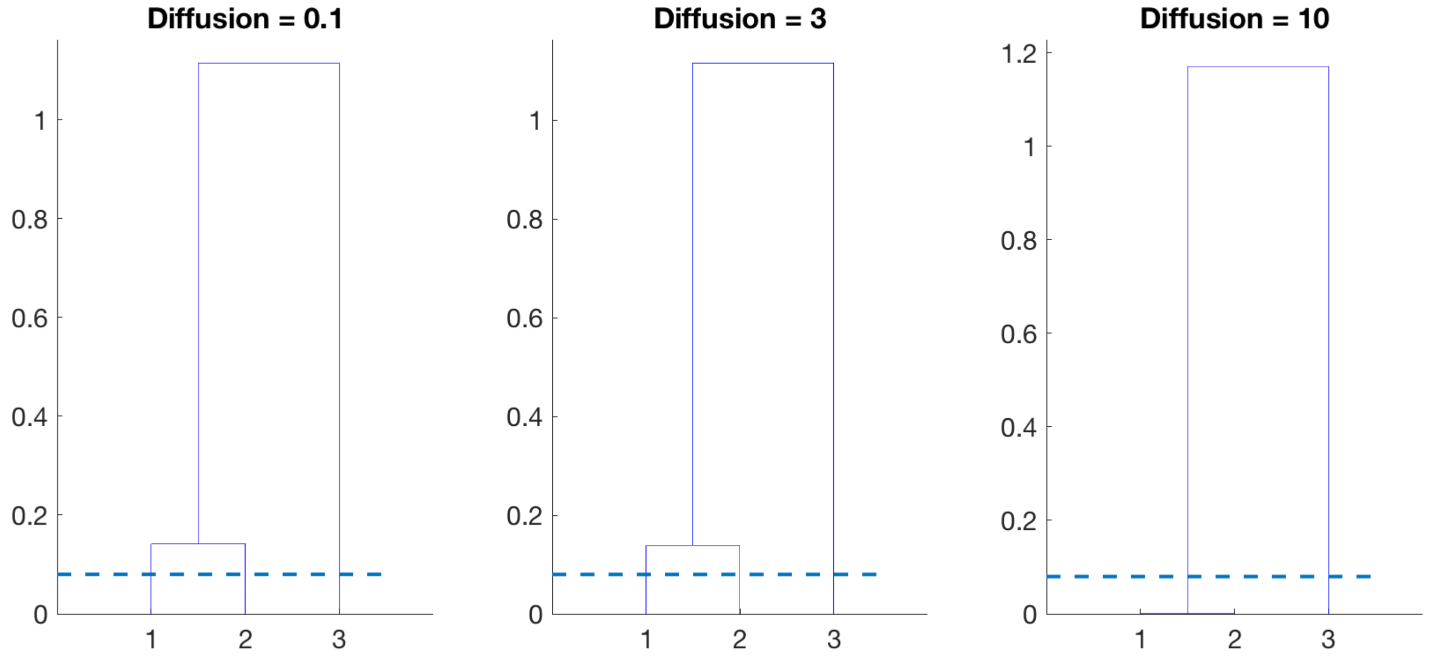
```
end
```

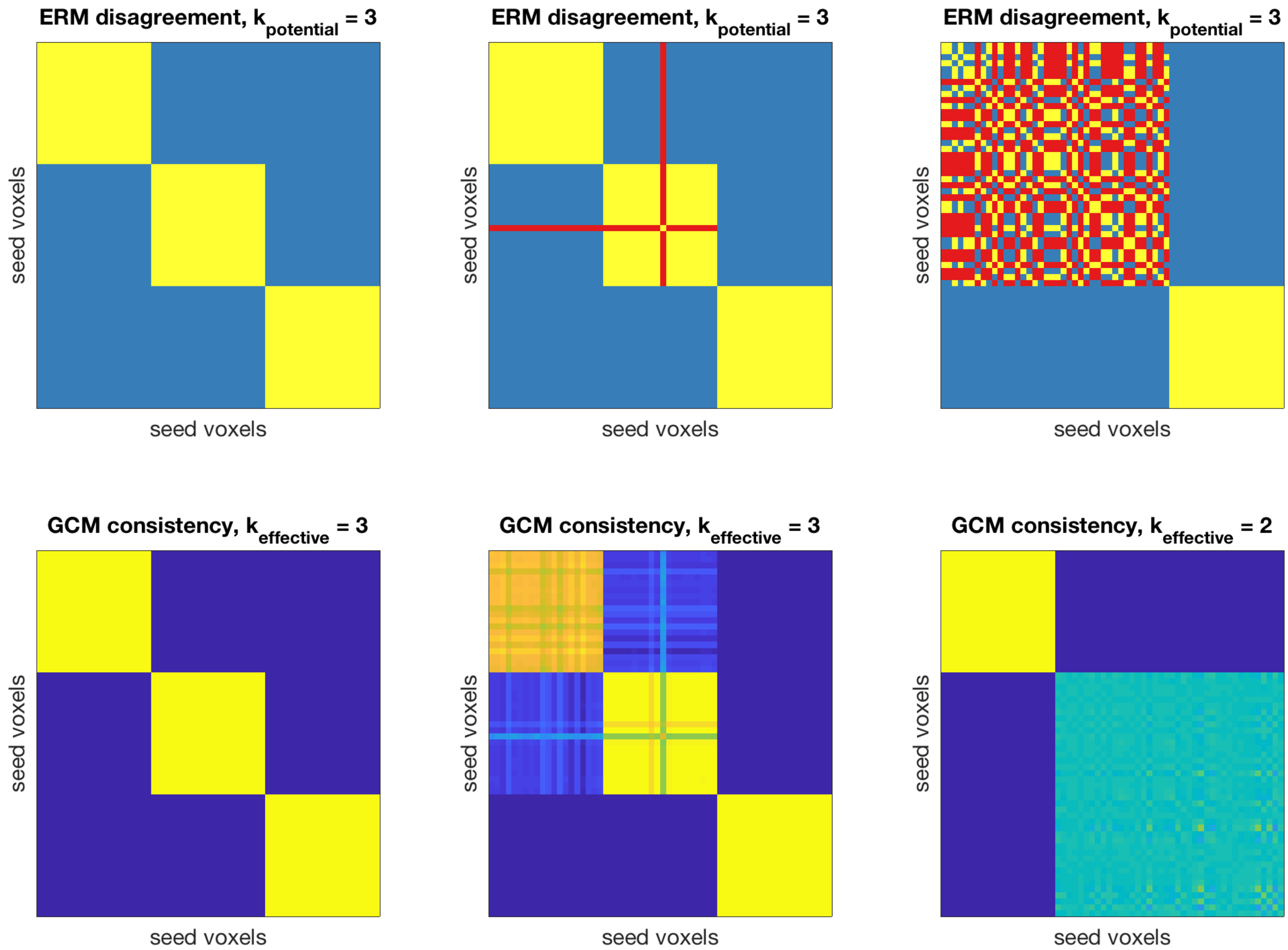
Results

```
display_result(gc,inv_temp,gibbs_dist_packed1,gibbs_dist_packed2,diffusion,...
    seed_coords,data1,trajectory_all,time,connectivity_matrix,rem_idx)
```




Diffusion = 0.1
Diffusion = 3
Diffusion = 10


Diffusion = 0.1
Diffusion = 3
Diffusion = 10
0
0.2
0.4
0.6
0.8
1
1.2
1
2
3




```
disp(['runtime: ' num2str(toc/60) ' minutes']);     % runtime
```

```
runtime: 0.16734 minutes
```

Discussion

The generalization capacity ranks the experiments in the order corresponding to the stochasticity (i.e. magnitude of SDE diffusion coefficient) in the Ornstein-Uhlenbeck process which is expected since a stochasticity in the OU process results in more ``noisy'' connectivity scores. The ranking is further supported by the disagreement among the ERM's with red indicating disagreement of clusterings. The GCM's of the experiments characterized by the low and medium stochasticity resolve three effective clusters of seed objects based upon their connectivity scores to target objects. The experiment with stochasticity, however, sufficiently corrupts the connectivity scores such that clusters 2 and 3 become indistinguishable as indicated by the GCM.

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