# read\_codex args

codex\_blanks="../Data/raw\_dataset/codex\_blanks.csv",

codex\_protein="../Data/`raw\_dataset/codex\_protein.csv",

codex\_size="../Data/raw\_dataset/codex\_size.csv",

codex\_spatial="../Data/raw\_dataset/codex\_spatial.csv",

codex\_preprocess=True,

codex\_border=564000,

# read\_cite args

cite\_latent="../Data/raw\_dataset/cite\_latent.csv",

cite\_protein="../Data/raw\_dataset/cite\_protein.csv",

cite\_mrna="../Data/raw\_dataset/cite\_mRNA.csv",

# take\_subset args

amount\_codex=-1, # -1 = default ≈ 9000 CODEX cells

amount\_cite=-1, # -1 ≈ 7000 cells

# filter\_codex args

size\_lim=(1000, 25000),

blank\_lower=(-1200, -1200, -1200, -1200),

blank\_upper=(6000, 2500, 5000, 2500),

# clean\_cite args

maxit=500,

factr=1e-9,

optim\_init=([10, 60, 2, 0.5, 0.5],

[4.8, 50, 0.5, 2, 0.5],

A screenshot of a cell phone

Description automatically generated [2, 18, 0.5, 2, 0.5],

A screenshot of a computer

Description automatically generated [1, 3, 2, 2, 0.5],

[1, 3, 0.5, 2, 0.5]),

ignore\_warnings=True,

clean\_cite\_method="l-bfgs-b",

# cluster\_codex args

cluster\_codex\_k=10,

cluster\_codex\_knn\_option=1,

# parameter\_scan args

parameter\_scan\_min\_cluster\_size\_range=tuple(range(5, 21, 4)),

parameter\_scan\_min\_sample\_range=tuple(range(10, 41, 3)),

parameter\_scan\_n\_neighbors=50,

parameter\_scan\_min\_dist=0.1,

parameter\_scan\_negative\_sample\_rate=50,

parameter\_scan\_metric="correlation",

# consensus\_cluster args

consensus\_cluster\_silhouette\_cutoff=0.126,

consensus\_cluster\_inconsistent\_value=0.1,

consensus\_cluster\_min\_cluster\_size=10,

# map\_codex\_to\_cite args

k\_find\_nn=80,

k\_find\_anchor=20,

k\_filter\_anchor=100,

k\_score\_anchor=80,

k\_find\_weights=100,

# transfer\_matrix

k\_transfer\_matrix=None,

c\_transfer\_matrix=0.1,

mask=False

result:

Macrophages: TPR: 41.24% TNR: 98.34

B cells: TPR: 99.08% TNR: 64.44

A screenshot of a graph

Description automatically generatedNeutrophils: TPR: 71.43% TNR: 99.84

A diagram of a heatmap

Description automatically generated

def test\_overall\_evaluation(self):

# initialize variable

cn = Controller.Controller()

# this pipeline will read files

cn.pipeline(

# read\_codex args

codex\_blanks="../Data/raw\_dataset/codex\_blanks.csv",

codex\_protein="../Data/raw\_dataset/codex\_protein.csv",

codex\_size="../Data/raw\_dataset/codex\_size.csv",

codex\_spatial="../Data/raw\_dataset/codex\_spatial.csv",

codex\_preprocess=True,

codex\_border=564000,

T cells: TPR: 68.59% TNR: 99.86

Transferred majority: T cells

B cells: TPR: 98.56% TNR: 87.73

Transferred majority: B cells

Neutrophils: TPR: 61.54% TNR: 99.96

Transferred majority: Neutrophils

NK cells: TPR: 41.18% TNR: 98.33

Transferred majority: NK cells

CODEX cluster 1 transferred majority: T cells

CODEX cluster 2 transferred majority: B cells

CODEX cluster 3 transferred majority: Macrophages

CODEX cluster 4 transferred majority: B cells

CODEX cluster 5 transferred majority: Macrophages

CODEX cluster 6 transferred majority: B cells

CODEX cluster 7 transferred majority: B cells

CODEX cluster 8 transferred majority: Neutrophils

CODEX cluster 9 transferred majority: B cells

CODEX cluster 10 transferred majority: NK cells

CODEX cluster 11 transferred majority: B cells

CODEX cluster 12 transferred majority:

