

OT-SA Taxonomy

We will show how to build a taxonomy of clusters from multiple samples. The data set in this example is the Baron Pancreas dataset. It only has 4 samples which allows us to visualize the taxonomy with a dendrogram. The method by which clusters are aligned here is regular OT.

We first load the Mosek Matlab package:

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

Load the formatted 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 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]=OT(cost,p,p);
    xx=res.sol.itr.xx;
    gammaij=reshape(xx,[nclust,nclust]);
    %normalization
    gammaijcol = gammaij./ max(abs(gammaij), [], 1);
    gammaijrow = gammaij./ max(abs(gammaij), [], 2);
    matchSelf{i} = (gammaijcol+gammaijrow)/2;
end
```

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```
Problem
  Name           :
  Objective sense : minimize
  Type           : LO (linear optimization problem)
  Constraints     : 28
  Affine conic cons. : 0
  Disjunctive cons. : 0
  Cones          : 0
  Scalar variables : 196
  Matrix variables : 0
```

```

Integer variables      : 0

Optimizer started.
Presolve started.
Linear dependency checker started.
Linear dependency checker terminated.
Eliminator started.
Freed constraints in eliminator : 0
Eliminator terminated.
Eliminator - tries          : 1          time           : 0.00
Lin. dep.  - tries          : 1          time           : 0.00
Lin. dep.  - primal attempts : 1          successes        : 1
Lin. dep.  - dual attempts   : 0          successes        : 0
Lin. dep.  - primal deps.    : 1          dual deps.       : 0
Presolve terminated. Time: 0.00
Optimizer - threads         : 4
Optimizer - solved problem   : the primal
Optimizer - Constraints      : 27
Optimizer - Cones           : 0
Optimizer - Scalar variables : 196        conic            : 0
Optimizer - Semi-definite variables: 0      scalarized       : 0
Factor - setup time         : 0.00
Factor - dense det. time    : 0.00        GP order time    : 0.00
Factor - nonzeros before factor : 209      after factor     : 287
Factor - dense dim.         : 0          flops            : 4.68e+03
ITE PFEAS  DFEAS  GFEAS  PRSTATUS  POBJ          DOBJ          MU          TIME
0  1.7e+00  4.4e-01  1.2e+01  0.00e+00  1.121735064e+01 -9.976372414e-01 1.6e-01 0.02
1  5.3e-01  1.4e-01  3.8e+00  1.38e+00  2.572686545e+00 -2.554371438e-01 4.9e-02 0.03
2  7.0e-02  1.8e-02  5.1e-01  1.70e+00  2.263839249e-01 -3.307175336e-02 6.6e-03 0.03
3  8.0e-03  2.1e-03  5.8e-02  1.29e+00  2.127138034e-02 -3.999807663e-03 7.4e-04 0.03
4  2.7e-04  1.7e-04  2.4e-03  1.17e+00  7.332874268e-04 -2.341756479e-04 3.1e-05 0.03
5  8.2e-07  5.0e-07  7.2e-06  1.02e+00  2.413527227e-06 -4.640102693e-07 9.4e-08 0.05
6  8.2e-11  5.0e-11  7.2e-10  1.00e+00  6.848507925e-08 6.819732199e-08 9.4e-12 0.05
Basis identification started.
Primal basis identification phase started.
Primal basis identification phase terminated. Time: 0.00
Dual basis identification phase started.
Dual basis identification phase terminated. Time: 0.00
Basis identification terminated. Time: 0.00
Optimizer terminated. Time: 0.09

Interior-point solution summary
Problem status : PRIMAL_AND_DUAL_FEASIBLE
Solution status : OPTIMAL
Primal.  obj: 6.8485079253e-08    nrm: 5e-01    Viol.  con: 3e-11    var: 0e+00
Dual.    obj: 6.8197321991e-08    nrm: 1e+00    Viol.  con: 0e+00    var: 2e-11

Basic solution summary
Problem status : PRIMAL_AND_DUAL_FEASIBLE
Solution status : OPTIMAL
Primal.  obj: 6.8250548272e-08    nrm: 5e-01    Viol.  con: 0e+00    var: 0e+00
Dual.    obj: 6.8197321992e-08    nrm: 2e+00    Viol.  con: 0e+00    var: 1e-09
Optimizer summary
Optimizer - time: 0.09
Interior-point - iterations : 6    time: 0.06
Basis identification - time: 0.00
Primal - iterations : 0    time: 0.00
Dual - iterations : 13    time: 0.00
Clean primal - iterations : 0    time: 0.00
Clean dual - iterations : 0    time: 0.00
Simplex - time: 0.00
Primal simplex - iterations : 0    time: 0.00
Dual simplex - iterations : 0    time: 0.00
Mixed integer - relaxations: 0    time: 0.00

```

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Problem

Name :
 Objective sense : minimize
 Type : LO (linear optimization problem)
 Constraints : 28
 Affine conic cons. : 0
 Disjunctive cons. : 0
 Cones : 0
 Scalar variables : 196
 Matrix variables : 0
 Integer variables : 0

Optimizer started.

Presolve started.

Linear dependency checker started.

Linear dependency checker terminated.

Eliminator started.

Freed constraints in eliminator : 0

Eliminator terminated.

