A Tutorial for Bayesian Integrative Factor Models

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Welcome

This is the tutorial to guide statisticians to use Baysian integrative factor models. Including Tetris (2023).

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Quick start

Step 1: Prepare the package and data

A small simulated data can be downloaded here:

RDS format

Step 2: Run BMSFA

Step 3: Post-processing

Step 4: Visualization

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A summary of the models

1 Package Installation

I have this separate section to introduce the package installation because installing some packages requires extra efforts.

1.1 Stack FA, Ind FA, and BMSFA

The Stack FA, Ind FA, and BMSFA models are implemented in the MSFA package, which is not available on CRAN. We can install it from GitHub using the remotes package. We use sp_fa() within the MSFA package to fit the Stack FA and Ind FA model, and sp_msfa() to fit the BMSFA model.

```
install.packages("remotes")
remotes::install_github("rdevito/MSFA")
library(MSFA)
```

I edited the functions a bit so that sp_fa() and sp_msfa() can accept the scaling and centering arguments. So that we can only center the data without scaling it, or centering and scaling, or neither.

```
devtools::install_github("Mavis-Liang/MSFA")
```

1.2 PFA

PFA does not provide any downloadable R packages and we need to download the R scripts from their GitHub repository, put them in the same directory as the main script, and source them for use.

We only need the three files: FBPFA-PFA.R, FBPFA-PFA with fixed latent dim.R, and PFA.cpp, which can be found in https://github.com/royarkaprava/Perturbed-factor-models. The FBPFA-PFA.R file contains the full Bayesian inference algorithm for the PFA model, directly set the latent dimensions equal to the dimensions or the original data. The FBPFA-PFA with fixed latent dim.R file contains the same algorithm that requires to set numbers of common factors K. We also notice that two version of the models are both PFA(), and some

functions in the FBPFA-PFA with fixed latent dim.R file depends on the FBPFA-PFA.R file. Therefore, since we want to run the dimension reduction version of the model, we must source the FBPFA-PFA.R file first, and then source the FBPFA-PFA with fixed latent dim.R file.

```
# Suppose the files are in the same directory as the main script
source("FBPFA-PFA.R")
source("FBPFA-PFA with fixed latent dim.R")
```

1.3 MOM-SS

```
BiocManager::install("sparseMatrixStats") # Dependency
install.packages("mombf")

install.packages("devtools")

devtools::install_github("AleAviP/BFR.BE")
library(BFR.BE)
```

1.4 SUFA

To install SUFA on Linux, you need to also install extra dependencies like PROJ, sqlite3 and GDAL onto PATH. On Windows, you might need to do several updates, particularly the updates for terra. We can skip building the vignettes to save time, as it contains the computation of a large dataset.

```
devtools::install_github("noirritchandra/SUFA", build_vignettes = FALSE)
library(SUFA)
```

1.5 Tetris

Similar to PFA, Tetris does not provide any downloadable R packages and we need to download the R scripts from their GitHub repository, put them in the same directory as the main script, and source them for use. The R scripts can be found in https://github.com/igrabski/tetris/tree/main.

Suppose the files are in the same directory as the main script source("Tetris.R")

1.6 Other utility packages

library(tidyverse)
library(Matrix)#for the bdiag function

2 Case study: nutrition data

2.1 Loading and previewing the data

The data used in this section is from a large multi-site study investigating health and diet among Hispanic/Latino adults in the United States(2022). This data is not publicly available. Please contact the authors of the original study for access.

However, you can use this simulated data instead: simulated_nutrition_data.rds (if it does not triggers instant download, you can find it in the repo site). To read in the data, use readRDS(). The loaded object contains data in both Y_mat and Y_list formats, as well as covariates and other information. It is generated with the Scenario 4 in the manuscript (see code). Note that instead of having 6 studies, this simulated data has 12 studies.

```
load("./Data/dataLAT_projale2.rda")
```

The resulting object is a list of 6 data frames, each corresponding to a different study. Each data frame contains information about the nutritional intake of individuals, and the columns represent different nutrients. From Study 1 to Study 6, the number of individuals (N_s) are 1364, 1517, 2210, 5184, 2478, and 959, respectively, and the number of nutrients (P) are all 42.

```
# Check how many studies in the list
length(X_s2)
```

[1] 6

```
# Dimension of each study
lapply(X_s2, dim)
```

```
[[1]]
[1] 1364 42
[[2]]
[1] 1517 42
```

```
[[3]]
[1] 2210 42

[[4]]
[1] 5184 42

[[5]]
[1] 2478 42

[[6]]
[1] 959 42
```

Let's take a look at the first few rows of the first data frame to get an idea of the data structure.

```
X_s2[[1]][1:5, 1:5]
```

	Animal	Protein (g)	Vegetable	Protein (g)	Cholesterol (mg)	SCSFA	MCSFA
1		28.9560		14.7440	256.761	0.2665	0.939
2		33.6675		8.9710	104.217	0.2180	0.520
3		70.0000		31.0635	207.902	0.9845	1.692
4		20.6700		13.8240	148.921	0.0625	0.239
5		15.4250		10.5550	65.060	0.0090	0.033

We note that the data we have available is different from the original data (cite). The original data is a collection of 12 studies, and there are known covariates for each individuals, like the one we simulated in the previous section. However, for the purpose of this case study, the data we used are collapsed into 6 studies, and only the nutritional intake data are available.

2.2 Data preprocessing

Some individuals have missing values for all nutrients, thus we will remove these individuals from the data. Also, there are some nutrition intake are less than zero, for which we will replace with 0. We then apply a log transformation to the data.