CODEX cluster 13 transferred majority: B cells

CODEX cluster 14 transferred majority: Plasma cells

CODEX cluster 15 transferred majority: B cells

CODEX cluster 16 transferred majority: T cells

CODEX cluster 17 transferred majority: T cells

CODEX cluster 18 transferred majority: B cells

CODEX cluster 19 transferred majority: B cells

CODEX cluster 20 transferred majority: B cells

CODEX cluster 21 transferred majority: B cells

CODEX cluster 22 transferred majority: B cells

# read\_cite args

cite\_latent="../Data/raw\_dataset/cite\_latent.csv",

cite\_protein="../Data/raw\_dataset/cite\_protein.csv",

cite\_mrna="../Data/raw\_dataset/cite\_mRNA.csv",

# take\_subset args

amount\_codex=-1, # -1 = default ≈ 9000 CODEX cells

amount\_cite=-1, # -1 ≈ 7000 cells

# filter\_codex args

size\_lim=(1000, 25000),

blank\_lower=(-1200, -1200, -1200, -1200),

blank\_upper=(6000, 2500, 5000, 2500),

# clean\_cite args

maxit=500,

factr=1e-9,

optim\_init=([10, 60, 2, 0.5, 0.5],

[4.8, 50, 0.5, 2, 0.5],

[2, 18, 0.5, 2, 0.5],

[1, 3, 2, 2, 0.5],

[1, 3, 0.5, 2, 0.5]),

ignore\_warnings=True,

clean\_cite\_method="l-bfgs-b",

# cluster\_codex args

cluster\_codex\_k=5,

cluster\_codex\_knn\_option=1,

# parameter\_scan args

parameter\_scan\_min\_cluster\_size\_range=tuple(range(5, 21, 4)),

parameter\_scan\_min\_sample\_range=tuple(range(10, 41, 3)),

parameter\_scan\_n\_neighbors=50,

parameter\_scan\_min\_dist=0.1,

parameter\_scan\_negative\_sample\_rate=50,

parameter\_scan\_metric="correlation",

# consensus\_cluster args

consensus\_cluster\_silhouette\_cutoff=0.126,

consensus\_cluster\_inconsistent\_value=0.1,

consensus\_cluster\_min\_cluster\_size=10,

# map\_codex\_to\_cite args

k\_find\_nn=80,

k\_find\_anchor=20,

k\_filter\_anchor=100,

k\_score\_anchor=80,

k\_find\_weights=100,

# transfer\_matrix

k\_transfer\_matrix=None,

c\_transfer\_matrix=0.1,

mask=False

A screenshot of a graph

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A screenshot of a graph

Description automatically generated

T cells: TPR: 84.75% TNR: 99.86

Transferred majority: T cells

B cells: TPR: 99.23% TNR: 97.08

Transferred majority: B cells

Neutrophils: TPR: 60.53% TNR: 99.95

Transferred majority: Neutrophils

NK cells: TPR: 62.5% TNR: 99.09

Transferred majority: NK cells

CODEX cluster 1 transferred majority: 83.858 % T cells

CODEX cluster 2 transferred majority: 17.759 % B cells

CODEX cluster 3 transferred majority: 54.962 % Macrophages

CODEX cluster 4 transferred majority: 100.0 % B cells

CODEX cluster 5 transferred majority: 48.308 % B cells

CODEX cluster 6 transferred majority: 100.0 % B cells

CODEX cluster 7 transferred majority: 58.974 % Neutrophils

CODEX cluster 8 transferred majority: 69.153 % Macrophages

CODEX cluster 9 transferred majority: 98.742 % B cells

CODEX cluster 10 transferred majority: 95.96 % B cells

CODEX cluster 11 transferred majority: 99.441 % B cells

CODEX cluster 12 transferred majority: 22.034 % Macrophages

CODEX cluster 13 transferred majority: 49.492 % B cells

CODEX cluster 14 transferred majority: 98.759 % B cells

CODEX cluster 15 transferred majority: 59.055 % T cells

CODEX cluster 16 transferred majority: 100.0 % B cells

CODEX cluster 17 transferred majority: 96.721 % B cells

CODEX cluster 18 transferred majority: 98.477 % B cells

CODEX cluster 19 transferred majority: 61.538 % NK cells

CODEX cluster 20 transferred majority: 69.231 % Plasma cells

CODEX cluster 21 transferred majority: 99.445 % B cells

CODEX cluster 22 transferred majority: 94.805 % B cells

CODEX cluster 23 transferred majority: 99.379 % B cells

CODEX cluster 24 transferred majority: 74.766 % B cells

CODEX cluster 25 transferred majority: 99.043 % B cells

CODEX cluster 26 transferred majority: 100.0 % B cells

Kick out distant CODEX cells.

cn.pipeline(

# read\_codex args

codex\_blanks="../Data/raw\_dataset/codex\_blanks.csv",

codex\_protein="../Data/raw\_dataset/codex\_protein.csv",

codex\_size="../Data/raw\_dataset/codex\_size.csv",

codex\_spatial="../Data/raw\_dataset/codex\_spatial.csv",

codex\_preprocess=True,

codex\_border=564000,

# read\_cite args

cite\_latent="../Data/raw\_dataset/cite\_latent.csv",

cite\_protein="../Data/raw\_dataset/cite\_protein.csv",

cite\_mrna="../Data/raw\_dataset/cite\_mRNA.csv",

# take\_subset args

amount\_codex=-1, # -1 = default ≈ 9000 CODEX cells

amount\_cite=-1, # -1 ≈ 7000 cells

# filter\_codex args

size\_lim=(1000, 25000),

blank\_lower=(-1200, -1200, -1200, -1200),

blank\_upper=(6000, 2500, 5000, 2500),

# clean\_cite args

maxit=500,

factr=1e-9,

optim\_init=([10, 60, 2, 0.5, 0.5],

[4.8, 50, 0.5, 2, 0.5],

[2, 18, 0.5, 2, 0.5],

[1, 3, 2, 2, 0.5],

[1, 3, 0.5, 2, 0.5]),

ignore\_warnings=True,

clean\_cite\_method="l-bfgs-b",

# cluster\_codex args

cluster\_codex\_k=5,

cluster\_codex\_knn\_option=1,

# parameter\_scan args

parameter\_scan\_min\_cluster\_size\_range=tuple(range(5, 21, 4)),

parameter\_scan\_min\_sample\_range=tuple(range(10, 41, 3)),

parameter\_scan\_n\_neighbors=50,

parameter\_scan\_min\_dist=0.1,

A screenshot of a graph

Description automatically generated parameter\_scan\_negative\_sample\_rate=50,

parameter\_scan\_metric="correlation",

# consensus\_cluster args

consensus\_cluster\_silhouette\_cutoff=0.126,

consensus\_cluster\_inconsistent\_value=0.1,

consensus\_cluster\_min\_cluster\_size=10,

# map\_codex\_to\_cite args

k\_find\_nn=80,

k\_find\_anchor=20,

k\_filter\_anchor=100,

k\_score\_anchor=80,

k\_find\_weights=100,

# transfer\_matrix

k\_transfer\_matrix=None,

c\_transfer\_matrix=0.1,

mask=True

)