Eliminator - tries	: 1	time	: 0.00
Lin. dep. - tries	: 1	time	: 0.00
Lin. dep. - primal attempts	: 1	successes	: 1
Lin. dep. - dual attempts	: 0	successes	: 0
Lin. dep. - primal deps.	: 1	dual deps.	: 0

Presolve terminated. Time: 0.00

Optimizer - threads	: 4							
Optimizer - solved problem	: the primal							
Optimizer - Constraints	: 27							
Optimizer - Cones	: 0							
Optimizer - Scalar variables	: 196	conic	: 0					
Optimizer - Semi-definite variables	: 0	scalarized	: 0					
Factor - setup time	: 0.00							
Factor - dense det. time	: 0.00	GP order time	: 0.00					
Factor - nonzeros before factor	: 209	after factor	: 287					
Factor - dense dim.	: 0	flops	: 4.68e+03					
ITE	PFEAS	DFEAS	GFEAS	PRSTATUS	POBJ	DOBJ	MU	TIME
0	1.7e+00	3.1e-01	1.2e+01	0.00e+00	1.082275814e+01	-1.024190053e+00	1.8e-01	0.01
1	2.7e-01	4.9e-02	1.9e+00	1.90e+00	9.784529916e-01	-9.439682157e-02	2.8e-02	0.03
2	2.6e-02	4.9e-03	1.9e-01	1.39e+00	7.194526261e-02	-1.194871059e-02	2.8e-03	0.03
3	4.1e-03	7.5e-04	2.9e-02	1.28e+00	9.856645279e-03	-1.404026706e-03	4.2e-04	0.03
4	1.1e-04	5.1e-05	9.0e-04	1.15e+00	2.046802322e-04	-1.179068294e-04	1.3e-05	0.05
5	7.1e-07	3.4e-07	6.0e-06	1.05e+00	1.468701830e-06	-6.511446844e-07	8.9e-08	0.05
6	7.6e-11	3.7e-11	6.5e-10	1.00e+00	5.784279741e-08	5.761609784e-08	9.6e-12	0.05

Basis identification started.

Primal basis identification phase started.

Primal basis identification phase terminated. Time: 0.00

Dual basis identification phase started.

Dual basis identification phase terminated. Time: 0.01

Basis identification terminated. Time: 0.01

Optimizer terminated. Time: 0.09

Interior-point solution summary

Problem status : PRIMAL_AND_DUAL_FEASIBLE

Solution status : OPTIMAL

Primal. obj:	5.7842797413e-08	nrm: 3e-01	Viol. con:	3e-11	var: 0e+00
Dual. obj:	5.7616097839e-08	nrm: 1e+00	Viol. con:	0e+00	var: 1e-11

Basic solution summary

Problem status : PRIMAL_AND_DUAL_FEASIBLE
 Solution status : OPTIMAL
 Primal. obj: 5.7691787587e-08 nrm: 3e-01 Viol. con: 0e+00 var: 0e+00
 Dual. obj: 5.7616097839e-08 nrm: 2e+00 Viol. con: 0e+00 var: 5e-08

Optimizer summary

Optimizer	-	time: 0.09
Interior-point	- iterations : 6	time: 0.06
Basis identification	-	time: 0.01
Primal	- iterations : 0	time: 0.00
Dual	- iterations : 13	time: 0.01
Clean primal	- iterations : 0	time: 0.00
Clean dual	- iterations : 0	time: 0.00
Simplex	-	time: 0.00
Primal simplex	- iterations : 0	time: 0.00
Dual simplex	- iterations : 0	time: 0.00
Mixed integer	- relaxations: 0	time: 0.00

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Platform: Windows/64-X86

Problem

Name	:
Objective sense	: minimize
Type	: LO (linear optimization problem)
Constraints	: 28
Affine conic cons.	: 0
Disjunctive cons.	: 0
Cones	: 0
Scalar variables	: 196
Matrix variables	: 0
Integer variables	: 0

Optimizer started.

Presolve started.

Linear dependency checker started.

Linear dependency checker terminated.

Eliminator started.

Freed constraints in eliminator : 0

Eliminator terminated.

Eliminator - tries	: 1	time	: 0.00
Lin. dep. - tries	: 1	time	: 0.02
Lin. dep. - primal attempts	: 1	successes	: 1
Lin. dep. - dual attempts	: 0	successes	: 0
Lin. dep. - primal deps.	: 1	dual deps.	: 0

Presolve terminated. Time: 0.02

Optimizer - threads	: 4
Optimizer - solved problem	: the primal
Optimizer - Constraints	: 27
Optimizer - Cones	: 0
Optimizer - Scalar variables	: 196
Optimizer - Semi-definite variables:	0
Factor - setup time	: 0.00
Factor - dense det. time	: 0.00
Factor - nonzeros before factor	: 209
Factor - dense dim.	: 0

conic	: 0
scalarized	: 0
GP order time	: 0.00
after factor	: 287
flops	: 4.68e+03

	ITE	PFEAS	DFEAS	GFEAS	PRSTATUS	POBJ	DOBJ	MU	TIME
0	1.7e+00	5.5e-01	1.5e+01	0.00e+00	1.393184117e+01	-1.068392929e+00	1.6e-01	0.03	
1	3.6e-01	1.2e-01	3.3e+00	1.06e+00	2.446021571e+00	-2.250300595e-01	3.6e-02	0.03	
2	4.2e-02	1.2e-02	3.8e-01	1.38e+00	2.040778770e-01	-3.582528235e-02	4.1e-03	0.05	
3	4.4e-03	9.8e-04	3.9e-02	1.31e+00	1.674574097e-02	-3.644862047e-03	4.2e-04	0.05	
4	1.0e-04	6.7e-05	1.2e-03	1.19e+00	3.741952955e-04	-2.050730830e-04	1.3e-05	0.05	
5	9.4e-08	6.0e-08	1.1e-06	1.02e+00	3.392677121e-07	-1.760652310e-07	1.2e-08	0.05	
6	1.0e-11	6.5e-12	1.2e-10	1.00e+00	1.095654685e-07	1.095093081e-07	1.3e-12	0.05	

Basis identification started.
 Primal basis identification phase started.
 Primal basis identification phase terminated. Time: 0.00
 Dual basis identification phase started.
 Dual basis identification phase terminated. Time: 0.01
 Basis identification terminated. Time: 0.01
 Optimizer terminated. Time: 0.09

