

```
In [ ]: !pip install mofapy2
```

```
In [ ]: from mofapy2.run.entry_point import entry_point
import pandas as pd
import io
import requests # to download the online data
```

```
In [ ]: # The input needs to be a data.frame with columns ["sample", "feature", "view", "group", "value"]
# In this case there is no need to have missing values in the data.frame, they will be automatically filled in wh
"""
# The data format is a nested list of matrices, where the first index refers to the view and the second index ref
# samples are stored in the rows and features are stored in the columns.
# Missing values must be explicitly filled using NAs, including samples missing an entire view

datadir = "/Users/ricard/data/mofaplus/test"
views = ["0", "1"]
groups = ["0", "1"]
data = [None]*len(views)
for m in range(len(views)):
    data[m] = [None]*len(groups)
    for g in range(len(groups)):
        datafile = "%s/%s_%s.txt.gz" % (datadir, views[m], groups[g])
        data[m][g] = pd.read_csv(datafile, header=None, sep=' ')
"""
file = "ftp://ftp.ebi.ac.uk/pub/databases/mofa/getting_started/data.txt.gz"
data = pd.read_csv(file, sep="\t")
```

```
In [ ]: data
```

Out[]:

	sample	group	feature	view	value
0	sample_0_group_0	group_0	feature_0_view_0	view_0	-2.05
1	sample_1_group_0	group_0	feature_0_view_0	view_0	0.10
2	sample_2_group_0	group_0	feature_0_view_0	view_0	1.44
3	sample_3_group_0	group_0	feature_0_view_0	view_0	-0.28
4	sample_4_group_0	group_0	feature_0_view_0	view_0	-0.88
...
399995	sample_95_group_1	group_1	feature_999_view_1	view_1	0.21
399996	sample_96_group_1	group_1	feature_999_view_1	view_1	0.47
399997	sample_97_group_1	group_1	feature_999_view_1	view_1	0.49
399998	sample_98_group_1	group_1	feature_999_view_1	view_1	0.19
399999	sample_99_group_1	group_1	feature_999_view_1	view_1	-1.60

400000 rows × 5 columns

```
In [ ]: #####
## Initialise MOFA model ##
#####

## (1) initialise the entry point
ent = entry_point()

## (2) Set data options
# - scale_views: if views have very different ranges, one can to scale each view to unit variance
ent.set_data_options(
    scale_views = False
)

## (3) Define names
views_names = ["view1", "view2"]
groups_names = ["groupA", "groupB"]

# samples_names nested list with length n_groups. Each entry g is a list with the sample names for the g-th group
# - if not provided, MOFA will fill it with default samples names
samples_names = (...)

# features_names nested list with length N_VIEWS. Each entry m is a list with the features names for the m-th view
# - if not provided, MOFA will fill it with default features names
features_names = (...)
```

[illegible]

```
In [ ]: ## (2) Set data options
# - scale_views: if views have very different ranges, one can to scale each view to unit variance
ent.set_data_options(
    scale_views = False
)

# (3) Set data using the data frame format
ent.set_data_df(data)

## (5) Set model options
# - factors: number of factors. Default is 15
# - likelihoods: likelihoods per view (options are "gaussian", "poisson", "bernoulli"). Default and recommended is "
# - spikeslab_weights: use spike-slab sparsity prior in the weights? (recommended TRUE)
# - ard_weights: use automatic relevance determination prior in the weights? (TRUE if using multiple views)

# using default values
# ent.set_model_options()

# using personalised values
ent.set_model_options(
    factors = 5,
    spikeslab_weights = True,
    ard_weights = True
)
```

```
Loaded group='group_0' view='view_0' with N=100 samples and D=1000 features...
Loaded group='group_0' view='view_1' with N=100 samples and D=1000 features...
Loaded group='group_1' view='view_0' with N=100 samples and D=1000 features...
Loaded group='group_1' view='view_1' with N=100 samples and D=1000 features...
```

```
WARNING: 'ard_factors' in model_options should be set to True if using multiple groups unless you are using MEFIST
0
```

```
Model options:
- Automatic Relevance Determination prior on the factors: False
- Automatic Relevance Determination prior on the weights: True
- Spike-and-slab prior on the factors: False
- Spike-and-slab prior on the weights: True
Likelihoods:
- View 0 (view_0): gaussian
- View 1 (view_1): gaussian
```

```
In [ ]:

## (5) Set training options ##
# - iter: number of iterations
# - convergence_mode: "fast", "medium", "slow". Fast mode is usually good enough.
# - dropR2: minimum variance explained criteria to drop factors while training. Default is None, inactive factors
# - gpu_mode: use GPU mode? this functionality needs cupy installed and a functional GPU, see https://biofam.github.io/biofam/FAQ.html
# - seed: random seed

# using default values
ent.set_train_options()

# using personalised values
ent.set_train_options(
    iter = 100,
    convergence_mode = "fast",
    dropR2 = None,
    gpu_mode = True,
    seed = 42
)
```