A screenshot of a graph

Description automatically generated

A screenshot of a cell phone

Description automatically generated

Around 9000 CODEX cells

A screenshot of a graph

Description automatically generated def test\_overall\_evaluation(self):

# initialize variable

cn = Controller.Controller()

# this pipeline will read files

cn.pipeline(

# read\_codex args

codex\_blanks="../Data/raw\_dataset/codex\_blanks.csv",

codex\_protein="../Data/raw\_dataset/codex\_protein.csv",

codex\_size="../Data/raw\_dataset/codex\_size.csv",

codex\_spatial="../Data/raw\_dataset/codex\_spatial.csv",

codex\_preprocess=True,

codex\_border=600000,

# read\_cite args

cite\_latent="../Data/raw\_dataset/cite\_latent.csv",

cite\_protein="../Data/raw\_dataset/cite\_protein.csv",

cite\_mrna="../Data/raw\_dataset/cite\_mRNA.csv",

# take\_subset args

amount\_codex=-1, # -1 = default ≈ 9000 CODEX cells

amount\_cite=-1, # -1 ≈ 7000 cells

# filter\_codex args

size\_lim=(1000, 25000),

blank\_lower=(-1200, -1200, -1200, -1200),

blank\_upper=(6000, 2500, 5000, 2500),

# clean\_cite args

maxit=500,

factr=1e-9,

optim\_init=([10, 60, 2, 0.5, 0.5],

[4.8, 50, 0.5, 2, 0.5],

[2, 18, 0.5, 2, 0.5],

[1, 3, 2, 2, 0.5],

[1, 3, 0.5, 2, 0.5]),

ignore\_warnings=True,

clean\_cite\_method="l-bfgs-b",

# cluster\_codex args

cluster\_codex\_k=5,

cluster\_codex\_knn\_option=1,

# parameter\_scan args

parameter\_scan\_min\_cluster\_size\_range=tuple(range(5, 21, 4)),

parameter\_scan\_min\_sample\_range=tuple(range(10, 41, 3)),

parameter\_scan\_n\_neighbors=50,

parameter\_scan\_min\_dist=0.1,

parameter\_scan\_negative\_sample\_rate=50,

parameter\_scan\_metric="correlation",

# consensus\_cluster args

consensus\_cluster\_silhouette\_cutoff=0.126,

consensus\_cluster\_inconsistent\_value=0.1,

consensus\_cluster\_min\_cluster\_size=10,

# map\_codex\_to\_cite args

T cells: TPR: 90.52% TNR: 99.53%

Transferred majority: T cells

B cells: TPR: 99.47% TNR: 93.68%

Transferred majority: B cells

Neutrophils: TPR: 61.76% TNR: 99.97%

Transferred majority: Neutrophils

NK cells: TPR: 57.14% TNR: 99.45%

Transferred majority: NK cells

CODEX cluster 1 transferred majority: 84.153 % T cells

CODEX cluster 2 transferred majority: 57.285 % B cells

CODEX cluster 3 transferred majority: 100.0 % B cells

CODEX cluster 4 transferred majority: 34.541 % B cells

CODEX cluster 5 transferred majority: 97.602 % B cells

CODEX cluster 6 transferred majority: 99.04 % B cells

CODEX cluster 7 transferred majority: 56.757 % Neutrophils

CODEX cluster 8 transferred majority: 63.277 % B cells

CODEX cluster 9 transferred majority: 41.558 % Erythrocytes

CODEX cluster 10 transferred majority: 56.738 % NK cells

CODEX cluster 11 transferred majority: 91.441 % B cells

CODEX cluster 12 transferred majority: 93.137 % B cells

CODEX cluster 13 transferred majority: 60.635 % T cells

CODEX cluster 14 transferred majority: 99.06 % B cells

CODEX cluster 15 transferred majority: 92.949 % T cells

CODEX cluster 16 transferred majority: 99.333 % B cells

CODEX cluster 17 transferred majority: 99.065 % B cells

CODEX cluster 18 transferred majority: 98.505 % B cells

CODEX cluster 19 transferred majority: 81.047 % B cells

CODEX cluster 20 transferred majority: 89.778 % B cells

CODEX cluster 21 transferred majority: 99.505 % B cells

CODEX cluster 22 transferred majority: 99.805 % B cells

k\_find\_nn=80,

k\_find\_anchor=20,

k\_filter\_anchor=100,

k\_score\_anchor=80,

k\_find\_weights=100,

# transfer\_matrix

k\_transfer\_matrix=None,

c\_transfer\_matrix=0.1,

mask=True

)

# invoke the partial evaluation

TestController.partial\_evaluation(cn.stvea, cn.annotation)