Interior-point solution summary

Problem status : PRIMAL_AND_DUAL_FEASIBLE
 Solution status : OPTIMAL
 Primal. obj: 1.0956546852e-07 nrm: 4e-01 Viol. con: 5e-12 var: 0e+00
 Dual. obj: 1.0950930807e-07 nrm: 1e+00 Viol. con: 0e+00 var: 3e-12

Basic solution summary

Problem status : PRIMAL_AND_DUAL_FEASIBLE
 Solution status : OPTIMAL
 Primal. obj: 1.0954043279e-07 nrm: 4e-01 Viol. con: 0e+00 var: 0e+00
 Dual. obj: 1.0950930801e-07 nrm: 2e+00 Viol. con: 0e+00 var: 9e-09

Optimizer summary

Optimizer	-	time: 0.09
Interior-point	- iterations : 6	time: 0.06
Basis identification	-	time: 0.01
Primal	- iterations : 0	time: 0.00
Dual	- iterations : 13	time: 0.01
Clean primal	- iterations : 0	time: 0.00
Clean dual	- iterations : 0	time: 0.00
Simplex	-	time: 0.00
Primal simplex	- iterations : 0	time: 0.00
Dual simplex	- iterations : 0	time: 0.00
Mixed integer	- relaxations: 0	time: 0.00

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Problem

Name :
 Objective sense : minimize
 Type : LO (linear optimization problem)
 Constraints : 28
 Affine conic cons. : 0
 Disjunctive cons. : 0
 Cones : 0
 Scalar variables : 196
 Matrix variables : 0
 Integer variables : 0

Optimizer started.

Presolve started.

Linear dependency checker started.

Linear dependency checker terminated.

Eliminator started.

Freed constraints in eliminator : 0

Eliminator terminated.

Eliminator - tries	: 1	time	: 0.00
Lin. dep. - tries	: 1	time	: 0.02
Lin. dep. - primal attempts	: 1	successes	: 1
Lin. dep. - dual attempts	: 0	successes	: 0
Lin. dep. - primal deps.	: 1	dual deps.	: 0

Presolve terminated. Time: 0.02

Optimizer - threads : 4

Optimizer - solved problem : the primal

```

Optimizer - Constraints          : 27
Optimizer - Cones               : 0
Optimizer - Scalar variables    : 196          conic          : 0
Optimizer - Semi-definite variables: 0          scalarized       : 0
Factor - setup time             : 0.01
Factor - dense det. time        : 0.00          GP order time    : 0.00
Factor - nonzeros before factor : 209          after factor     : 287
Factor - dense dim.             : 0            flops            : 4.68e+03
ITE PFEAS   DFEAS   GFEAS   PRSTATUS   POBJ          DOBJ          MU          TIME
0   1.7e+00  5.1e-01  1.5e+01  0.00e+00  1.334854790e+01 -1.081459940e+00 1.7e-01 0.03
1   3.6e-01  1.1e-01  3.1e+00  1.20e+00  2.201014664e+00 -2.006778581e-01 3.6e-02 0.05
2   4.2e-02  1.3e-02  3.7e-01  1.35e+00  2.036286790e-01 -2.453735077e-02 4.2e-03 0.05
3   4.6e-03  9.3e-04  3.8e-02  1.25e+00  1.715037941e-02 -3.559793348e-03 4.4e-04 0.05
4   2.2e-04  6.5e-05  2.0e-03  1.27e+00  6.248034125e-04 -2.923466449e-04 2.3e-05 0.05
5   4.2e-07  1.2e-07  3.8e-06  1.06e+00  1.351620741e-06 -3.382616587e-07 4.3e-08 0.05
6   4.2e-11  1.2e-11  3.8e-10  1.00e+00  5.917840012e-08 5.900885571e-08 4.3e-12 0.05
Basis identification started.
Primal basis identification phase started.
Primal basis identification phase terminated. Time: 0.00
Dual basis identification phase started.
Dual basis identification phase terminated. Time: 0.00
Basis identification terminated. Time: 0.00
Optimizer terminated. Time: 0.09

```

Interior-point solution summary

```

Problem status : PRIMAL_AND_DUAL_FEASIBLE
Solution status : OPTIMAL
Primal.  obj: 5.9178400122e-08   nrm: 4e-01   Viol.  con: 2e-11   var: 0e+00
Dual.    obj: 5.9008855706e-08   nrm: 1e+00   Viol.  con: 0e+00   var: 6e-12

```

Basic solution summary

```

Problem status : PRIMAL_AND_DUAL_FEASIBLE
Solution status : OPTIMAL
Primal.  obj: 5.9048715346e-08   nrm: 4e-01   Viol.  con: 0e+00   var: 0e+00
Dual.    obj: 5.9008855656e-08   nrm: 2e+00   Viol.  con: 0e+00   var: 9e-09

```

Optimizer summary

```

Optimizer - time: 0.09
Interior-point - iterations : 6   time: 0.06
Basis identification - time: 0.00
Primal - iterations : 0   time: 0.00
Dual - iterations : 13   time: 0.00
Clean primal - iterations : 0   time: 0.00
Clean dual - iterations : 0   time: 0.00
Simplex - time: 0.00
Primal simplex - iterations : 0   time: 0.00
Dual simplex - iterations : 0   time: 0.00
Mixed integer - relaxations: 0   time: 0.00

```

We compute the matching matrices for the different pairwise sample combinations. For each pair of samples we obtain a similarity matrix

```

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 sam
vars2 = supp(dim+1:dim+dim^2,start2:start2+nclust2-1);
p1 = ww(start1:start1+nclust1-1); %proportions of clusters in sample 1
p2 = ww(start2:start2+nclust2-1);
cost = CostMat(ms1,ms2,vars1,vars2,nclust1,nclust2); %cost matrix computation
cost = real(cost/max(cost,[],"all"));
[~,res]=OT(cost,p1,p2);
xx=res.sol.itr.xx;
gammaij=reshape(xx,[nclust1,nclust2]);
%normalization
if sum(sum(gammaij)) ~=0
    gammaijcol = gammaij./ max(abs(gammaij), [], 1);
    gammaijrow = gammaij./ max(abs(gammaij), [], 2);
    matchM{i} = (gammaijcol+gammaijrow)/2;
else
    matchM{i} = gammaij;
end
end

```

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 Platform: Windows/64-X86

Problem

```

Name           :
Objective sense : minimize
Type           : LO (linear optimization problem)
Constraints     : 28
Affine conic cons. : 0
Disjunctive cons. : 0
Cones          : 0
Scalar variables : 196
Matrix variables : 0
Integer variables : 0

```

Optimizer started.