GPU mode is activated

```
In [ ]: #####  
        ## Build and train the MOFA model ##
```

```
#####
```

```
# Build the model  
ent.build()
```

```
# Run the model  
ent.run()
```

```
#####  
## Training the model with seed 42 ##  
#####
```

ELBO before training: -2022955.14

```
Iteration 1: time=2.69, ELBO=-559016.69, deltaELBO=1463938.452 (72.36633287%), Factors=5  
Iteration 2: time=0.03, ELBO=-472290.49, deltaELBO=86726.204 (4.28710467%), Factors=5  
Iteration 3: time=0.03, ELBO=-466508.44, deltaELBO=5782.042 (0.28582155%), Factors=5  
Iteration 4: time=0.02, ELBO=-464279.86, deltaELBO=2228.580 (0.11016459%), Factors=5  
Iteration 5: time=0.02, ELBO=-463375.42, deltaELBO=904.447 (0.04470920%), Factors=5  
Iteration 6: time=0.03, ELBO=-463041.39, deltaELBO=334.025 (0.01651173%), Factors=5  
Iteration 7: time=0.03, ELBO=-462888.81, deltaELBO=152.587 (0.00754277%), Factors=5  
Iteration 8: time=0.03, ELBO=-462790.30, deltaELBO=98.502 (0.00486921%), Factors=5  
Iteration 9: time=0.02, ELBO=-462708.91, deltaELBO=81.392 (0.00402342%), Factors=5  
Iteration 10: time=0.02, ELBO=-462633.86, deltaELBO=75.051 (0.00370996%), Factors=5  
Iteration 11: time=0.02, ELBO=-462562.20, deltaELBO=71.663 (0.00354248%), Factors=5  
Iteration 12: time=0.02, ELBO=-462493.45, deltaELBO=68.752 (0.00339861%), Factors=5  
Iteration 13: time=0.02, ELBO=-462427.53, deltaELBO=65.914 (0.00325829%), Factors=5  
Iteration 14: time=0.02, ELBO=-462364.21, deltaELBO=63.324 (0.00313028%), Factors=5  
Iteration 15: time=0.02, ELBO=-462303.08, deltaELBO=61.123 (0.00302148%), Factors=5  
Iteration 16: time=0.03, ELBO=-462243.82, deltaELBO=59.265 (0.00292962%), Factors=5  
Iteration 17: time=0.03, ELBO=-462186.23, deltaELBO=57.594 (0.00284703%), Factors=5  
Iteration 18: time=0.02, ELBO=-462130.26, deltaELBO=55.968 (0.00276667%), Factors=5  
Iteration 19: time=0.02, ELBO=-462075.97, deltaELBO=54.287 (0.00268355%), Factors=5  
Iteration 20: time=0.02, ELBO=-462023.44, deltaELBO=52.535 (0.00259692%), Factors=5  
Iteration 21: time=0.02, ELBO=-461972.63, deltaELBO=50.804 (0.00251137%), Factors=5  
Iteration 22: time=0.02, ELBO=-461923.45, deltaELBO=49.180 (0.00243109%), Factors=5  
Iteration 23: time=0.02, ELBO=-461875.77, deltaELBO=47.686 (0.00235726%), Factors=5  
Iteration 24: time=0.02, ELBO=-461829.40, deltaELBO=46.363 (0.00229184%), Factors=5  
Iteration 25: time=0.02, ELBO=-461784.14, deltaELBO=45.260 (0.00223732%), Factors=5  
Iteration 26: time=0.02, ELBO=-461739.74, deltaELBO=44.404 (0.00219499%), Factors=5  
Iteration 27: time=0.02, ELBO=-461695.94, deltaELBO=43.795 (0.00216488%), Factors=5  
Iteration 28: time=0.02, ELBO=-461652.54, deltaELBO=43.405 (0.00214562%), Factors=5  
Iteration 29: time=0.02, ELBO=-461609.36, deltaELBO=43.180 (0.00213452%), Factors=5  
Iteration 30: time=0.02, ELBO=-461566.31, deltaELBO=43.053 (0.00212821%), Factors=5  
Iteration 31: time=0.02, ELBO=-461523.36, deltaELBO=42.950 (0.00212311%), Factors=5  