1. A purple and orange squares

   Description automatically generated

Around 4000 CODEX cells

# this pipeline will read files

cn.pipeline(

# read\_codex args

codex\_blanks="../Data/raw\_dataset/codex\_blanks.csv",

codex\_protein="../Data/raw\_dataset/codex\_protein.csv",

codex\_size="../Data/raw\_dataset/codex\_size.csv",

codex\_spatial="../Data/raw\_dataset/codex\_spatial.csv",

codex\_preprocess=True,

codex\_border=390000,

# read\_cite args

cite\_latent="../Data/raw\_dataset/cite\_latent.csv",

cite\_protein="../Data/raw\_dataset/cite\_protein.csv",

cite\_mrna="../Data/raw\_dataset/cite\_mRNA.csv",

# take\_subset args

amount\_codex=-1, # -1 = default ≈ 9000 CODEX cells

amount\_cite=-1, # -1 ≈ 7000 cells

# filter\_codex args

size\_lim=(1000, 25000),

blank\_lower=(-1200, -1200, -1200, -1200),

blank\_upper=(6000, 2500, 5000, 2500),

# clean\_cite args

maxit=500,

factr=1e-9,

optim\_init=([10, 60, 2, 0.5, 0.5],

[4.8, 50, 0.5, 2, 0.5],

[2, 18, 0.5, 2, 0.5],

[1, 3, 2, 2, 0.5],

[1, 3, 0.5, 2, 0.5]),

ignore\_warnings=True,

clean\_cite\_method="l-bfgs-b",

# cluster\_codex args

cluster\_codex\_k=5,

cluster\_codex\_knn\_option=1,

# parameter\_scan args

T cells: TPR: 87.56% TNR: 99.54%

Transferred majority: T cells

B cells: TPR: 97.7% TNR: 95.48%

Transferred majority: B cells

Neutrophils: TPR: 51.85% TNR: 100.0%

Transferred majority: Neutrophils

NK cells: TPR: 88.57% TNR: 98.22%

Transferred majority: NK cells

CODEX cluster 1 transferred majority: 86.275 % T cells

CODEX cluster 2 transferred majority: 47.059 % B cells

CODEX cluster 3 transferred majority: 30.252 % B cells

CODEX cluster 4 transferred majority: 100.0 % B cells

CODEX cluster 5 transferred majority: 85.714 % B cells

CODEX cluster 6 transferred majority: 95.977 % B cells

CODEX cluster 7 transferred majority: 51.852 % Neutrophils

CODEX cluster 8 transferred majority: 61.6 % B cells

CODEX cluster 9 transferred majority: 31.0 % B cells

CODEX cluster 10 transferred majority: 87.324 % NK cells

CODEX cluster 11 transferred majority: 44.156 % B cells

CODEX cluster 12 transferred majority: 93.452 % B cells

CODEX cluster 13 transferred majority: 99.153 % B cells

CODEX cluster 14 transferred majority: 56.25 % T cells

CODEX cluster 15 transferred majority: 46.552 % B cells

CODEX cluster 16 transferred majority: 85.926 % T cells

CODEX cluster 17 transferred majority: 94.604 % B cells

CODEX cluster 18 transferred majority: 97.84 % B cells

CODEX cluster 19 transferred majority: 78.571 % NK cells

CODEX cluster 20 transferred majority: 78.261 % B cells

CODEX cluster 21 transferred majority: 100.0 % B cells

CODEX cluster 22 transferred majority: 82.222 % B cells

CODEX cluster 23 transferred majority: 99.194 % B cells

CODEX cluster 24 transferred majority: 99.415 % B cells

parameter\_scan\_min\_cluster\_size\_range=tuple(range(5, 21, 4)),

parameter\_scan\_min\_sample\_range=tuple(range(10, 41, 3)),

parameter\_scan\_n\_neighbors=50,

parameter\_scan\_min\_dist=0.1,

parameter\_scan\_negative\_sample\_rate=50,

parameter\_scan\_metric="correlation",

# consensus\_cluster args

consensus\_cluster\_silhouette\_cutoff=0.126,

consensus\_cluster\_inconsistent\_value=0.1,

consensus\_cluster\_min\_cluster\_size=10,

# map\_codex\_to\_cite args

k\_find\_nn=80,

k\_find\_anchor=20,

k\_filter\_anchor=100,

k\_score\_anchor=80,

k\_find\_weights=100,

# transfer\_matrix

k\_transfer\_matrix=None,

c\_transfer\_matrix=0.1,

mask=True

)