We first count how many NA values and negative values are in each study.

```
count_na_and_negatives <- function(df) {
    # Count NA values
    na_count <- sum(is.na(df))
    # Count negative values
    negative_count <- sum(df < 0, na.rm = TRUE)

# Print counts
    cat("Number of NAs:", na_count, "\n")
    cat("Number of negative values:", negative_count, "\n")
}
invisible(lapply(X_s2, count_na_and_negatives))</pre>
```

```
Number of NAs: 1344
Number of negative values: 0
Number of NAs: 1344
Number of negative values: 1
Number of NAs: 1344
Number of negative values: 0
Number of NAs: 1344
Number of negative values: 2
Number of NAs: 1344
Number of negative values: 1
Number of NAs: 1344
Number of negative values: 1
Number of negative values: 0
```

We will define a function to process the data, which removes rows where all values are NA. We also define a function that replaces negative values with 0, and applies a log transformation to the data.

```
process_study_data <- function(df) {
    # Remove rows where all values are NA
    cleaned_df <- df[!apply(df, 1, function(row) all(is.na(row))), , drop = FALSE]
    # Count remaining rows
    remaining_rows <- nrow(cleaned_df)
    # Print results for the study
    cat("Remaining rows:", remaining_rows, "\n")
    return(cleaned_df)
}
Y_list <- lapply(X_s2, process_study_data)</pre>
```

Remaining rows: 1332

Remaining rows: 1485 Remaining rows: 2178 Remaining rows: 5152 Remaining rows: 2446 Remaining rows: 927

The numbers of individuals in each study left for analysis (N_s) are 1332, 1485, 2178, 5152, 2446, and 927, respectively.

```
# Replace negative values with 0, then log(x+0.01) + 0.01
replace_negatives <- function(df) {
    # Replace negative values with 0
    df[df < 0] <- 0
    # Apply log transformation. Add 0.01 to avoid log(0).
    transformed_df <- log(df + 0.01)
    return(transformed_df)
}

Y_list <- lapply(Y_list, replace_negatives)</pre>
```

```
# Check the processed data
invisible(lapply(Y_list, count_na_and_negatives))
```

```
Number of NAs: 0
Number of negative values: 11910
Number of NAs: 0
Number of negative values: 11222
Number of NAs: 0
Number of negative values: 15006
Number of negative values: 36230
Number of negative values: 36230
Number of negative values: 19349
Number of NAs: 0
Number of negative values: 6707
```

Now we don't have any NA values or negative values in the data.

The assumptions for factor models require that each variable has a mean of 0. Therefore, for each study, we will center the data for each column. We note that for some model (Stack FA, Ind FA, BMSFA, and Tetris), this step is handeled internally, and for MOM-SS, the random intercepts are estimated, so we do not need to center the data.

```
Y_list_scaled <- lapply(
   Y_list, function(x) scale(x, center = TRUE, scale = FALSE)
)
Y_mat_scaled <- Y_list_scaled %>% do.call(rbind, .) %>% as.matrix()
```

2.3 Model fitting

We recommend running model fitting and post-processing in a high-performance computing environment, as the model fitting process can be computationally intensive. PFA and Tetris are particularly computationally expensive, where PFA requires more than 10 hours to run, and Tetris requires more than 4 days to run. Other models can be completed in half an hour. We recommend at least 5GB of memory for running the models and post-processing.

For each model, we over-specify the numbers of factors to .. [to be written].

```
# Stack FA
Y_mat = Y_list %>% do.call(rbind, .) %>% as.matrix()
fit_stackFA <- MSFA::sp_fa(Y_mat, k = 6, scaling = FALSE, centering = TRUE,</pre>
                                control = list(nrun = 10000, burn = 800))
# Ind FA
fit_indFA <-
      lapply(1:6, function(s){
        j_s = c(8, 8, 8, 8, 8, 8)
        MSFA::sp_fa(Y_list[[s]], k = j_s[s], scaling = FALSE, centering = TRUE,
                     control = list(nrun = 10000, burn = 8000))
      })
# PFA
N_s <- sapply(Y_list, nrow)</pre>
fit_PFA <- PFA(Y=t(Y_mat_scaled),</pre>
                         latentdim = 6,
                         grpind = rep(1:6,
                                      times = N_s),
                 Thin = 5,
                 Total_itr = 10000, burn = 8000)
# MOM-SS
Y_mat = Y_list %>% do.call(rbind, .) %>% as.matrix()
# Construct the membership matrix
N_s <- sapply(Y_list, nrow)</pre>
M_list <- list()</pre>
```

Fitting Tetris requires a 3-step process. First, we run tetris() to draw posterior samples of the model parameters, including \mathcal{T} . Then we run choose.A() to choose the best \mathcal{T} based on the posterior samples. Finally, we run tetris() again with the chosen \mathcal{T} to obtain the final model. Hyperparameters $\alpha_{\mathcal{T}}$ are set to 1.25 times the number of studies.

2.4 Post processing

Post processing includes calculating the point estimates of the factor loadings and covariance matrix from the posterior samples, and determing the number of factors for each model.

For methods of MOM-SS, SUFA, and Tetris, the number of factors is determined internally in the algorithms, therefore, the output of the models are final results.