Presolve started.

Linear dependency checker started.

Linear dependency checker terminated.

Eliminator started.

Freed constraints in eliminator : 0

Eliminator terminated.

Eliminator - tries	: 1	time	: 0.00
Lin. dep. - tries	: 1	time	: 0.00
Lin. dep. - primal attempts	: 1	successes	: 1
Lin. dep. - dual attempts	: 0	successes	: 0
Lin. dep. - primal deps.	: 1	dual deps.	: 0

Presolve terminated. Time: 0.00

```

Optimizer - threads           : 4
Optimizer - solved problem    : the primal
Optimizer - Constraints       : 27
Optimizer - Cones            : 0
Optimizer - Scalar variables  : 196
Optimizer - Semi-definite variables: 0
Factor - setup time           : 0.00
Factor - dense det. time      : 0.00
Factor - nonzeros before factor : 209
Factor - dense dim.          : 0

```

```

conic           : 0
scalarized      : 0
GP order time   : 0.00
after factor    : 287
flops           : 4.68e+03

```

ITE	PFEAS	DFEAS	GFEAS	PRSTATUS	POBJ	DOBJ	MU	TIME
0	1.9e+00	1.2e-01	1.4e+01	0.00e+00	1.268799652e+01	-6.826861994e-01	1.7e-01	0.01
1	4.7e-01	2.9e-02	3.4e+00	3.19e+00	1.597515029e+00	2.300236060e-01	4.1e-02	0.01

2	2.2e-01	1.4e-02	1.6e+00	1.42e+00	8.822250278e-01	3.294305934e-01	1.9e-02	0.03
3	3.9e-02	2.4e-03	2.8e-01	1.46e+00	4.543950590e-01	3.771362880e-01	3.4e-03	0.03
4	8.6e-03	5.3e-04	6.1e-02	1.26e+00	3.992315161e-01	3.844139444e-01	7.5e-04	0.03
5	1.8e-03	1.1e-04	1.3e-02	1.17e+00	3.889030037e-01	3.860807292e-01	1.6e-04	0.03
6	4.4e-04	2.7e-05	3.1e-03	1.12e+00	3.870214420e-01	3.863671288e-01	3.8e-05	0.03
7	2.5e-05	1.5e-06	1.8e-04	1.02e+00	3.864625466e-01	3.864258400e-01	2.2e-06	0.03
8	7.1e-07	4.4e-08	5.1e-06	1.00e+00	3.864301402e-01	3.864290796e-01	6.2e-08	0.03
9	7.6e-11	4.7e-12	5.4e-10	1.00e+00	3.864291918e-01	3.864291917e-01	6.6e-12	0.03

Basis identification started.

Primal basis identification phase started.

Primal basis identification phase terminated. Time: 0.00

Dual basis identification phase started.

Dual basis identification phase terminated. Time: 0.00

Basis identification terminated. Time: 0.02

Optimizer terminated. Time: 0.08

Interior-point solution summary

Problem status : PRIMAL_AND_DUAL_FEASIBLE

Solution status : OPTIMAL

Primal. obj: 3.8642919181e-01 nrm: 5e-01 Viol. con: 2e-11 var: 0e+00

Dual. obj: 3.8642919170e-01 nrm: 1e+00 Viol. con: 0e+00 var: 1e-12

Basic solution summary

Problem status : PRIMAL_AND_DUAL_FEASIBLE

Solution status : OPTIMAL

Primal. obj: 3.8642919171e-01 nrm: 5e-01 Viol. con: 6e-17 var: 0e+00

Dual. obj: 3.8642919170e-01 nrm: 1e+00 Viol. con: 0e+00 var: 1e-08

Optimizer summary

Optimizer	-	time: 0.08
Interior-point	- iterations : 9	time: 0.05
Basis identification	-	time: 0.02
Primal	- iterations : 0	time: 0.00
Dual	- iterations : 0	time: 0.00
Clean primal	- iterations : 0	time: 0.00
Clean dual	- iterations : 0	time: 0.00
Simplex	-	time: 0.00
Primal simplex	- iterations : 0	time: 0.00
Dual simplex	- iterations : 0	time: 0.00
Mixed integer	- relaxations: 0	time: 0.00

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Platform: Windows/64-X86

Problem

Name	:
Objective sense	: minimize
Type	: LO (linear optimization problem)
Constraints	: 28
Affine conic cons.	: 0
Disjunctive cons.	: 0
Cones	: 0
Scalar variables	: 196
Matrix variables	: 0
Integer variables	: 0

Optimizer started.

Presolve started.

Linear dependency checker started.

Linear dependency checker terminated.

Eliminator started.