Around 2000 cells

cn.pipeline(

T cells: TPR: 91.95% TNR: 99.49%

Transferred majority: T cells

B cells: TPR: 95.71% TNR: 95.94%

Transferred majority: B cells

NK cells: TPR: 52.17% TNR: 98.72%

Transferred majority: NK cells

CODEX cluster 1 transferred majority: 91.304 % T cells

CODEX cluster 2 transferred majority: 29.412 % Erythroblasts

CODEX cluster 3 transferred majority: 98.565 % B cells

CODEX cluster 4 transferred majority: 75.0 % B cells

CODEX cluster 5 transferred majority: 39.706 % B cells

CODEX cluster 6 transferred majority: 93.396 % B cells

CODEX cluster 7 transferred majority: 67.347 % NK cells

CODEX cluster 8 transferred majority: 53.049 % B cells

CODEX cluster 9 transferred majority: 63.158 %

CODEX cluster 10 transferred majority: 68.657 % B cells

CODEX cluster 11 transferred majority: 23.529 % Monocytes

CODEX cluster 12 transferred majority: 80.488 % B cells

CODEX cluster 13 transferred majority: 61.039 % B cells

CODEX cluster 14 transferred majority: 89.412 % T cells

CODEX cluster 15 transferred majority: 63.043 % B cells

CODEX cluster 16 transferred majority: 52.174 % NK cells

CODEX cluster 17 transferred majority: 95.205 % B cells

CODEX cluster 18 transferred majority: 89.109 % B cells

CODEX cluster 19 transferred majority: 71.93 % B cells

CODEX cluster 20 transferred majority: 96.825 % B cells

CODEX cluster 21 transferred majority: 99.02 % B cells

# read\_codex args

codex\_blanks="../Data/raw\_dataset/codex\_blanks.csv",

codex\_protein="../Data/raw\_dataset/codex\_protein.csv",

codex\_size="../Data/raw\_dataset/codex\_size.csv",

codex\_spatial="../Data/raw\_dataset/codex\_spatial.csv",

codex\_preprocess=True,

codex\_border=300000,

# read\_cite args

cite\_latent="../Data/raw\_dataset/cite\_latent.csv",

cite\_protein="../Data/raw\_dataset/cite\_protein.csv",

cite\_mrna="../Data/raw\_dataset/cite\_mRNA.csv",

# take\_subset args

amount\_codex=-1, # -1 = default ≈ 9000 CODEX cells

amount\_cite=-1, # -1 ≈ 7000 cells

# filter\_codex args

size\_lim=(1000, 25000),

blank\_lower=(-1200, -1200, -1200, -1200),

blank\_upper=(6000, 2500, 5000, 2500),

# clean\_cite args

maxit=500,

factr=1e-9,

optim\_init=([10, 60, 2, 0.5, 0.5],

[4.8, 50, 0.5, 2, 0.5],

[2, 18, 0.5, 2, 0.5],

[1, 3, 2, 2, 0.5],

[1, 3, 0.5, 2, 0.5]),

ignore\_warnings=True,

clean\_cite\_method="l-bfgs-b",

# cluster\_codex args

cluster\_codex\_k=5,

A purple and yellow squares

Description automatically generated cluster\_codex\_knn\_option=1,

# parameter\_scan args

parameter\_scan\_min\_cluster\_size\_range=tuple(range(5, 21, 4)),

parameter\_scan\_min\_sample\_range=tuple(range(10, 41, 3)),

parameter\_scan\_n\_neighbors=50,

parameter\_scan\_min\_dist=0.1,

parameter\_scan\_negative\_sample\_rate=50,

parameter\_scan\_metric="correlation",

# consensus\_cluster args

consensus\_cluster\_silhouette\_cutoff=0.126,

consensus\_cluster\_inconsistent\_value=0.1,

consensus\_cluster\_min\_cluster\_size=10,

# map\_codex\_to\_cite args

k\_find\_nn=80,

k\_find\_anchor=20,

k\_filter\_anchor=100,

k\_score\_anchor=80,

k\_find\_weights=100,

# transfer\_matrix

k\_transfer\_matrix=None,

c\_transfer\_matrix=0.1,

mask=True

)

Try to implement nested clustering

cn.pipeline(

# read\_codex args

codex\_blanks="../Data/raw\_dataset/codex\_blanks.csv",

codex\_protein="../Data/raw\_dataset/codex\_protein.csv",

codex\_size="../Data/raw\_dataset/codex\_size.csv",

codex\_spatial="../Data/raw\_dataset/codex\_spatial.csv",

codex\_preprocess=True,

codex\_border=564000,

# read\_cite args

cite\_latent="../Data/raw\_dataset/cite\_latent.csv",

cite\_protein="../Data/raw\_dataset/cite\_protein.csv",

cite\_mrna="../Data/raw\_dataset/cite\_mRNA.csv",

# take\_subset args

amount\_codex=-1, # -1 = default ≈ 9000 CODEX cells

amount\_cite=-1, # -1 ≈ 7000 cells

# filter\_codex args

size\_lim=(1000, 25000),

blank\_lower=(-1200, -1200, -1200, -1200),

blank\_upper=(6000, 2500, 5000, 2500),

# clean\_cite args

maxit=500,

factr=1e-9,

optim\_init=([10, 60, 2, 0.5, 0.5],

[4.8, 50, 0.5, 2, 0.5],

[2, 18, 0.5, 2, 0.5],

[1, 3, 2, 2, 0.5],

[1, 3, 0.5, 2, 0.5]),

ignore\_warnings=True,

clean\_cite\_method="l-bfgs-b",

A screenshot of a graph

Description automatically generated # cluster\_codex args

cluster\_codex\_k=5,

cluster\_codex\_knn\_option=3,

# parameter\_scan args

parameter\_scan\_min\_cluster\_size\_range=tuple(range(5, 21, 4)),

parameter\_scan\_min\_sample\_range=tuple(range(10, 41, 3)),

parameter\_scan\_n\_neighbors=50,

parameter\_scan\_min\_dist=0.1,

parameter\_scan\_negative\_sample\_rate=50,

parameter\_scan\_metric="correlation",

# consensus\_cluster args

consensus\_cluster\_silhouette\_cutoff=0.126,

consensus\_cluster\_inconsistent\_value=0.1,

consensus\_cluster\_min\_cluster\_size=10,

# map\_codex\_to\_cite args

k\_find\_nn=80,

k\_find\_anchor=20,

k\_filter\_anchor=100,

k\_score\_anchor=80,

k\_find\_weights=100,

# transfer\_matrix

k\_transfer\_matrix=None,

c\_transfer\_matrix=0.1,

mask=True

)