For MOM-SS, Φ is directly obtained with its post-processed common loadings in the fitted output. The common covariance is calculated with $\Phi\Phi^{\top}$. The marginal covariance matrix

 $\Sigma_{\rm marginal}$ is calculated by adding the estimated study-specific error covariances to the common variance. The study-specific intercepts α and the coefficients for the known covariates B are also extracted from the fitted output.

```
post_MOMSS <- function(fit, version = 2){ # version 1: M, version 2: Mpost</pre>
  est_Phi <- fit$M
  if (version==2){est Phi <- fit$Mpost}</pre>
  est_SigmaPhi <- tcrossprod(est_Phi)</pre>
  # Marginal covariance
  S <- dim(fit$sigma)[2]
  est_PsiList <- est_SigmaMarginal <- list()</pre>
  for(s in 1:S){
    est_PsiList[[s]] <- fit$sigma[,s]</pre>
    est_SigmaMarginal[[s]] <- est_SigmaPhi + diag(fit$sigma[,s])</pre>
  # last S columns of fit$Theta are the study-specific intercepts
  est_alphas <- fit$Theta[, (dim(fit$Theta)[2]-S+1):dim(fit$Theta)[2]]
  # The rest are coeficients for the known covariates
  est B <- fit$Theta[, 1:(dim(fit$Theta)[2]-S)]</pre>
  return(list(Phi = est_Phi, SigmaPhi = est_SigmaPhi, Psi = est_PsiList, alpha = est_alphas,
               SigmaMarginal = est_SigmaMarginal))
}
res_MOMSS <- post_MOMSS(fit_MOMSS)</pre>
saveRDS(res_MOMSS, "Data/Rnutrition_MOMSS.rds")
```

For SUFA, the shared and study-specific loading matrices, as well as the common and marginal covariance can be conveniently obtained via the lam.est.all(), SUFA_shared_covmat() and sufa_marginal_covs() functions. Error covariance is obtained by taking averages of the "residuals" fitted output. And the study-specific covariance matrices are calculated by subtracting the common covariance from the marginal covariance. Note that in the definition of SUFA, common covariance is $\Phi\Phi^{\top} + \Sigma$.

```
post_SUFA <- function(fit){
   all <- dim(fit$Lambda)[3]
   burnin <- floor(all * 0.8) # We will use the last 20% samples
   # shared and study-specific loading matrices
   loadings <- lam.est.all(fit, burn = burnin)
   # Obtain common covariance matrix and loading from fitting
   est_Phi <- loadings$Shared
   est_SigmaPhi <- SUFA_shared_covmat(fit, burn = burnin)</pre>
```

```
est_Psi <- diag(colMeans(fit$residuals))</pre>
  # Study-specific loadings
  est_LambdaList <- loadings$Study_specific</pre>
  # Obtain study-specific covariance matrices
  S <- length(fit$A)
  marginal_cov <- sufa_marginal_covs(fit, burn = burnin)</pre>
  est SigmaLambdaList <- list()</pre>
  for (s in 1:S) {
    est_SigmaLambdaList[[s]] <- marginal_cov[,,s] - est_SigmaPhi</pre>
  return(list(SigmaPhi = est_SigmaPhi, Phi = est_Phi,
               SigmaLambdaList = est_SigmaLambdaList,
               LambdaList = est_LambdaList,
               Psi = est_Psi,
               SigmaMarginal = lapply(1:S, function(s) marginal_cov[,,s])
               ))
}
res_SUFA <- post_SUFA(fit_SUFA)</pre>
saveRDS(res_SUFA, "Data/Rnutrition_SUFA.rds")
```

For Tetris, the common loading matrix Φ can be obtained through the getLambda() function. The common covariance matrix is calculated as $\Phi\Phi^{\top}$. The study-specific loading matrices Λ_s are obtained by multiplying the common loading matrix with the study-specific matrices T_s-P . The study-specific covariance matrices are calculated as $\Lambda_s\Lambda_s^{\top}$. The marginal covariance matrix is calculated as $\Lambda T\Lambda^{\top} + \Psi$.

```
post_Tetris <- function(fit){
    # Estimated common covariance
    A <- fit$A[[1]]
    Lambda <- getLambda(fit,A)
    S <- dim(A)[1]
    est_Phi <- as.matrix(Lambda[,colSums(A)==S])
    est_SigmaPhi <- tcrossprod(est_Phi)
    # Estimated study-specific covariance
    P = diag((colSums(A) == S)*1)
    T_s <- list()
    est_LambdaList <- list()
    for(s in 1:S){
        T_s[[s]] <- diag(A[s,])
        Lambda_s <- Lambda %*% (T_s[[s]] - P)</pre>
```

```
Lambda_s <- Lambda_s[,-which(colSums(Lambda_s == 0) == nrow(Lambda_s))]
    Lambda_s <- matrix(Lambda_s, nrow=nrow(Lambda))</pre>
    est_LambdaList[[s]] <- Lambda_s}</pre>
  est_SigmaLambdaList <- lapply(1:S, function(s){</pre>
    tcrossprod(est LambdaList[[s]])})
  # Estimated marginal covariance
  Psi <- list()
  est_SigmaMarginal <- lapply(1:S, function(s){</pre>
    Psi[[s]] <- diag(Reduce("+", fit$Psi[[s]])/length(fit$Psi[[s]]))</pre>
    Sigma_s <- Lambda %*% T_s[[s]] %*% t(Lambda) + Psi[[s]]
    })
  return(list(Phi = est_Phi, SigmaPhi = est_SigmaPhi,
               LambdaList = est_LambdaList, SigmaLambdaList = est_SigmaLambdaList,
               Psi = Psi, T_s = T_s,
               SigmaMarginal = est_SigmaMarginal))
res_Tetris <- post_Tetris(run_fixed)</pre>
saveRDS(res_Tetris, "Data/Rnutrition_Tetris.rds")
```

For PFA, the post-processing is a little bit tricky. According to the original paper, the common loading matrix Φ can be just the average of the estimated loadings from the posterior samples. However, we still apply OP as in BMSFA to get the common loadings, and the loadings in PFA should be the product of the estimated loadings and the square root of the variance of the factors. Therefore, we carry out multiplication for Φ for each posterior sample, and then OP the sequence. We also carry out multiplication for Q_s , Σ_{Φ} , Σ_s , Σ_{Λ_s} , and Ψ as in the definition of PFA, and then take the average of the results.