Iteration 32: time=0.02, ELBO=-461480.57, deltaELBO=42.790 (0.00211523%), Factors=5  
Iteration 33: time=0.02, ELBO=-461438.06, deltaELBO=42.510 (0.00210139%), Factors=5  
Iteration 34: time=0.02, ELBO=-461395.95, deltaELBO=42.107 (0.00208145%), Factors=5  
Iteration 35: time=0.02, ELBO=-461354.32, deltaELBO=41.632 (0.00205798%), Factors=5  
Iteration 36: time=0.02, ELBO=-461313.17, deltaELBO=41.149 (0.00203408%), Factors=5  
Iteration 37: time=0.03, ELBO=-461272.46, deltaELBO=40.709 (0.00201234%), Factors=5  
Iteration 38: time=0.03, ELBO=-461232.11, deltaELBO=40.349 (0.00199454%), Factors=5  
Iteration 39: time=0.02, ELBO=-461192.02, deltaELBO=40.087 (0.00198159%), Factors=5  
Iteration 40: time=0.02, ELBO=-461152.10, deltaELBO=39.924 (0.00197355%), Factors=5  
Iteration 41: time=0.02, ELBO=-461112.25, deltaELBO=39.849 (0.00196986%), Factors=5  
Iteration 42: time=0.03, ELBO=-461072.41, deltaELBO=39.843 (0.00196953%), Factors=5  
Iteration 43: time=0.02, ELBO=-461032.52, deltaELBO=39.885 (0.00197162%), Factors=5  
Iteration 44: time=0.02, ELBO=-460992.55, deltaELBO=39.973 (0.00197595%), Factors=5  
Iteration 45: time=0.02, ELBO=-460952.43, deltaELBO=40.124 (0.00198345%), Factors=5  
Iteration 46: time=0.02, ELBO=-460912.04, deltaELBO=40.383 (0.00199625%), Factors=5  
Iteration 47: time=0.02, ELBO=-460871.22, deltaELBO=40.820 (0.00201785%), Factors=5  
Iteration 48: time=0.02, ELBO=-460829.69, deltaELBO=41.534 (0.00205311%), Factors=5  
Iteration 49: time=0.02, ELBO=-460787.08, deltaELBO=42.610 (0.00210632%), Factors=5  
Iteration 50: time=0.02, ELBO=-456462.22, deltaELBO=4324.856 (0.21378904%), Factors=5  
Iteration 51: time=0.02, ELBO=-456092.40, deltaELBO=369.828 (0.01828158%), Factors=5  
Iteration 52: time=0.02, ELBO=-455970.50, deltaELBO=121.896 (0.00602565%), Factors=5  
Iteration 53: time=0.02, ELBO=-455906.68, deltaELBO=63.815 (0.00315454%), Factors=5  
Iteration 54: time=0.02, ELBO=-455861.58, deltaELBO=45.106 (0.00222971%), Factors=5  
Iteration 55: time=0.02, ELBO=-455822.77, deltaELBO=38.804 (0.00191821%), Factors=5  
Iteration 56: time=0.03, ELBO=-455785.80, deltaELBO=36.978 (0.00182793%), Factors=5  
Iteration 57: time=0.02, ELBO=-455748.71, deltaELBO=37.089 (0.00183340%), Factors=5  
Iteration 58: time=0.02, ELBO=-455710.52, deltaELBO=38.187 (0.00188767%), Factors=5  
Iteration 59: time=0.02, ELBO=-455670.89, deltaELBO=39.633 (0.00195918%), Factors=5  
Iteration 60: time=0.02, ELBO=-455629.84, deltaELBO=41.049 (0.00202915%), Factors=5  
Iteration 61: time=0.03, ELBO=-455587.32, deltaELBO=42.518 (0.00210180%), Factors=5  
Iteration 62: time=0.02, ELBO=-455543.05, deltaELBO=44.271 (0.00218843%), Factors=5  
Iteration 63: time=0.02, ELBO=-455496.67, deltaELBO=46.383 (0.00229282%), Factors=5  
Iteration 64: time=0.02, ELBO=-455448.01, deltaELBO=48.659 (0.00240533%), Factors=5  
Iteration 65: time=0.02, ELBO=-455397.26, deltaELBO=50.748 (0.00250860%), Factors=5  
Iteration 66: time=0.02, ELBO=-455344.76, deltaELBO=52.497 (0.00259506%), Factors=5  