T cells: TPR: 83.96% TNR: 100.0%

Transferred majority: T cells

B cells: TPR: 99.78% TNR: 97.95%

Transferred majority: B cells

Neutrophils: TPR: 60.53% TNR: 99.87%

Transferred majority: Neutrophils

NK cells: TPR: 64.29% TNR: 97.89%

Transferred majority: NK cells

CODEX cluster 1 transferred majority: 83.048 % T cells

CODEX cluster 2 transferred majority: 17.797 % B cells

CODEX cluster 3 transferred majority: 55.728 % Macrophages

CODEX cluster 4 transferred majority: 100.0 % B cells

CODEX cluster 5 transferred majority: 45.223 % B cells

CODEX cluster 6 transferred majority: 100.0 % B cells

CODEX cluster -1 transferred majority: 79.62 % B cells

CODEX cluster 7 transferred majority: 58.974 % Neutrophils

CODEX cluster 8 transferred majority: 70.27 % Macrophages

CODEX cluster 9 transferred majority: 98.131 % B cells

CODEX cluster 12 transferred majority: 22.034 % Macrophages

CODEX cluster 15 transferred majority: 55.435 % T cells

CODEX cluster 14 transferred majority: 98.611 % B cells

CODEX cluster 16 transferred majority: 100.0 % B cells

CODEX cluster 13 transferred majority: 49.554 % B cells

CODEX cluster 11 transferred majority: 99.315 % B cells

CODEX cluster 10 transferred majority: 92.655 % B cells

CODEX cluster 17 transferred majority: 96.933 % B cells

CODEX cluster 19 transferred majority: 63.158 % NK cells

CODEX cluster 20 transferred majority: 69.231 % Plasma cells

CODEX cluster 18 transferred majority: 97.175 % B cells

CODEX cluster 21 transferred majority: 99.488 % B cells

CODEX cluster 22 transferred majority: 94.444 % B cells

CODEX cluster 23 transferred majority: 99.324 % B cells

CODEX cluster 24 transferred majority: 74.092 % B cells

CODEX cluster 25 transferred majority: 98.966 % B cells

CODEX cluster 26 transferred majority: 100.0 % B cells

Looks like it’s working. But not very effective. C

8.

Use corrected codex proteins to perform CODEX cluster

cluster.cluster\_codex(k=4, knn\_option=1)

A screenshot of a computer

Description automatically generated

9.

def test\_overall\_evaluation(self):

# initialize variable

cn = Controller.Controller()

# this pipeline will read files

cn.pipeline(

# read\_codex args

codex\_blanks="../Data/raw\_dataset/codex\_blanks.csv",

codex\_protein="../Data/raw\_dataset/codex\_protein.csv",

codex\_size="../Data/raw\_dataset/codex\_size.csv",

codex\_spatial="../Data/raw\_dataset/codex\_spatial.csv",

codex\_preprocess=True,

codex\_border=564000,

# read\_cite args

cite\_latent="../Data/raw\_dataset/cite\_latent.csv",

cite\_protein="../Data/raw\_dataset/cite\_protein.csv",

cite\_mrna="../Data/raw\_dataset/cite\_mRNA.csv",

# take\_subset args

amount\_codex=-1, # -1 = default ≈ 9000 CODEX cells

amount\_cite=-1, # -1 ≈ 7000 cells

# filter\_codex args

size\_lim=(1000, 25000),

blank\_lower=(-1200, -1200, -1200, -1200),

blank\_upper=(6000, 2500, 5000, 2500),

# clean\_cite args

maxit=500,

factr=1e-9,

optim\_init=([10, 60, 2, 0.5, 0.5],

[4.8, 50, 0.5, 2, 0.5],

[2, 18, 0.5, 2, 0.5],

[1, 3, 2, 2, 0.5],

[1, 3, 0.5, 2, 0.5]),

ignore\_warnings=True,

clean\_cite\_method="l-bfgs-b",

# cluster\_codex args

cluster\_codex\_k=4,

cluster\_codex\_knn\_option=3,

# parameter\_scan args

parameter\_scan\_min\_cluster\_size\_range=tuple(range(5, 21, 4)),

parameter\_scan\_min\_sample\_range=tuple(range(10, 41, 3)),

parameter\_scan\_n\_neighbors=50,

parameter\_scan\_min\_dist=0.1,

parameter\_scan\_negative\_sample\_rate=50,

parameter\_scan\_metric="correlation",

# consensus\_cluster args

consensus\_cluster\_silhouette\_cutoff=0.126,

consensus\_cluster\_inconsistent\_value=0.1,

consensus\_cluster\_min\_cluster\_size=10,

# map\_codex\_to\_cite args

k\_find\_nn=80,

k\_find\_anchor=20,

k\_filter\_anchor=100,

k\_score\_anchor=80,

k\_find\_weights=100,

# transfer\_matrix

k\_transfer\_matrix=None,

c\_transfer\_matrix=0.1,

mask=True

)

Neutrophils: TPR: 87.5% TNR: 100.0%

Transferred majority: Neutrophils

T cells: TPR: 96.03% TNR: 100.0%

Transferred majority: T cells

NK cells: TPR: 72.97% TNR: 99.88%

Transferred majority: NK cells

B cells: TPR: 99.82% TNR: 100.0%

Transferred majority: B cells

CODEX cluster 1 transferred majority: 64.881 % Macrophages

CODEX cluster 2 transferred majority: 42.023 % Erythrocytes

CODEX cluster 3 transferred majority: 65.783 % Macrophages

CODEX cluster 4 transferred majority: 99.265 % B cells

CODEX cluster 5 transferred majority: 24.364 % B cells

CODEX cluster 6 transferred majority: 96.209 % B cells

CODEX cluster -1 transferred majority: 47.105 % B cells

CODEX cluster 8 transferred majority: 87.5 % Neutrophils

CODEX cluster 9 transferred majority: 85.47 % B cells

CODEX cluster 10 transferred majority: 35.317 %

CODEX cluster 11 transferred majority: 86.567 % B cells

CODEX cluster 12 transferred majority: 92.281 % B cells

CODEX cluster 15 transferred majority: 98.02 % T cells

CODEX cluster 7 transferred majority: 100.0 % B cells

CODEX cluster 16 transferred majority: 91.667 % B cells

CODEX cluster 14 transferred majority: 100.0 % B cells

CODEX cluster 18 transferred majority: 95.616 % B cells

CODEX cluster 19 transferred majority: 70.732 % Plasma cells

CODEX cluster 20 transferred majority: 98.276 % B cells

CODEX cluster 21 transferred majority: 99.476 % B cells

CODEX cluster 22 transferred majority: 40.23 % NK cells

CODEX cluster 23 transferred majority: 100.0 % B cells

CODEX cluster 24 transferred majority: 100.0 % B cells

CODEX cluster 25 transferred majority: 31.818 %

CODEX cluster 17 transferred majority: 71.053 % NK cells

CODEX cluster 26 transferred majority: 99.821 % B cells

CODEX cluster 13 transferred majority: 88.0 % T cells

CODEX cluster 27 transferred majority: 98.784 % B cells

CODEX cluster 28 transferred majority: 100.0 % B cells

CODEX cluster 29 transferred majority: 96.0 % B cells

CODEX cluster 30 transferred majority: 97.625 % B cells

10.