After that, the number of factors is determined by counting the number of columns in Φ that have all loadings less than 10^{-3} .

```
post_PFA <- function(fit){
  p <- nrow(fit$Loading[[1]])
  k <- ncol(fit$Loading[[1]])
  npost <- length(fit$Loading)
  Q_list <- fit$Pertmat
  S <- dim(Q_list[[1]])[2]
  posteriorPhis <- array(0, dim = c(p, k, npost))

#---estimated common loadings and shared variance---
# Element-wise multiplication</pre>
```

```
for(i in 1:npost){
    posteriorPhis[,,i] <- fit$Loading[[i]] %*% diag(fit$Latentsigma[[i]])</pre>
  # Varimax for common loadings
  est_Phi <- MSFA::sp_OP(posteriorPhis, itermax = 10, trace = FALSE)$Phi
  # Estimated shared covariance, study-specific covariance matrix, and SigmaMarginal
  sharevar <- list()</pre>
  est_SigmaLambdaList <- list()</pre>
  est_SigmaMarginal <- list()</pre>
  est_Psi <- list()</pre>
  for(s in 1:S){ # Loop over each study
  post_SigmaLambda_s <- list()</pre>
  post_SigmaMarginal_s <- list()</pre>
  Psi <- list()
  for(i in 1:npost){ # Loop over each posterior sample
    sharevar[[i]] <- fit$Loading[[i]]%*%diag(fit$Latentsigma[[i]]^2)%*%t(fit$Loading[[i]]) +
      diag(fit$Errorsigma[[i]]^2) # Get the shared variance
    Q_temp_inv <- solve(</pre>
      matrix(Q_list[[i]][, s], p, p)
    post_SigmaMarginal_s[[i]] <- Q_temp_inv%*%sharevar[[i]]%*%t(Q_temp_inv)</pre>
    post_SigmaLambda_s[[i]] <- post_SigmaMarginal_s[[i]] - sharevar[[i]]</pre>
    Psi[[i]] <- diag(fit$Errorsigma[[i]]^2)</pre>
  est_SigmaMarginal[[s]] <- Reduce('+', post_SigmaMarginal_s)/length(post_SigmaMarginal_s)</pre>
  est_SigmaLambdaList[[s]] <- Reduce('+', post_SigmaLambda_s)/length(post_SigmaLambda_s)</pre>
  }
  est_Psi <- Reduce('+', Psi)/length(Psi)</pre>
  est_SigmaPhi <- Reduce('+', sharevar)/length(sharevar)</pre>
  est_Q <- Reduce('+', Q_list)/length(Q_list)</pre>
  est_Q_list <- lapply(1:S, function(s) matrix(est_Q[, s], p, p))</pre>
  # Return the results
  return(list(Phi = est_Phi, SigmaPhi = est_SigmaPhi, Psi = est_Psi, Q = est_Q_list,
               SigmaLambdaList = est_SigmaLambdaList,
               SigmaMarginal = est_SigmaMarginal))
res_PFA <- post_PFA(fit_PFA)</pre>
saveRDS(res_PFA, "Data/Rnutrition_PFA.rds")
```

```
# columns have all loadings less than 10^-3
fun_neibour <- function(Phi, threshold = 1e-3) {
    return(
        sum(apply(Phi, 2, function(x) {
            sum(abs(x) <= threshold) < length(x)}
        ))
      )
}

# The post_PFA(fit_PFA) object
res_PFA <- readRDS("Data/Rnutrition_PFA.rds")
Phi_PFA <- res_PFA$Phi
K_PFA <- fun_neibour(Phi_PFA)
K_PFA</pre>
```

[1] 6

The estimated K for PFA is 6.

Next, we show how to process the output of Stack FA, Ind FA, and BMSFA. While point estimates for the loadings and covariances can be obtained in the similar way as in PFA, the number of factors is determined with eigen value decompositions of the covariance matrix. Once the numbers of factors are determined, we have to run the models again with the correct number of factors, and then extract the final results.

Therefore, for Stack FA, we first extract the point estimates of the Φ by applying OP to the posterior samples of the loadings. The common covariance matrix is calculated as $\Phi\Phi^{\top}$. The marginal covariance matrix is calculated as the average of its posterior samples.

```
}
res_stackFA <- post_stackFA(fit_stackFA, S=6)
saveRDS(res_stackFA, "Data/Rnutrition_StackFA.rds")</pre>
```

After that, we determine the number of factors by eigen value decomposition of the common covariance matrix. We then run the model again with the correct number of factors, and extract the final results.

```
fun_eigen <- function(Sig_mean) {
   val_eigen <- eigen(Sig_mean)$values
   prop_var <- val_eigen/sum(val_eigen)
   choose_K <- length(which(prop_var > 0.05))
   return(choose_K)
}
res_stackFA <- readRDS("Data/Rnutrition_StackFA.rds")
SigmaPhi_StackFA <- res_stackFA$SigmaPhi
K_StackFA <- fun_eigen(SigmaPhi_StackFA)
K_StackFA</pre>
```

[1] 4

The estimated K for Stack FA is 4.