Iteration 67: time=0.02, ELBO=-455290.64, deltaELBO=54.121 (0.00267537%), Factors=5  
Iteration 68: time=0.02, ELBO=-455235.49, deltaELBO=55.153 (0.00272638%), Factors=5  
Iteration 69: time=0.03, ELBO=-455183.22, deltaELBO=52.268 (0.00258372%), Factors=5  
Iteration 70: time=0.02, ELBO=-455139.35, deltaELBO=43.870 (0.00216862%), Factors=5  
Iteration 71: time=0.02, ELBO=-455105.23, deltaELBO=34.118 (0.00168652%), Factors=5  
Iteration 72: time=0.03, ELBO=-455078.69, deltaELBO=26.542 (0.00131203%), Factors=5  
Iteration 73: time=0.02, ELBO=-455056.96, deltaELBO=21.731 (0.00107424%), Factors=5  
Iteration 74: time=0.02, ELBO=-455037.89, deltaELBO=19.068 (0.00094256%), Factors=5  
Iteration 75: time=0.02, ELBO=-455020.17, deltaELBO=17.720 (0.00087594%), Factors=5  
Iteration 76: time=0.02, ELBO=-455003.12, deltaELBO=17.052 (0.00084294%), Factors=5
```

```
Iteration 76: time=0.02, ELBO=-454986.12, deltaELBO=17.032 (0.0004294%), Factors=5
Iteration 77: time=0.02, ELBO=-454986.42, deltaELBO=16.694 (0.00082525%), Factors=5
Iteration 78: time=0.02, ELBO=-454969.96, deltaELBO=16.463 (0.00081380%), Factors=5
Iteration 79: time=0.02, ELBO=-454953.69, deltaELBO=16.276 (0.00080458%), Factors=5
Iteration 80: time=0.02, ELBO=-454937.58, deltaELBO=16.104 (0.00079604%), Factors=5
Iteration 81: time=0.02, ELBO=-454921.65, deltaELBO=15.934 (0.00078765%), Factors=5
Iteration 82: time=0.02, ELBO=-454905.88, deltaELBO=15.765 (0.00077932%), Factors=5
Iteration 83: time=0.02, ELBO=-454890.28, deltaELBO=15.599 (0.00077109%), Factors=5
Iteration 84: time=0.02, ELBO=-454874.85, deltaELBO=15.435 (0.00076301%), Factors=5
Iteration 85: time=0.02, ELBO=-454859.57, deltaELBO=15.276 (0.00075514%), Factors=5
Iteration 86: time=0.02, ELBO=-454844.45, deltaELBO=15.121 (0.00074748%), Factors=5
Iteration 87: time=0.03, ELBO=-454829.48, deltaELBO=14.970 (0.00074002%), Factors=5
Iteration 88: time=0.02, ELBO=-454814.66, deltaELBO=14.823 (0.00073275%), Factors=5
Iteration 89: time=0.02, ELBO=-454799.98, deltaELBO=14.679 (0.00072563%), Factors=5
Iteration 90: time=0.02, ELBO=-454785.44, deltaELBO=14.538 (0.00071865%), Factors=5
Iteration 91: time=0.02, ELBO=-454771.04, deltaELBO=14.399 (0.00071177%), Factors=5
Iteration 92: time=0.03, ELBO=-454756.78, deltaELBO=14.262 (0.00070499%), Factors=5
Iteration 93: time=0.03, ELBO=-454742.65, deltaELBO=14.127 (0.00069832%), Factors=5
Iteration 94: time=0.03, ELBO=-454728.66, deltaELBO=13.994 (0.00069176%), Factors=5
Iteration 95: time=0.03, ELBO=-454714.80, deltaELBO=13.864 (0.00068531%), Factors=5
Iteration 96: time=0.03, ELBO=-454701.06, deltaELBO=13.736 (0.00067900%), Factors=5
Iteration 97: time=0.02, ELBO=-454687.45, deltaELBO=13.611 (0.00067284%), Factors=5
Iteration 98: time=0.02, ELBO=-454673.96, deltaELBO=13.490 (0.00066685%), Factors=5
Iteration 99: time=0.02, ELBO=-454660.59, deltaELBO=13.373 (0.00066107%), Factors=5
```

```
#####
## Training finished ##
#####
```