Freed constraints in eliminator : 0

Eliminator terminated.


```

Eliminator - tries          : 1          time          : 0.00
Lin. dep.  - tries          : 1          time          : 0.00
Lin. dep.  - primal attempts : 1          successes       : 1
Lin. dep.  - dual attempts   : 0          successes       : 0
Lin. dep.  - primal deps.    : 1          dual deps.      : 0
Presolve terminated. Time: 0.01
Optimizer - threads          : 4
Optimizer - solved problem   : the primal
Optimizer - Constraints       : 27
Optimizer - Cones            : 0
Optimizer - Scalar variables : 196          conic           : 0
Optimizer - Semi-definite variables: 0          scalarized      : 0
Factor - setup time          : 0.00
Factor - dense det. time     : 0.00          GP order time   : 0.00
Factor - nonzeros before factor : 209          after factor    : 287
Factor - dense dim.          : 0          flops           : 4.68e+03
ITE PFEAS DFEAS GFEAS PRSTATUS POBJ DOBJ MU TIME
0  1.9e+00 1.1e-01 1.5e+01 0.00e+00 1.372254016e+01 -7.123448206e-01 1.7e-01 0.01
1  4.9e-01 2.7e-02 3.8e+00 3.56e+00 1.584299799e+00 2.196694186e-01 4.4e-02 0.05
2  1.4e-01 7.6e-03 1.0e+00 1.46e+00 6.363877889e-01 3.284988441e-01 1.2e-02 0.05
3  2.6e-02 1.5e-03 2.0e-01 1.31e+00 4.014970253e-01 3.519709868e-01 2.3e-03 0.05
4  7.2e-03 4.0e-04 5.5e-02 1.21e+00 3.708099789e-01 3.584259379e-01 6.4e-04 0.05
5  1.2e-03 6.5e-05 8.9e-03 1.15e+00 3.617234232e-01 3.598671502e-01 1.0e-04 0.05
6  5.9e-05 3.3e-06 4.6e-04 1.02e+00 3.602170245e-01 3.601213500e-01 5.3e-06 0.06
7  5.8e-07 3.3e-08 4.5e-06 1.00e+00 3.601357940e-01 3.601348550e-01 5.2e-08 0.06
8  1.4e-09 7.8e-11 1.1e-08 1.00e+00 3.601350240e-01 3.601350217e-01 1.2e-10 0.06
9  2.0e-13 7.8e-15 1.1e-12 1.00e+00 3.601350219e-01 3.601350219e-01 1.2e-14 0.08
Basis identification started.
Primal basis identification phase started.
Primal basis identification phase terminated. Time: 0.06
Dual basis identification phase started.
Dual basis identification phase terminated. Time: 0.02
Basis identification terminated. Time: 0.08
Optimizer terminated. Time: 0.22

```

Interior-point solution summary

```

Problem status : PRIMAL_AND_DUAL_FEASIBLE
Solution status : OPTIMAL
Primal.  obj: 3.6013502187e-01    nrm: 5e-01    Viol.  con: 4e-14    var: 0e+00
Dual.    obj: 3.6013502187e-01    nrm: 8e-01    Viol.  con: 0e+00    var: 2e-15

```

Basic solution summary

```

Problem status : PRIMAL_AND_DUAL_FEASIBLE
Solution status : OPTIMAL
Primal.  obj: 3.6013502187e-01    nrm: 5e-01    Viol.  con: 1e-16    var: 0e+00
Dual.    obj: 3.6013502187e-01    nrm: 8e-01    Viol.  con: 0e+00    var: 7e-12

```

Optimizer summary

```

Optimizer - time: 0.22
Interior-point - iterations : 9    time: 0.17
Basis identification - time: 0.08
Primal - iterations : 0    time: 0.06
Dual - iterations : 0    time: 0.02
Clean primal - iterations : 0    time: 0.00
Clean dual - iterations : 0    time: 0.00
Simplex - time: 0.00
Primal simplex - iterations : 0    time: 0.00
Dual simplex - iterations : 0    time: 0.00
Mixed integer - relaxations: 0    time: 0.00

```

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```

Problem
  Name           :
  Objective sense : minimize
  Type           : LO (linear optimization problem)
  Constraints     : 28
  Affine conic cons. : 0
  Disjunctive cons. : 0
  Cones          : 0
  Scalar variables : 196
  Matrix variables : 0
  Integer variables : 0

```

Optimizer started.

Presolve started.

Linear dependency checker started.

Linear dependency checker terminated.

Eliminator started.

Freed constraints in eliminator : 0

Eliminator terminated.

Eliminator - tries	: 1	time	: 0.00
Lin. dep. - tries	: 1	time	: 0.00
Lin. dep. - primal attempts	: 1	successes	: 1
Lin. dep. - dual attempts	: 0	successes	: 0
Lin. dep. - primal deps.	: 1	dual deps.	: 0

Presolve terminated. Time: 0.02

```

Optimizer - threads           : 4
Optimizer - solved problem    : the primal
Optimizer - Constraints       : 27
Optimizer - Cones            : 0
Optimizer - Scalar variables  : 196
Optimizer - Semi-definite variables: 0
Factor - setup time          : 0.00
Factor - dense det. time     : 0.00
Factor - nonzeros before factor : 209
Factor - dense dim.         : 0

```