Then we re-run the model with the correct number of factors, and extract the final results.

We repeat this process for Ind FA and BMSFA.

```
# Ind FA
post_indFA <- function(fit){
    # Estimated study-specific covariance and loading
    S <- length(fit_list)
    est_LambdaList <- lapply(1:S, function(s){
        MSFA::sp_OP(fit_list[[s]]$Lambda, trace=FALSE)$Phi
    })
    est_SigmaLambdaList <- lapply(est_LambdaList, function(x) tcrossprod(x))</pre>
```

```
# Marginal covariance matrices
  est_SigmaMarginal <- lapply(1:S, function(s) {</pre>
    fit <- fit_list[[s]]</pre>
    apply(fit$Sigma, c(1, 2), mean)
  })
  Psi <- list()
  for(s in 1:S){
    Psi_chain <- list()</pre>
    for(i in 1:dim(fit_list[[1]]$Sigma)[3]){
      Psi_chain[[i]] <- fit_list[[s]]$Sigma[, , i] - tcrossprod(fit_list[[s]]$Lambda[, , i])</pre>
    Psi[[s]] <- Reduce('+', Psi_chain)/length(Psi_chain)</pre>
  }
  return(list(LambdaList = est_LambdaList, SigmaLambdaList = est_SigmaLambdaList, Psi = Psi,
               SigmaMarginal = est_SigmaMarginal))
}
res_indFA <- post_indFA(fit_indFA)</pre>
saveRDS(res_indFA, "Data/Rnutrition_IndFA.rds")
# BMSFA
post_BMSFA <- function(fit){</pre>
  # Common covariance matrix and loading
  est_Phi <- sp_OP(fit$Phi, trace=FALSE)$Phi
  est_SigmaPhi <- tcrossprod(est_Phi)</pre>
  # Study-specific covariance matrices and loadings
  est_LambdaList <- lapply(fit$Lambda, function(x) sp_OP(x, trace=FALSE)$Phi)
  est_SigmaLambdaList <- lapply(est_LambdaList, function(x) tcrossprod(x))</pre>
  # Marginal covariance matrices
  S <- length(est_SigmaLambdaList)</pre>
  # Get point estimate of each Psi_s
  est_PsiList <- lapply(1:S, function(s) {</pre>
    apply(fit$psi[[s]], c(1, 2), mean)
  est_margin_cov <- lapply(1:S, function(s) {</pre>
    est_SigmaPhi + est_SigmaLambdaList[[s]] + diag(est_PsiList[[s]] %>% as.vector())
  })
```

```
SigmaLambda_IndFA <- readRDS("Data/Rnutrition_IndFA.rds")$SigmaLambda
Js_IndFA <- lapply(SigmaLambda_IndFA, fun_eigen)
Js_IndFA %>% unlist()
```

[1] 4 5 5 5 4 4

```
SigmaPhi_BMSFA <- readRDS("Data/Rnutrition_BMSFA.rds")$SigmaPhi
K_BMSFA <- fun_eigen(SigmaPhi_BMSFA)
SigmaLambda_BMSFA <- readRDS("Data/Rnutrition_BMSFA.rds")$SigmaLambda
Js_BMSFA <- lapply(SigmaLambda_BMSFA, fun_eigen)
K_BMSFA %>% unlist()
```

[1] 4

```
Js_BMSFA %>% unlist()
```

[1] 2 2 2 2 2 2

The estimated J_s for Ind FA are 4, 5, 5, 5, 4, and 4. The estimated K for BMSFA is 4 and the estimated J_s are 2, 2, 2, 2, and 2

Then we re-run the models with the correct number of factors, and extract the final results.

Now the final results are obtained and you can get the saved files mentioned above from the GitHub repository.

2.5 Visualization

We can make some heatmap for the loadings. Please see the figures in the paper.

2.6 Mean squared error (MSE)

We can assess the goodness-of-fit of the models by reconstructing data and calculating the reconstruction errors. With estimated loadings and error covariances, we can estimate the factor scores for a new observation, $\hat{\mathbf{f}}_{is,(new)}$ and $\hat{\mathbf{l}}_{is,(new)}$, derived by adapting the Bartlett method?,?. Then we can use the estimated factor scores, together with the estimated loadings, to reconstruct $\hat{\mathbf{y}}_{is,(new)}$ and calculate the reconstruction error which represents the fit of the models. To be specific, suppose that we have the multivariate data of a new observation from a specific study, $\mathbf{y}_{is,(new)}$, we can estimate its factor score and reconstruct its $\hat{\mathbf{y}}_{is,(new)}$ in the following ways:

$$\bullet \ \ \mathrm{Stack} \ \ \mathrm{FA:} \ \widehat{\mathbf{f}}_{is,(new)} = (\widehat{\Phi}^{\top}\widehat{\Psi}^{-1}\widehat{\Phi})^{-1}\widehat{\Phi}^{\top}\widehat{\Psi}^{-1}\mathbf{y}_{is,(new)}, \ \mathrm{and} \ \ \widehat{\mathbf{y}}_{is,(new)} = \widehat{\Phi}\widehat{\mathbf{f}}_{is,(new)}.$$

$$\bullet \ \ \mathrm{Ind} \ \ \mathrm{FA:} \ \hat{\mathbf{l}}_{is,(new)} = (\widehat{\Lambda_s}^{\top} \widehat{\Psi_s}^{-1} \widehat{\Lambda_s})^{-1} \widehat{\Lambda_s}^{\top} \widehat{\Psi_s}^{-1} \mathbf{y}_{is,(new)}, \ \mathrm{and} \ \ \hat{\mathbf{y}}_{is,(new)} = \widehat{\Lambda_s} \hat{\mathbf{l}}_{is,(new)}.$$