In []:

```
#####
## Save the model ##
#####

outfile = "/content/sample_data/test.hdf5"

# - save_data: logical indicating whether to save the training data in the hdf5 file.
# this is useful for some downstream analysis in R, but it can take a lot of disk space.
ent.save(outfile, save_data=True)
```

Saving model in /content/sample_data/test.hdf5...

In []:

```
#####
## Downstream analysis ##
#####

# Check the mofax package for the downstream analysis in Python: https://qithub.com/bioFAM/mofax
```



main ▾

DEEP_LEARNING / MOFA.ipynb

↑ Top

Preview

Code

Blame

1558 lines (1558 loc) · 86.1 KB

Raw



```
# Extract weights (a list with one matrix per view)
weights = ent.model.nodes["W"].getExpectation()

# Extract variance explained values
r2 = ent.model.calculate_variance_explained()
```

In []:

```
# Interact directly with the hdf5 file
import h5py
f = h5py.File(outfile, 'r')
f.keys()
```

Out[]:

```
<KeysViewHDF5 ['data', 'expectations', 'features', 'groups', 'intercepts', 'model_options', 'samples', 'training_
opts', 'training_stats', 'variance_explained', 'views']>
```

In []:

```
print(f["expectations"]["Z"]["group_0"][0])
```

```
[-1.79188109e+00 -1.69409634e+00 -1.00564149e+00  1.61705455e+00
-1.87105228e+00  3.95501421e-01  2.11015144e-01  2.17984515e-01
 3.42887708e+00  2.19041169e+00 -3.02742479e+00  1.08594359e+00
 3.15197423e+00 -2.17457997e+00 -4.43571929e+00 -1.14671974e+00
 1.93565968e-01 -2.29818100e+00  4.31612915e-01  8.44580630e+00
-2.79237235e+00  3.42681296e-01  4.79637718e+00  1.03940462e+00
-3.09047627e-01  2.33922426e-01  2.79046900e+00  2.31043856e-01
-4.60120562e+00  3.49098984e+00  7.87833734e-01  5.07077396e-02
-1.27499036e+00 -1.43631160e+00  1.78578712e-01 -2.31647033e-02
-1.81807588e-02  1.28537355e-01 -5.33851345e+00  3.84306821e+00
-1.49434318e+00 -6.15472141e-02  2.91812922e-02  2.30038037e+00
 8.71793104e-01  4.91132431e-01 -3.50273013e+00 -2.03584080e+00
-7.02789738e-01 -6.41093630e-01  3.03863967e+00  2.63918136e+00]
```



```
-7.02709730e-01 -0.41093030e-01 3.03003907e+00 2.03910130e+00
2.09834453e-01 1.70730904e-02 3.49013243e-01 1.10511115e+00
4.19982531e-01 -2.51797339e+00 -6.56413418e-01 -4.81323816e-01
2.59394928e-01 -1.05463311e+00 8.36554799e-01 -1.93314113e+00
3.51483432e-01 3.81075806e+00 9.71822906e+00 1.32389083e+00
3.03920454e-01 2.26662515e-01 3.54487510e-01 -4.15901710e+00
-1.09189846e+00 1.27420952e+00 -2.83225899e+00 -3.48414661e+00
1.77020680e+00 -3.35506024e-01 4.20187254e-01 -8.36474878e-02