```

conic           : 0
scalarized      : 0
GP order time   : 0.00
after factor    : 287
flops           : 4.68e+03

```

ITE	PFEAS	DFEAS	GFEAS	PRSTATUS	POBJ	DOBJ	MU	TIME
0	1.9e+00	1.2e-01	1.5e+01	0.00e+00	1.411364457e+01	-6.926314022e-01	1.7e-01	0.03
1	5.4e-01	3.5e-02	4.3e+00	3.72e+00	1.730735547e+00	2.257353780e-01	4.8e-02	0.05
2	1.6e-01	1.0e-02	1.3e+00	1.38e+00	6.954790948e-01	3.074386989e-01	1.4e-02	0.05
3	2.7e-02	1.7e-03	2.1e-01	1.28e+00	3.866737163e-01	3.310979283e-01	2.4e-03	0.05
4	7.4e-03	4.8e-04	5.8e-02	1.32e+00	3.487017049e-01	3.355688522e-01	6.6e-04	0.05
5	6.7e-04	4.4e-05	5.3e-03	1.22e+00	3.377742004e-01	3.367150213e-01	6.1e-05	0.06
6	3.5e-05	2.3e-06	2.7e-04	1.01e+00	3.368527677e-01	3.367981082e-01	3.1e-06	0.06
7	3.4e-07	2.2e-08	2.7e-06	1.00e+00	3.368014725e-01	3.368009361e-01	3.0e-08	0.06
8	3.4e-11	2.2e-12	2.7e-10	1.00e+00	3.368009909e-01	3.368009908e-01	3.0e-12	0.06

Basis identification started.

Primal basis identification phase started.

Primal basis identification phase terminated. Time: 0.00

Dual basis identification phase started.

Dual basis identification phase terminated. Time: 0.01

Basis identification terminated. Time: 0.01

Optimizer terminated. Time: 0.11

Interior-point solution summary

Problem status : PRIMAL_AND_DUAL_FEASIBLE

Solution status : OPTIMAL

Primal. obj:	3.3680099087e-01	nrm: 5e-01	Viol.	con: 7e-12	var: 0e+00
Dual. obj:	3.3680099082e-01	nrm: 7e-01	Viol.	con: 0e+00	var: 4e-13

Basic solution summary

Problem status : PRIMAL_AND_DUAL_FEASIBLE

Solution status : OPTIMAL

Primal. obj:	3.3680099082e-01	nrm: 5e-01	Viol.	con: 7e-18	var: 0e+00
Dual. obj:	3.3680099082e-01	nrm: 7e-01	Viol.	con: 0e+00	var: 5e-09

Optimizer summary

Optimizer	-	time: 0.11
Interior-point	- iterations : 8	time: 0.08
Basis identification	-	time: 0.01
Primal	- iterations : 0	time: 0.00
Dual	- iterations : 0	time: 0.01
Clean primal	- iterations : 0	time: 0.00
Clean dual	- iterations : 0	time: 0.00
Simplex	-	time: 0.00
Primal simplex	- iterations : 0	time: 0.00
Dual simplex	- iterations : 0	time: 0.00
Mixed integer	- relaxations: 0	time: 0.00

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Platform: Windows/64-X86

Problem

Name	:
Objective sense	: minimize
Type	: LO (linear optimization problem)
Constraints	: 28
Affine conic cons.	: 0
Disjunctive cons.	: 0
Cones	: 0
Scalar variables	: 196
Matrix variables	: 0
Integer variables	: 0

Optimizer started.

Presolve started.

Linear dependency checker started.

Linear dependency checker terminated.

Eliminator started.

Freed constraints in eliminator : 0

Eliminator terminated.

Eliminator - tries	: 1	time	: 0.00
Lin. dep. - tries	: 1	time	: 0.00
Lin. dep. - primal attempts	: 1	successes	: 1
Lin. dep. - dual attempts	: 0	successes	: 0
Lin. dep. - primal deps.	: 1	dual deps.	: 0

Presolve terminated. Time: 0.00

Optimizer - threads	: 4
Optimizer - solved problem	: the primal
Optimizer - Constraints	: 27
Optimizer - Cones	: 0
Optimizer - Scalar variables	: 196
Optimizer - Semi-definite variables	: 0
Factor - setup time	: 0.00
Factor - dense det. time	: 0.00
Factor - nonzeros before factor	: 209
Factor - dense dim.	: 0

conic	: 0
scalarized	: 0
GP order time	: 0.00
after factor	: 287
flops	: 4.68e+03

ITE	PFEAS	DFEAS	GFEAS	PRSTATUS	POBJ	DOBJ	MU	TIME
0	1.9e+00	2.1e-01	1.5e+01	0.00e+00	1.415848620e+01	-6.143545484e-01	1.8e-01	0.01
1	5.7e-01	6.4e-02	4.5e+00	4.29e+00	1.746813893e+00	3.270480327e-01	5.4e-02	0.01
2	1.2e-01	1.4e-02	9.9e-01	1.33e+00	6.434993241e-01	3.772571921e-01	1.2e-02	0.03
3	3.1e-02	3.5e-03	2.4e-01	1.36e+00	4.479671525e-01	3.925924472e-01	2.9e-03	0.03
4	5.2e-03	5.9e-04	4.1e-02	1.24e+00	4.052927317e-01	3.970696975e-01	4.9e-04	0.03
5	1.4e-03	1.5e-04	1.1e-02	1.18e+00	3.996443735e-01	3.976536024e-01	1.3e-04	0.03
6	2.9e-04	3.3e-05	2.3e-03	1.07e+00	3.982030979e-01	3.977913377e-01	2.8e-05	0.03
7	1.2e-05	1.4e-06	9.8e-05	1.01e+00	3.978323154e-01	3.978144766e-01	1.2e-06	0.03
8	5.2e-09	5.9e-10	4.1e-08	1.00e+00	3.978154487e-01	3.978154413e-01	4.9e-10	0.03

Basis identification started.

Primal basis identification phase started.

Primal basis identification phase terminated. Time: 0.00
Dual basis identification phase started.
Dual basis identification phase terminated. Time: 0.02
Basis identification terminated. Time: 0.02
Optimizer terminated. Time: 0.08

Interior-point solution summary

Problem status : PRIMAL_AND_DUAL_FEASIBLE
Solution status : OPTIMAL
Primal. obj: 3.9781544869e-01 nrm: 4e-01 Viol. con: 9e-10 var: 0e+00
Dual. obj: 3.9781544126e-01 nrm: 7e-01 Viol. con: 0e+00 var: 1e-10

Basic solution summary

Problem status : PRIMAL_AND_DUAL_FEASIBLE
Solution status : OPTIMAL
Primal. obj: 3.9781544184e-01 nrm: 4e-01 Viol. con: 1e-16 var: 0e+00
Dual. obj: 3.9781544126e-01 nrm: 7e-01 Viol. con: 0e+00 var: 3e-07

Optimizer summary

Optimizer	-	time: 0.08
Interior-point	- iterations : 8	time: 0.05
Basis identification	-	time: 0.02
Primal	- iterations : 0	time: 0.00
Dual	- iterations : 0	time: 0.02
Clean primal	- iterations : 0	time: 0.00
Clean dual	- iterations : 0	time: 0.00
Simplex	-	time: 0.00
Primal simplex	- iterations : 0	time: 0.00
Dual simplex	- iterations : 0	time: 0.00
Mixed integer	- relaxations: 0	time: 0.00

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Platform: Windows/64-X86

Problem

Name	:
Objective sense	: minimize
Type	: LO (linear optimization problem)
Constraints	: 28
Affine conic cons.	: 0
Disjunctive cons.	: 0
Cones	: 0
Scalar variables	: 196
Matrix variables	: 0
Integer variables	: 0

Optimizer started.

Presolve started.

Linear dependency checker started.

Linear dependency checker terminated.

Eliminator started.

Freed constraints in eliminator : 0

Eliminator terminated.

Eliminator - tries	: 1	time	: 0.00
Lin. dep. - tries	: 1	time	: 0.00
Lin. dep. - primal attempts	: 1	successes	: 1
Lin. dep. - dual attempts	: 0	successes	: 0
Lin. dep. - primal deps.	: 1	dual deps.	: 0

Presolve terminated. Time: 0.02

Optimizer - threads	: 4
Optimizer - solved problem	: the primal
Optimizer - Constraints	: 27
Optimizer - Cones	: 0