Increase the silhouette score threashold

cn.pipeline(

# read\_codex args

codex\_blanks="../Data/raw\_dataset/codex\_blanks.csv",

codex\_protein="../Data/raw\_dataset/codex\_protein.csv",

codex\_size="../Data/raw\_dataset/codex\_size.csv",

codex\_spatial="../Data/raw\_dataset/codex\_spatial.csv",

codex\_preprocess=True,

codex\_border=564000,

# read\_cite args

cite\_latent="../Data/raw\_dataset/cite\_latent.csv",

cite\_protein="../Data/raw\_dataset/cite\_protein.csv",

cite\_mrna="../Data/raw\_dataset/cite\_mRNA.csv",

# take\_subset args

amount\_codex=-1, # -1 = default ≈ 9000 CODEX cells

amount\_cite=-1, # -1 ≈ 7000 cells

# filter\_codex args

size\_lim=(1000, 25000),

blank\_lower=(-1200, -1200, -1200, -1200),

blank\_upper=(6000, 2500, 5000, 2500),

# clean\_cite args

maxit=500,

factr=1e-9,

optim\_init=([10, 60, 2, 0.5, 0.5],

[4.8, 50, 0.5, 2, 0.5],

[2, 18, 0.5, 2, 0.5],

[1, 3, 2, 2, 0.5],

[1, 3, 0.5, 2, 0.5]),

ignore\_warnings=True,

clean\_cite\_method="l-bfgs-b",

# cluster\_codex args

cluster\_codex\_k=4,

cluster\_codex\_knn\_option=1,

# parameter\_scan args

parameter\_scan\_min\_cluster\_size\_range=tuple(range(5, 21, 4)),

parameter\_scan\_min\_sample\_range=tuple(range(10, 41, 3)),

parameter\_scan\_n\_neighbors=50,

parameter\_scan\_min\_dist=0.1,

parameter\_scan\_negative\_sample\_rate=50,

parameter\_scan\_metric="correlation",

# consensus\_cluster args

consensus\_cluster\_silhouette\_cutoff=0.130,

consensus\_cluster\_inconsistent\_value=0.1,

consensus\_cluster\_min\_cluster\_size=10,

# map\_codex\_to\_cite args

k\_find\_nn=80,

k\_find\_anchor=20,

k\_filter\_anchor=100,

k\_score\_anchor=80,

k\_find\_weights=100,

# transfer\_matrix

k\_transfer\_matrix=None,

c\_transfer\_matrix=0.1,

mask=True

)

Neutrophils: TPR: 82.61% TNR: 99.88%

Transferred majority: Neutrophils

T cells: TPR: 87.18% TNR: 100.0%

Transferred majority: T cells

A screenshot of a graph

Description automatically generated

B cells: TPR: 99.44% TNR: 99.38%

Transferred majority: B cells

NK cells: TPR: 70.0% TNR: 98.22%

Transferred majority: NK cells

CODEX cluster 1 transferred majority: 63.517 % Macrophages

CODEX cluster 2 transferred majority: 41.265 % Erythrocytes

CODEX cluster 3 transferred majority: 66.284 % Macrophages

CODEX cluster 4 transferred majority: 99.459 % B cells

CODEX cluster 5 transferred majority: 29.63 % Langerhans

1: T cells  
2: B cells  
3: NK cells  
4: CD4  
5: Monocytes  
6: Neutrophils  
8: T1 B cells  
9: T1 B cells  
12: Plasma cells  
13: CD8  
14: Neutrophils  
15: Erythrocytes  
16: Macrophages  
17: Macrophages  
18: pDCs  
19: Langerhans

13: T cells  
15: T cells  
26: B cells  
8: Neutrophils  
17: NK cells  
31: T cells

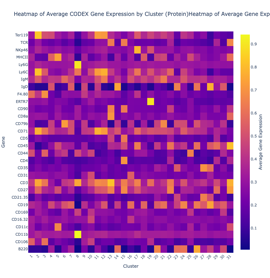
CODEX cluster 6 transferred majority: 76.744 % B cells

CODEX cluster 7 transferred majority: 98.256 % B cells

CODEX cluster 8 transferred majority: 73.077 % Neutrophils

CODEX cluster 9 transferred majority: 86.792 % B cells

CODEX cluster 10 transferred majority: 30.712 % Langerhans

CODEX cluster 11 transferred majority: 85.135 % B cells

CODEX cluster 12 transferred majority: 63.158 % B cells

CODEX cluster 13 transferred majority: 64.516 % T cells

CODEX cluster 14 transferred majority: 100.0 % B cells

CODEX cluster 15 transferred majority: 90.451 % T cells

CODEX cluster 16 transferred majority: 54.167 % B cells

CODEX cluster 17 transferred majority: 62.5 % NK cells

CODEX cluster 18 transferred majority: 94.179 % B cells

CODEX cluster 19 transferred majority: 69.565 % Plasma cells

CODEX cluster 20 transferred majority: 96.54 % B cells

CODEX cluster 21 transferred majority: 94.226 % B cells

CODEX cluster 22 transferred majority: 44.33 % NK cells

CODEX cluster 23 transferred majority: 100.0 % B cells

CODEX cluster 24 transferred majority: 95.122 % B cells

CODEX cluster 25 transferred majority: 34.286 % B cells

CODEX cluster 26 transferred majority: 99.298 % B cells

CODEX cluster 27 transferred majority: 98.118 % B cells

CODEX cluster 28 transferred majority: 100.0 % B cells

CODEX cluster 29 transferred majority: 82.0 % B cells

CODEX cluster 30 transferred majority: 97.143 % B cells

CODEX cluster 31 transferred majority: 75.0 %

11. further, increase silhouette score.