$$\bullet \ \ \mathrm{PFA:} \ \hat{\mathbf{f}}_{is,(new)} = (\widehat{\Phi}^{\top}\widehat{\Psi}^{-1}\widehat{\Phi})^{-1}\widehat{\Phi}^{\top}\widehat{\Psi}^{-1}\widehat{Q_{s}}\mathbf{y}_{is,(new)}, \ \mathrm{and} \ \hat{\mathbf{y}}_{is,(new)} = \widehat{Q_{s}}^{-1}\widehat{\Phi}\hat{\mathbf{f}}_{is,(new)}.$$

$$\begin{array}{l} \bullet \ \ \mathrm{MOM\text{-}SS:} \ \widehat{\mathbf{f}}_{is,(new)} = (\widehat{\Phi}^{\top} \widehat{\Psi_s}^{-1} \widehat{\Phi})^{-1} \widehat{\Phi}^{\top} \widehat{\Psi_s}^{-1} (\mathbf{y}_{is,(new)} - \widehat{\mathbf{s}} - \mathbf{\hat{x}}_{is,(new)}), \ \mathrm{and} \ \ \widehat{\mathbf{y}}_{is,(new)} = \widehat{\mathbf{s}} + \mathbf{\hat{x}}_{is,(new)} + \widehat{\Phi} \widehat{\mathbf{f}}_{is,(new)}. \end{array}$$

• SUFA: let
$$\Omega = [\widehat{\Phi}, \widehat{\Phi}\widehat{A_s}]$$
, then $\begin{bmatrix} \widehat{\mathbf{f}}_{is,(new)} \\ \widehat{\mathbf{l}}_{is,(new)} \end{bmatrix} = (\Omega^{\top}\widehat{\Psi}^{-1}\Omega)^{-1}\Omega^{\top}\widehat{\Psi}^{-1}\mathbf{y}_{is,(new)}$, and $\widehat{\mathbf{y}}_{is,(new)} = \widehat{\Phi}\widehat{\mathbf{f}}_{is,(new)} + \widehat{\Phi}\widehat{A_s}\widehat{\mathbf{l}}_{is,(new)}$.

- $\begin{array}{lll} \bullet & \mathrm{BMSFA:} \ \, \mathrm{let} \ \, \Omega \ \, = \ \, [\widehat{\Phi}, \widehat{\Lambda_s}], \ \, \mathrm{then} \ \, \begin{bmatrix} \widehat{\mathbf{f}}_{is,(new)} \\ \widehat{\mathbf{l}}_{is,(new)} \end{bmatrix} \ \, = \ \, (\Omega^{\top} \widehat{\Psi_s}^{-1} \Omega)^{-1} \Omega^{\top} \widehat{\Psi_s}^{-1} \mathbf{y}_{is,(new)}, \ \, \mathrm{and} \\ \widehat{\mathbf{y}}_{is,(new)} = \widehat{\Phi} \widehat{\mathbf{f}}_{is,(new)} + \widehat{\Lambda_s} \widehat{\mathbf{l}}_{is,(new)}. \end{array}$
- $\begin{array}{lll} \bullet & \text{Tetris:} & \widehat{\mathbf{f}}_{is,(new)} & = & (\widehat{T_s}^\top (\widehat{\Phi^*})^\top \widehat{\Psi_s}^{-1} \widehat{\Phi^*} \widehat{T_s})^{-1} \widehat{T_s}^\top (\widehat{\Phi^*})^\top \widehat{\Psi_s}^{-1} \mathbf{y}_{is,(new)}, & \text{and} & \widehat{\mathbf{y}}_{is,(new)} & = & \\ \widehat{\Phi^*} \widehat{T_s} \widehat{\mathbf{f}}_{is,(new)}. & \end{array}$

If we divide the whole data into training set and test set, we can obtain the **mean square** difference (MSE) between the true and estimated $\mathbf{y}_{is,(new)}$ in the test set for all individuals in all studies with $\frac{1}{P\sum_{s}^{S}N_{s}}\sum_{s}^{N_{s}}\sum_{i}^{N_{s}}\sum_{p}^{P}(\hat{y}_{isp,(new)}-y_{isp,(new)})^{2}$.

In the following, we divide the nutrition data into training set (70%) and test set (30%) and calculate the MSE of each model. Note that \mathbf{y}_{new} should also be centered except for MOM-SS.

```
train_ratio <- 0.7
train_list <- list()

test_list <- list()

for (s in seq_along(Y_list)) {
    N_s <- nrow(Y_list[[s]]) # Number of rows in the study
    train_indices <- sample(1:N_s, size = floor(train_ratio * N_s), replace = FALSE)

    train_list[[s]] <- Y_list[[s]][train_indices, ]
    test_list[[s]] <- Y_list[[s]][-train_indices, ]
}

# Test data has to be centered
test_list <- lapply(test_list, as.matrix)
test_list_scaled <- lapply(
    test_list, function(x) scale(x, center = TRUE, scale = FALSE)
)</pre>
```