```

Optimizer - Scalar variables      : 196          conic          : 0
Optimizer - Semi-definite variables: 0          scalarized       : 0
Factor    - setup time           : 0.00
Factor    - dense det. time      : 0.00          GP order time    : 0.00
Factor    - nonzeros before factor : 209        after factor     : 287
Factor    - dense dim.           : 0            flops            : 4.68e+03
ITE PFEAS DFEAS GFEAS PRSTATUS POBJ DOBJ MU TIME
0  1.9e+00 2.0e-01 1.5e+01 0.00e+00 1.448100040e+01 -6.346398643e-01 1.8e-01 0.03
1  5.2e-01 5.4e-02 4.2e+00 4.16e+00 1.679141086e+00 3.460975762e-01 4.9e-02 0.05
2  1.3e-01 1.3e-02 1.0e+00 1.28e+00 6.777261578e-01 3.916089298e-01 1.2e-02 0.05
3  2.8e-02 3.0e-03 2.3e-01 1.30e+00 4.653370254e-01 4.092696915e-01 2.7e-03 0.05
4  8.6e-03 9.0e-04 7.0e-02 1.23e+00 4.280328336e-01 4.128461875e-01 8.2e-04 0.05
5  9.2e-04 9.6e-05 7.4e-03 1.25e+00 4.154070819e-01 4.140497261e-01 8.7e-05 0.05
6  1.4e-04 1.4e-05 1.1e-03 1.08e+00 4.143548861e-01 4.141540396e-01 1.3e-05 0.05
7  1.1e-05 1.1e-06 8.5e-05 1.03e+00 4.141916311e-01 4.141761446e-01 1.0e-06 0.05
8  1.0e-07 1.1e-08 8.5e-07 1.00e+00 4.141769098e-01 4.141767562e-01 1.0e-08 0.05
9  1.1e-11 1.1e-12 8.6e-11 1.00e+00 4.141767637e-01 4.141767637e-01 1.0e-12 0.05
Basis identification started.
Primal basis identification phase started.
Primal basis identification phase terminated. Time: 0.02
Dual basis identification phase started.
Dual basis identification phase terminated. Time: 0.00
Basis identification terminated. Time: 0.02
Optimizer terminated. Time: 0.08

```

Interior-point solution summary

```

Problem status : PRIMAL_AND_DUAL_FEASIBLE
Solution status : OPTIMAL
Primal.  obj: 4.1417676367e-01    nrm: 4e-01    Viol.  con: 2e-12    var: 0e+00
Dual.    obj: 4.1417676365e-01    nrm: 8e-01    Viol.  con: 0e+00    var: 2e-13

```

Basic solution summary

```

Problem status : PRIMAL_AND_DUAL_FEASIBLE
Solution status : OPTIMAL
Primal.  obj: 4.1417676365e-01    nrm: 4e-01    Viol.  con: 1e-17    var: 0e+00
Dual.    obj: 4.1417676365e-01    nrm: 8e-01    Viol.  con: 0e+00    var: 8e-10

```

Optimizer summary

```

Optimizer - time: 0.08
Interior-point - iterations : 9    time: 0.06
Basis identification - time: 0.02
Primal - iterations : 0    time: 0.02
Dual - iterations : 0    time: 0.00
Clean primal - iterations : 0    time: 0.00
Clean dual - iterations : 0    time: 0.00
Simplex - time: 0.00
Primal simplex - iterations : 0    time: 0.00
Dual simplex - iterations : 0    time: 0.00
Mixed integer - relaxations: 0    time: 0.00

```

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Platform: Windows/64-X86

Problem

```

Name :
Objective sense : minimize
Type : LO (linear optimization problem)
Constraints : 28
Affine conic cons. : 0
Disjunctive cons. : 0
Cones : 0
Scalar variables : 196
Matrix variables : 0

```

