

OT-RMC-SA Taxonomy and Sample Classification

We first load Mosek Matlab package.

```
addpath C:/Users/sebastian/Mosek/10.2/toolbox/r2017a
```

Load the Baron Pancreas dataset:

```
load baronpc ;  
dim = 50; %number of PCs  
numPat = length(stride); %number of samples in dataset  
celltypes= unique(cellnames); %unique cell types present in dataset  
numcells = length(celltypes); %number of unique cell types.
```

We will now apply the OT-RMC algorithm for each sample. The output for a sample is a similarity matrix with respect to the clusters present in that sample.

```
lambda2=0;  
lambda = .075;  
matchSelf = cell(numPat,1);  
for i =1:numPat  
    nclust=stride(i); %number of clusters in sample i  
    start = sum(stride(1:i-1))+1;  
    ms = supp(1:dim,start:start+nclust-1); %mean vectors of clusters in sample i  
    vars = supp(dim+1:dim^2+dim,start:start+nclust-1); %cov matrices of clusters in sample i  
    p = ww(start:start+nclust-1);%proportions of clusters in sample i  
    cost = CostMat(ms,ms,vars,vars,nclust,nclust); %compute cost matrix  
    cost = real(cost/max(cost,[],"all")); %standardize  
    [~,res]=otrmcl1(cost,lambda,lambda2,p,p); %apply OTRMC  
    xx=res.sol.itr.xx;  
    gammaij=reshape(xx(nclust+nclust+1:nclust+nclust+nclust*nclust),[nclust,nclust]); %weight m  
    %row and vector standardization  
    gammaijcol = gammaij./ max(abs(gammaij), [], 1);  
    gammaijrow = gammaij./ max(abs(gammaij), [], 2);  
    matchSelf{i} = (gammaijcol+gammaijrow)/2;  
end
```

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We compute the matching matrices for the different patients combinations

```
combs = nchoosek(1:numPat,2);
matchM = cell(length(combs),1);
for i=1:length(combs)
    nclust1=stride(combs(i,1)); %number of clusters in 1st sample
    nclust2=stride(combs(i,2)); %number of clusters in 2nd sample
    start1 = sum(stride(1:combs(i,1)-1))+1; %how many columns to ignore +1
    start2 = sum(stride(1:combs(i,2)-1))+1;
    ms1 = supp(1:dim,start1:start1+nclust1-1); %mean vectors of clusters in first sample
    ms2 = supp(1:dim,start2:start2+nclust2-1);
    vars1=supp(dim+1:dim+dim^2,start1:start1+nclust1-1); %cov matrices of clusters in first sample
    vars2 = supp(dim+1:dim+dim^2,start2:start2+nclust2-1);
    p1 = ww(start1:start1+nclust1-1);
    p2 = ww(start2:start2+nclust2-1);
    cost = CostMat(ms1,ms2,vars1,vars2,nclust1,nclust2);
    cost = real(cost/max(cost,[],"all"));
    [~,res]=otrmcl1(cost,lambda,lambda2,p1,p2);
    xx=res.sol.itr.xx;
    gammaij=reshape(xx((nclust1+nclust2+1):(nclust1+nclust2+nclust1*nclust2)),[nclust1,nclust2]);
    %row and vector standardization
    gammaijcol = gammaij./ max(abs(gammaij), [], 1);
    gammaijrow = gammaij./ max(abs(gammaij), [], 2);
    matchM{i} = (gammaijcol+gammaijrow)/2;
end
```

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We now combine all of the different matching matrices into one big matching matrix, B . We refer to B as the overall cluster similarity matrix

```

Biggammaij = blkdiag(matchSelf{:}); % this functions takes a finite list of matrices
                                     % and creates a larger matrix with the
                                     % matrices as diagonal blocks. {:}
                                     % spits out all the matrices from the
                                     % cell array

startPat=1;
endPat = numPat-1;
for j =1:(numPat-1)
    nclust1=stride(j); %number of clusters for individual j
    start1 = sum(stride(1:j-1))+1; %how many columns to ignore +1
    endClust=start1+nclust1-1;
    Biggammaij(start1:endClust,endClust+1:end)=Biggammaij(start1:endClust,endClust+1:end)+ [mat
    Biggammaij(endClust+1:end,start1:endClust)=Biggammaij(endClust+1:end,start1:endClust)+ [mat
    startPat = endPat+1;
    endPat = startPat+numPat-2-j;
end
Biggammaij(abs(Biggammaij) < min(ww)* 1E-7) = min(ww)* 1E-7;

```

Dendrogram

We now need to transform **B** into a distance symmetric matrix **A**.

```

%Now we will create a distance matrix
A = real(-log(Biggammaij));
A= A/ max(max(A));
B = squareform(A);
tree=linkage(B,'ward');
cellClusters=cluster(tree,"MaxClust", numcells);

```

We build the dendrogram from the tree.

```

cutoff = max(tree(end-numcells+2, 3)); % Determine the cutoff height
figure;
H = dendrogram(tree, 0, 'ColorThreshold', cutoff);
set(H, 'LineWidth', 2);
set(gca, 'FontSize', 14)
yline(cutoff, 'r--', 'LineWidth', 2); % Add the horizontal line
set(gca, 'XTickLabel', []);

```