We fit the models in the training data (on high-performance computing clusters), and then we load the fitted models and calculate the MSE on the test set for each model. The numbers of factors we input are determined by the previous results.

```
fit_StackFA_train <- readRDS("Data/Rnutrition_stackFA_train.rds")
fit_IndFA_train <- readRDS("Data/Rnutrition_IndFA_train.rds")
fit_PFA_train <- readRDS("Data/Rnutrition_PFA_train.rds")
fit_MOMSS_train <- readRDS("Data/Rnutrition_MOMSS_train.rds")
fit_SUFA_train <- readRDS("Data/Rnutrition_SUFA_train.rds")</pre>
```

```
fit_BMSFA_train <- readRDS("Data/Rnutrition_BMSFA_train.rds")
fit_Tetris_train <- readRDS("Data/Rnutrition_Tetris_train.rds")</pre>
```

We used the derived MSE function to calculate the MSE for each model.

```
# Stack FA
Phi <- fit_StackFA_train$Phi
Psi <- fit_StackFA_train$Psi</pre>
mse_stackFA <- 1/(42 * sum(sapply(test_list, nrow)))*sum(</pre>
  sapply(1:6, function(s){
    scores <- test_list_scaled[[s]] %*% solve(Psi) %*% Phi %*% mnormt::pd.solve(signif(t(Phi</pre>
    norm(test_list_scaled[[s]] - scores %*% t(Phi), "F")^2
  })
)
# Ind FA
LambdaList <- fit_IndFA_train$LambdaList</pre>
Psi <- fit_IndFA_train$Psi
mse_IndFA <- 1/(42 * sum(sapply(test_list, nrow)))*sum(</pre>
  sapply(1:6, function(s){
    scores <- test_list_scaled[[s]] %*% solve(Psi[[s]]) %*% LambdaList[[s]] %*% mnormt::pd.se
    norm(test_list_scaled[[s]] - scores %*% t(LambdaList[[s]]), "F")^2
  })
)
# PFA
Phi <- fit_PFA_train$Phi
Psi <- fit_PFA_train$Psi
Q_list <- fit_PFA_train$Q</pre>
mse_PFA <- 1/(42 * sum(sapply(test_list, nrow)))*sum(</pre>
  sapply(1:6, function(s){
    scores <- test_list_scaled[[s]] %*% t(Q_list[[s]]) %*% Phi %*% mnormt::pd.solve(signif(t</pre>
    Y_est <- scores %*% t(Phi) %*% t(solve(Q_list[[s]]))</pre>
    norm(test_list_scaled[[s]] - Y_est, "F")^2
  })
)
# MOM-SS
Phi <- fit_MOMSS_train$Phi
```

```
Psi <- fit_MOMSS_train$Psi %>% lapply(diag)
alpha <- lapply(1:6, function(s) {</pre>
  fit_MOMSS_train$alpha[,s]
})
mse_MOMSS <- 1/(42 * sum(sapply(test_list, nrow)))*sum(</pre>
  sapply(1:6, function(s){
    scores <- t(apply(test_list[[s]], 1, function(row) {row - alpha[[s]]})) %*% solve(Psi[[s]
    Y_est <- t(apply(scores %*% t(Phi), 1, function(row) {row + alpha[[s]]}))
    norm(test_list[[s]] - Y_est, "F")^2
  })
)
# SUFA
Phi <- fit_SUFA_train$Phi
LambdaList <- fit_SUFA_train$LambdaList</pre>
Psi <- fit_SUFA_train$Psi
mse_SUFA <- 1/(42 * sum(sapply(test_list, nrow)))*sum(</pre>
  sapply(1:6, function(s){
    Omega <- cbind(Phi, LambdaList[[s]])</pre>
    scores <- test_list_scaled[[s]] %*% solve(Psi) %*% Omega %*% mnormt::pd.solve(signif(t(One)))
    norm(test_list_scaled[[s]] - scores %*% t(Omega), "F")^2
  })
)
# BMSFA
Phi <- fit_BMSFA_train$Phi
LambdaList <- fit_BMSFA_train$LambdaList</pre>
Psi <- fit_BMSFA_train$PsiList %>% lapply(as.vector) %>% lapply(diag)
mse_BMSFA <- 1/(42 * sum(sapply(test_list, nrow)))*sum(</pre>
  sapply(1:6, function(s){
    Omega <- cbind(Phi, LambdaList[[s]])</pre>
    scores <- test_list_scaled[[s]] %*% solve(Psi[[s]]) %*% Omega %*% mnormt::pd.solve(signi)</pre>
    norm(test_list_scaled[[s]] - scores %*% t(Omega), "F")^2
  })
# Tetris
Phi <- fit_Tetris_train$Phi
LambdaList <- fit_Tetris_train$LambdaList</pre>
```

We display the MSE of each model.

```
print(paste0("Stack FA: ", mse_stackFA %>% round(3)))
print(paste0("Ind FA: ", mse_IndFA %>% round(3)))
print(paste0("PFA: ", mse_PFA %>% round(3)))
print(paste0("MOM-SS: ", mse_MOMSS %>% round(3)))
print(paste0("SUFA: ", mse_SUFA %>% round(3)))
print(paste0("BMSFA: ", mse_BMSFA %>% round(3)))
print(paste0("Tetris: ", mse_Tetris %>% round(3)))
```

```
[1] "Stack FA: 0.493"
[1] "Ind FA: 0.474"
[1] "PFA: 0.668"
[1] "MOM-SS: 0.465"
[1] "SUFA: 0.432"
[1] "BMSFA: 0.446"
[1] "Tetris: 0.277"
```

3 Case study: gene expression data

Similarly, we load utility package tidyverse to help with data manipulation and visualization.

```
library(tidyverse)
```

In this demonstration, we use the curate Ovarian data(2013) to demonstrate (1) the common gene co-expression network drawn by Σ_{Φ} and (2) the fit of the models via calculating MSE. This data contains the gene expression and clinical outcomes of 2970 patients collected from 23 studies. Different studies have different sequencing platforms, sample sizes, stage/subtype of the tumor, survival and censoring information.