```

Integer variables      : 0

Optimizer started.
Presolve started.
Linear dependency checker started.
Linear dependency checker terminated.
Eliminator started.
Freed constraints in eliminator : 0
Eliminator terminated.
Eliminator - tries          : 1          time           : 0.00
Lin. dep. - tries          : 1          time           : 0.00
Lin. dep. - primal attempts : 1          successes        : 1
Lin. dep. - dual attempts  : 0          successes        : 0
Lin. dep. - primal deps.   : 1          dual deps.       : 0
Presolve terminated. Time: 0.00
Optimizer - threads        : 4
Optimizer - solved problem : the primal
Optimizer - Constraints     : 27
Optimizer - Cones          : 0
Optimizer - Scalar variables : 196        conic           : 0
Optimizer - Semi-definite variables: 0      scalarized      : 0
Factor - setup time        : 0.00
Factor - dense det. time   : 0.00        GP order time   : 0.00
Factor - nonzeros before factor : 209      after factor    : 287
Factor - dense dim.       : 0          flops           : 4.68e+03
ITE PFEAS  DFEAS  GFEAS  PRSTATUS  POBJ          DOBJ          MU          TIME
0  1.9e+00  1.1e-01  1.7e+01  0.00e+00  1.606574097e+01  -7.739208945e-01  1.8e-01  0.02
1  3.0e-01  1.7e-02  2.7e+00  3.20e+00  1.323177771e+00  2.349941742e-01  2.8e-02  0.03
2  8.3e-02  4.8e-03  7.6e-01  1.36e+00  5.585328347e-01  3.071749189e-01  7.8e-03  0.03
3  3.1e-02  1.8e-03  2.8e-01  1.14e+00  4.137462696e-01  3.222389300e-01  3.0e-03  0.03
4  5.0e-03  2.9e-04  4.5e-02  1.20e+00  3.411821789e-01  3.286411097e-01  4.7e-04  0.03
5  6.5e-04  3.8e-05  6.0e-03  1.26e+00  3.317081676e-01  3.302648941e-01  6.2e-05  0.03
6  6.5e-05  3.7e-06  5.9e-04  1.04e+00  3.305020670e-01  3.303593410e-01  6.1e-06  0.03
7  1.0e-06  5.8e-08  9.2e-06  1.01e+00  3.303856739e-01  3.303834664e-01  9.5e-08  0.03
8  1.0e-10  6.0e-12  9.5e-10  1.00e+00  3.303837308e-01  3.303837306e-01  9.9e-12  0.03
Basis identification started.
Primal basis identification phase started.
Primal basis identification phase terminated. Time: 0.00
Dual basis identification phase started.
Dual basis identification phase terminated. Time: 0.00
Basis identification terminated. Time: 0.00
Optimizer terminated. Time: 0.05

Interior-point solution summary
Problem status : PRIMAL_AND_DUAL_FEASIBLE
Solution status : OPTIMAL
Primal.  obj: 3.3038373083e-01    nrm: 4e-01    Viol.  con: 3e-11    var: 0e+00
Dual.    obj: 3.3038373060e-01    nrm: 1e+00    Viol.  con: 0e+00    var: 1e-12

Basic solution summary
Problem status : PRIMAL_AND_DUAL_FEASIBLE
Solution status : OPTIMAL
Primal.  obj: 3.3038373062e-01    nrm: 4e-01    Viol.  con: 1e-16    var: 0e+00
Dual.    obj: 3.3038373060e-01    nrm: 1e+00    Viol.  con: 0e+00    var: 1e-08

Optimizer summary
Optimizer - time: 0.05
Interior-point - iterations : 8    time: 0.03
Basis identification - time: 0.00
Primal - iterations : 0    time: 0.00
Dual - iterations : 0    time: 0.00
Clean primal - iterations : 0    time: 0.00
Clean dual - iterations : 0    time: 0.00
Simplex - time: 0.00
Primal simplex - iterations : 0    time: 0.00

```

Dual simplex	- iterations : 0	time: 0.00
Mixed integer	- relaxations: 0	time: 0.00

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.

```
Biggamma_ij = 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;
    Biggamma_ij(start1:endClust,endClust+1:end)=Biggamma_ij(start1:endClust,endClust+1:end)+ [mat
    Biggamma_ij(endClust+1:end,start1:endClust)=Biggamma_ij(endClust+1:end,start1:endClust)+ [mat
    startPat = endPat+1;
    endPat = startPat+numPat-2-j;
end
%We bound below very small values in the large matrix:
Biggamma_ij(abs(Biggamma_ij) < min(ww)* 1E-7) = min(ww)* 1E-7;
```

Construct Tree from Overall Similarity Matrix

We now need to transform B into a cluster distance matrix A from which we construct a taxonomy.

```
A = real(-log(Biggamma_ij));
A= A/ max(max(A));
B = squareform(A);
tree=linkage(B, 'ward');
cellClusters=cluster(tree, "MaxClust", numcells);
```

cellClusters is a vector with a length equivalent to that of the number of clusters. The entries in it give the metacluster label for all of the clusters.

Measure Performance

We compute the ARI, cell-level accuracy, as well as cluster level accuracy.

```
failcount = 0;
fail = 0;
for i=1:numcells
    PLindices = find(cellClusters==i); %indices for clusters with metacluster label i
    predictedLabels = string(cellnames(PLindices)); % Ground truth labels for clusters in metacluster i
    predLabel=mode(categorical(predictedLabels)); %Predicted label for metacluster i
    failcount = failcount+ sum(predictedLabels~=string(predLabel)); %add number of clusters in metacluster i
    propLabels = ww(PLindices); %cluster proportions
    cumstride = cumsum(stride);
    for j=1:length(PLindices)
```

```

        if predictedLabels(j)~=string(predLabel)
            cellsp=numerclust(min(find(cumstride>= PLindices(j)))); %this is the
            %total number of cells in the sample where cell type j is from.
            fail=fail+round(propLabels(j)*cellsp);
        end
    end
end

```

```

end
%ARI
[RI, ARI] = randindex(string(cellClusters),string(cellnames));
ARI

```

```
ARI = 0.7637
```

```

%Cluster accuracy
1-failcount/length(cellnames)

```

```
ans = 0.8750
```

```

%Cell accuracy. %numerclust gives the # of cells per cluster.
1-double(fail)/double(sum(numerclust))

```

```
ans = 0.9940
```

Dendrogram

We can visualize our dendrogram:

```

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', []);

```


