# Package: ManlyMix (via r-universe)

October 28, 2026

**Version** 0.1.15.1

**Date** 2023-04-27

**Title** Manly Mixture Modeling and Model-Based Clustering

**Depends** R (>= 3.0.0)

**LazyLoad** yes

**LazyData** no

**Description** The utility of this package includes finite mixture modeling and model-based clustering through Manly mixture models by Zhu and Melnykov (2016) <DOI:10.1016/j.csda.2016.01.015>. It also provides capabilities for forward and backward model selection procedures.

**License** GPL (>= 2)

**Author** Xuwen Zhu [aut, cre], Volodymyr Melnykov [aut], Michael Hutt [ctb, cph] (NM optimization in c), Stephen Moshier [ctb, cph] (eigen calculations in c), Rouben Rostamian [ctb, cph] (memory allocation in c)

**Maintainer** Xuwen Zhu <xzhu20@cba.ua.edu>

**NeedsCompilation** yes

**Repository** https://cran.r-universe.dev

**Date/Publication** 2024-09-24 02:59:53 UTC

**RemoteUrl** https://github.com/cran/ManlyMix

**RemoteRef** HEAD

**RemoteSha** 4fa9d7e7f73d36fdedc4ef6ffc0b5b57cddf3764

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`ManlyMix-package` *Finite mixture modeling and model-based clustering based on Manly mixture models.*

---

## Description

The utility of this package includes finite mixture modeling and model-based clustering based on Manly mixtures as well as forward and backward model selection procedures.

## Details

| | |
|---|---|
| Package: | ManlyMix |
| Type: | Package |
| Version: | 0.1.7 |
| Date: | 2016-12-01 |
| License: | GPL (>= 2) |
| LazyLoad: | no |

Function 'Manly.sim' simulates Manly mixture datasets.

Function 'Manly.overlap' estimates the pairwise overlaps for a Manly mixture.

Function 'Manly.EM' runs the EM algorithm for Manly mixture models.

Function 'Manly.select' runs forward and backward model selection procedures.

Function 'Manly.Kmeans' runs k-means model with Manly transformation.

Function 'Manly.var' produces the variance-covariance matrix of the parameter estimates from Manly mixture model.

Function 'Manly.plot' produces the density plot or contour plot of Manly mixture.

Function 'Manly.model' incorporates all Manly mixture related functionality.

## Author(s)

Xuwen Zhu and Volodymyr Melnykov.

Maintainer: Xuwen Zhu <xuwen.zhu@louisville.edu>

## References

Zhu, X. and Melnykov, V. (2016) "Manly Transformation in Finite Mixture Modeling", *Journal of Computational Statistics and Data Analysis*, doi:10.1016/j.csda.2016.01.015.

Maitra, R. and Melnykov, V. (2010) "Simulating data to study performance of finite mixture modeling and clustering algorithms", *Journal of Computational and Graphical Statistics*, 2:19, 354-376.

Melnykov, V., Chen, W.-C., and Maitra, R. (2012) "MixSim: An R Package for Simulating Data to Study Performance of Clustering Algorithms", *Journal of Statistical Software*, 51:12, 1-25.

## Examples

```
set.seed(123)

K <- 3; p <- 4
X <- as.matrix(iris[,-5])
id.true <- rep(1:K, each = 50)

# Obtain initial memberships based on the K-means algorithm
id.km <- kmeans(X, K)$cluster

# Run the CEM algorithm for Manly K-means model
la <- matrix(0.1, K, p)
C <- Manly.Kmeans(X, id = id.km, la = la)

# Run the EM algorithm for a Gaussian mixture model based on K-means solution
G <- Manly.EM(X, id = id.km)
id.G <- G$id

# Run FORWARD SELECTION ('silent' is on)
F <- Manly.select(X, model = G, method = "forward", silent = TRUE)

# Run the EM algorithm for a full Manly mixture model based on Gaussian mixture solution
la <- matrix(0.1, K, p)
M <- Manly.EM(X, id = id.G, la = la)

# Run BACKWARD SELECTION ('silent' is off)
B <- Manly.select(X, model = M, method = "backward")

BICs <- c(G$bic, M$bic, F$bic, B$bic)
names(BICs) <- c("Gaussian", "Manly", "Forward", "Backward")
BICs
```

---

`acidity` *Acidity data*

---

## Description

Acidity index measured in a sample of 155 lakes in the Northeastern United States. The data are on the log scale.

## Usage

```
data(acidity)
```

## Format

A data vector with 155 observations on the acidity index.

## Details

The data was first analysed by Crawford et al. (1994).

## References

Crawford, S. L. (1994) *An application of the Laplace method to finite mixture distribution*, Journal of the American Statistical Association, 89, 259-267.

## Examples

```
data(acidity)
```

---

# ais *Australian Institute of Sport data*

---

## Description

Data on 102 male and 100 female athletes collected at the Australian Institute of Sport, courtesy of Richard Telford and Ross Cunningham.

## Usage

```
data(ais)
```

## Format

A data frame with 202 observations on the following 13 variables.