3.1 Loading and previewing the data

We load the curatedOvarianData package to get the data. Description of each study can be found with data(package="curatedOvarianData").

library(curatedOvarianData)

```
#data(package="curatedOvarianData")
data(GSE13876_eset)
data(GSE26712_eset)
data(GSE9891_eset)
data(PMID17290060_eset)
```

The four datasets are of similar sizes. All of them have the majority of patients in the late stage of the cancer, and histological subtypes observed in the tissue samples are mostly serous carcinoma. The datasets differs in respect sequencing platforms, which are Operonv3two-color, AffymetrixHG-U133A, AffymetrixHG-U133Plus2 and AffymetrixHG-U133A.

3.2 Data pre-processing

First we find intersection of genes that are exist in all four studies. We use featureNames to extract the gene names and exprs to extract the data matrices. More operations of the ExpressionSets can be found in (Falcon, Morgan, and Gentleman 2007).

We then filter the genes so that only high variance genes are kept for later analysis.

```
# calculate Coefficient of Variation of each gene
cv1 <- apply(study1, 2, sd) / apply(study1, 2, mean)
cv2 <- apply(study2, 2, sd) / apply(study2, 2, mean)
cv3 <- apply(study3, 2, sd) / apply(study3, 2, mean)
cv4 <- apply(study4, 2, sd) / apply(study4, 2, mean)
cv_matrix <- rbind(cv1, cv2, cv3, cv4)

# Find genes with CV >= threshold in at least one study
threshold <- 0.16
genes_to_keep <- apply(cv_matrix, 2, function(cv) any(cv >= threshold))
sum(genes_to_keep)
```

[1] 1060

```
# Filtered
study1 <- GSE13876_eset[genes_to_keep,]
study2 <- GSE26712_eset[genes_to_keep,]
study3 <- GSE9891_eset[genes_to_keep,]
study4 <- PMID17290060_eset[genes_to_keep,]</pre>
```

Next, we log-transform the data (for a better normality) and store them in $4 N_s \times P$ matrices.

```
df1 <- study1 %>% exprs() %>% t() %>%
  log() %>% as.data.frame()
df2 <- study2 %>% exprs() %>% t() %>%
  log() %>% as.data.frame()
df3 <- study3 %>% exprs() %>% t() %>%
  log() %>% as.data.frame()
df4 <- study4 %>% exprs() %>% t() %>%
  log() %>% as.data.frame()
df4 <- study4 %>% exprs() %>% t() %>%
  log() %>% as.data.frame()
list_gene <- list(df1, df2, df3, df4)
saveRDS(list(df1, df2, df3, df4), "./Data/CuratedOvarian_processed.rds")</pre>
```

Now we can see the dimensions of each study:

```
sapply(list_gene, dim)

[,1] [,2] [,3] [,4]
[1,] 157 195 285 117
[2,] 1060 1060 1060 1060
```

The ultimate data for analysis has $N_s=(157,195,285,117)$ for s=1,2,3,4, and P=1060.

We scale the data so that we focus on the correlations between the genes. When the data are scaled, the variance of the genes are 1 and the off-diagonal values scales up, so does the estimated covariances matrices, which facilitates a more interpretable network analysis.

```
Y_list <- readRDS("./Data/CuratedOvarian_processed.rds")
Y_list_scaled <- lapply(
  Y_list, function(x) scale(x, center = TRUE, scale = TRUE)
)
Y_mat_scaled <- Y_list_scaled %>% do.call(rbind, .) %>% as.matrix()
```

3.3 Fitting the models

For models fitted with MSFA::sp_fa, the function provides scaling and centering arguments. Therefore, we do not need to use the scaled data before fitting (here I use Mavis's version of MSFA).

MOM-SS:

```
# Construct the membership matrix
N_s <- sapply(Y_list, nrow)
M_list <- list()
   for(s in 1:4){
      M_list[[s]] <- matrix(1, nrow = N_s[s], ncol = 1)
   }
M <- as.matrix(bdiag(M_list))

fit_MOMSS <- BFR.BE::BFR.BE.EM.CV(x = Y_mat, v = NULL, b = M, q = 20, scaling = TRUE)</pre>
```

PFA (we don't recommend running it. It takes 4 days and more.)

SUFA (takes about 10 hours):

```
fit_SUFA <- SUFA::fit_SUFA(Y_list_scaled, qmax=20,nrun = 10000)</pre>
```

BMSFA:

Tetris (we don't recommend running it. It could take more than 10 days.):

3.4 Post-processing

We use the post_xxx() functions defined in the chapter of nutrition applications to post-process for point estimates of the factor loadings, common factors, and covariance matrices.

For Stack FA, Ind FA and BMSFA, we need to determine the number of common factors K and the number of latent dimensions j_s for each study after the post-processing, and we need to re-run those models.

Here we start with Stack FA, Ind FA and BMSFA:

```
# Stack FA
```

References

- De Vito, Roberta, Briana Stephenson, Daniela Sotres-Alvarez, Anna-Maria Siega-Riz, Josiemer Mattei, Maria Parpinel, Brandilyn A Peters, et al. 2022. "Shared and Ethnic Background Site-Specific Dietary Patterns in the Hispanic Community Health Study/Study of Latinos (HCHS/SOL)." medRxiv, 2022–06.
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