def test\_overall\_evaluation(self):

# initialize variable

cn = Controller.Controller()

# this pipeline will read files

cn.pipeline(

# read\_codex args

codex\_blanks="../Data/raw\_dataset/codex\_blanks.csv",

A screenshot of a graph

Description automatically generated codex\_protein="../Data/raw\_dataset/codex\_protein.csv",

codex\_size="../Data/raw\_dataset/codex\_size.csv",

codex\_spatial="../Data/raw\_dataset/codex\_spatial.csv",

codex\_preprocess=True,

codex\_border=564000,

# read\_cite args

cite\_latent="../Data/raw\_dataset/cite\_latent.csv",

cite\_protein="../Data/raw\_dataset/cite\_protein.csv",

cite\_mrna="../Data/raw\_dataset/cite\_mRNA.csv",

# take\_subset args

amount\_codex=-1, # -1 = default ≈ 9000 CODEX cells

amount\_cite=-1, # -1 ≈ 7000 cells

# filter\_codex args

size\_lim=(1000, 25000),

blank\_lower=(-1200, -1200, -1200, -1200),

blank\_upper=(6000, 2500, 5000, 2500),

# clean\_cite args

maxit=500,

factr=1e-9,

optim\_init=([10, 60, 2, 0.5, 0.5],

[4.8, 50, 0.5, 2, 0.5],

[2, 18, 0.5, 2, 0.5],

[1, 3, 2, 2, 0.5],

[1, 3, 0.5, 2, 0.5]),

ignore\_warnings=True,

clean\_cite\_method="l-bfgs-b",

# cluster\_codex args

cluster\_codex\_k=4,

cluster\_codex\_knn\_option=1,

# parameter\_scan args

parameter\_scan\_min\_cluster\_size\_range=tuple(range(5, 21, 4)),

parameter\_scan\_min\_sample\_range=tuple(range(10, 41, 3)),

parameter\_scan\_n\_neighbors=50,

parameter\_scan\_min\_dist=0.1,

parameter\_scan\_negative\_sample\_rate=50,

parameter\_scan\_metric="correlation",

# consensus\_cluster args

consensus\_cluster\_silhouette\_cutoff=0.145,

consensus\_cluster\_inconsistent\_value=0.1,

A screenshot of a graph

Description automatically generated consensus\_cluster\_min\_cluster\_size=10,

# map\_codex\_to\_cite args

k\_find\_nn=80,

k\_find\_anchor=20,

k\_filter\_anchor=100,

k\_score\_anchor=80,

k\_find\_weights=100,

# transfer\_matrix

k\_transfer\_matrix=None,

c\_transfer\_matrix=0.1,

mask=True

)

# invoke the partial evaluation

TestController.partial\_evaluation(cn.stvea, cn.annotation)

Neutrophil: TPR: 0.0% TNR: 100.0%

Transferred majority: Neutrophils

T cells: TPR: 85.76% TNR: 100.0%

Transferred majority: T cells

NK cells: TPR: 60.71% TNR: 98.3%

Transferred majority: NK cells

B cells: TPR: 99.16% TNR: 99.4%

Transferred majority: B cells

CODEX cluster 1 transferred majority: 63.255 % Macrophages

CODEX cluster 2 transferred majority: 40.663 % Erythrocytes

CODEX cluster 3 transferred majority: 65.138 % Macrophages

CODEX cluster 4 transferred majority: 99.459 % B cells

CODEX cluster 5 transferred majority: 29.012 % Langerhans

CODEX cluster 6 transferred majority: 75.814 % B cells

CODEX cluster 7 transferred majority: 98.256 % B cells

CODEX cluster 8 transferred majority: 73.077 % Neutrophils

CODEX cluster 9 transferred majority: 86.792 % B cells

CODEX cluster 10 transferred majority: 29.963 % Langerhans

CODEX cluster 11 transferred majority: 85.135 % B cells

CODEX cluster 12 transferred majority: 61.988 % B cells

CODEX cluster 13 transferred majority: 64.516 % T cells

CODEX cluster 14 transferred majority: 100.0 % B cells

CODEX cluster 15 transferred majority: 90.451 % T cells

CODEX cluster 16 transferred majority: 54.167 % B cells

CODEX cluster 17 transferred majority: 60.714 % NK cells

CODEX cluster 18 transferred majority: 93.139 % B cells

CODEX cluster 19 transferred majority: 63.043 % Plasma cells

CODEX cluster 20 transferred majority: 94.464 % B cells

CODEX cluster 21 transferred majority: 93.995 % B cells

CODEX cluster 22 transferred majority: 44.33 % NK cells

CODEX cluster 23 transferred majority: 100.0 % B cells

CODEX cluster 24 transferred majority: 95.122 % B cells

CODEX cluster 25 transferred majority: 35.714 % B cells

CODEX cluster 26 transferred majority: 99.157 % B cells

CODEX cluster 27 transferred majority: 98.118 % B cells

CODEX cluster 28 transferred majority: 100.0 % B cells

CODEX cluster 29 transferred majority: 82.0 % B cells

CODEX cluster 30 transferred majority: 96.883 % B cells

CODEX cluster 31 transferred majority: 75.0 % CD8