2.59657766e+00 -4.50150672e+00 1.10350072e+00 -7.10027635e-01
6.25874076e-01 2.19577301e+00 -1.14403468e+00 3.41360766e+00
-2.56026640e-02 -4.29973547e-01 8.97656233e-01 8.11806981e-01
3.02861063e-01 -4.50295369e+00 -6.10567304e+00 3.66891561e+00
-3.35695355e-03 -3.89630010e+00 -3.73624309e+00 3.41816564e-01]
```

```
In [ ]: print(f["expectations"]["Z"]["group_0"][1])
```

```
[-0.55469587 -0.8887377 -1.0096505 -3.6901897 -0.98524385 -2.8191164
 0.04115362 -0.94654135 3.30682949 -0.9543282 -2.9232901 -3.83823163
 2.59633701 -1.03581209 -0.60283609 -0.75379845 1.67553375 1.34186203
 2.30976577 -0.045632 -1.4204892 -0.37550976 -0.17602659 -1.32537449
-1.93665784 -1.52421722 -0.02820841 3.88210402 0.33641594 2.00109088
-0.62445645 8.3733117 2.11912486 3.87362739 -0.30030667 2.01154669
-0.19215391 -0.08013081 0.19292655 -3.29615829 4.9691618 -2.44511929
-6.86499579 -2.41230179 -0.6125343 -2.04572959 -2.3923186 0.43736056
-0.43832175 -2.7178174 -0.64139906 2.79395683 -0.9843593 -1.82004897
 1.4069403 -1.30550652 -1.86701693 1.98893206 -2.26955503 0.22790282
 3.57296148 -1.84896067 1.15074788 -0.9335171 -2.58045661 -2.31876499
-2.59567471 -0.86823764 -0.40346444 -0.24838922 2.63861593 -0.81076053
 2.66104076 0.29996451 -0.14275049 -0.39731444 1.20878903 2.02083152
 0.18637028 3.00256581 4.95961633 6.2708145 -0.51955091 1.8407172
 0.1958329 0.75185053 3.4832341 -2.14887926 -0.00952942 0.22453215
-2.82052593 2.77163293 -3.11585734 0.36160606 -0.52855886 2.59833696
 1.84933584 -0.4777054 -1.48100481 -2.5405601 ]
```

```
In [ ]: # Extract weights
print(f["expectations"]["W"]["view_0"][0])
```

```
[ 3.09837045e-01 6.63885684e-02 4.06790077e-04 -6.88770871e-02
-6.16362909e-02 2.32191362e-01 -8.50406578e-02 -6.90491062e-03
-1.80849936e-01 8.06206148e-03 -6.98577534e-02 1.46926213e-01
-9.68840586e-02 -2.91750549e-01 8.06906300e-04 -4.58979901e-01
 2.20915726e-02 -4.80833986e-04 3.53174375e-01 2.59051422e-03
-7.25375178e-02 -8.09257329e-02 4.77171301e-04 -4.23269969e-02
 9.74836783e-02 1.35303517e-01 -2.96517979e-03 4.53022802e-01
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```
In [ ]: # Extract variance explained estimates
        print(f["variance_explained"]["r2_per_factor"])
```

<HDF5 group "/variance_explained/r2_per_factor" (2 members)>

```
In [ ]: print(f["variance_explained"]["r2_total"]["group_0"][0])
```

75.71346753165543

```
In [ ]: print(f["variance_explained"]["r2_total"]["group_0"][1])
```

76.4853236368788