**sex** Factor with levels: `female`, `male`;

**sport** Factor with levels: `B_Ball`, `Field`, `Gym`, `Netball`, `Row Swim`, `T_400m`, `Tennis`, `T_Sprnt`, `W_Polo`;

**RCC** Red cell count;

**WCC** White cell count;

**Hc** Hematocrit;

**Hg** Hemoglobin;

**Fe** Plasma ferritin concentration;

**BMI** Body Mass Index;

**SSF** Sum of skin folds;

**Bfat** Body fat percentage;

**LBM** Lean body mass;

**Ht** Height, cm;

**Wt** Weight, kg

## Details

The data have been made publicly available in connection with the book by Cook and Weisberg (1994).

## References

Cook and Weisberg (1994) *An Introduction to Regression Graphics*, John Wiley & Sons, New York.

## Examples

```
data(ais)
```

---

`bankruptcy` *Bankruptcy data*

---

## Description

The data set contain the ratio of retained earnings (RE) to total assets, and the ratio of earnings before interests and taxes (EBIT) to total assets of 66 American firms recorded in the form of ratios. Half of the selected firms had filed for bankruptcy.

## Usage

```
data(bankruptcy)
```

## Format

A data frame with the following variables:

**Y** The status of the firm: `0` bankruptcy or `1` financially sound;

**RE** Ratio of retained earnings to total assets;

**EBIT** Ratio of earnings before interests and taxes to total assets

## References

Altman E.I. (1968) Financial ratios, discriminant analysis and the prediction of corporate bankruptcy, *J Finance* **23**(4): 589-609

## Examples

```
data(bankruptcy)
```

---

`ClassAgree` *Calculates the confusion matrix and number of misclassifications*

---

## Description

Calculates the confusion matrix and number of misclassifications.

## Usage

```
ClassAgree(est.id, trueid)
```

## Arguments

| | |
|---|---|
| `est.id` | estimated membership vector |
| `trueid` | true membership vector |

## Value

`ClassificationTable`
: confusion table between true and estimated partitions

`MisclassificationNum`
: number of misclassifications

## Examples

```
set.seed(123)

K <- 3; p <- 4
X <- as.matrix(iris[,-5])
id.true <- rep(1:K, each = 50)

# Obtain initial memberships based on the K-means algorithm
id.km <- kmeans(X, K)$cluster

ClassAgree(id.km, id.true)
```

`Manly.EM` *EM algorithm for Manly mixture model*

## Description

Runs the EM algorithm for a Manly mixture model with specified initial membership and transformation parameters.

## Usage

```
Manly.EM(X, id = NULL, la = NULL, tau = NULL, Mu = NULL, S = NULL,
tol = 1e-5, max.iter = 1000)
```

## Arguments

| | |
|---|---|
| `X` | dataset matrix (n x p) |
| `id` | initial membership vector (length n) |
| `la` | initial transformation parameters (K x p) |
| `tau` | initial vector of mixing proportions (length K) |
| `Mu` | initial matrix of mean vectors (K x p) |
| `S` | initial array of covariance matrices (p x p x K) |
| `tol` | tolerance level |
| `max.iter` | maximum number of iterations |

## Details

Runs the EM algorithm for a Manly mixture model for a provided dataset. Manly mixture model assumes that a multivariate Manly transformation applied to each component allows to reach near-normality. A user has a choice to specify either initial id vector 'id' and transformation parameters 'la' or initial mode parameters 'la', 'tau', 'Mu', and 'S'. In the case when transformation parameters are not provided, the function runs the EM algorithm without any transformations, i.e., it is equivalent to the EM algorithm for a Gaussian mixtuire model. If some transformation parameters have to be excluded from the consideration, in the corresponding positions of matrix 'la', the user has to specify value 0. Notation: n - sample size, p - dimensionality of the dataset X, K - number of mixture components.

## Value

| | |
|---|---|
| `la` | matrix of the estimated transformation parameters (K x p) |
| `tau` | vector of mixing proportions (length K) |
| `Mu` | matrix of the estimated mean vectors (K x p) |
| `S` | array of the estimated covariance matrices (p x p x K) |
| `gamma` | matrix of posterior probabilities (n x K) |
| `id` | estimated membership vector (length n) |

| | |
|---|---|
| ll | log likelihood value |
| bic | Bayesian Information Criterion |
| iter | number of EM iterations run |
| flag | convergence flag (0 - success, 1 - failure) |

## See Also

Manly.select

## Examples

```
set.seed(123)

K <- 3; p <- 4
X <- as.matrix(iris[,-5])
id.true <- rep(1:K, each = 50)

# Obtain initial memberships based on the K-means algorithm
id.km <- kmeans(X, K)$cluster

# Run the EM algorithm for a Gaussian mixture model based on K-means solution
A <- Manly.EM(X, id.km)
id.Gauss <- A$id

ClassAgree(id.Gauss, id.true)

# Run the EM algorithm for a Manly mixture model based on Gaussian mixture solution
la <- matrix(0.1, K, p)
B <- Manly.EM(X, id.Gauss, la)
id.Manly <- B$id

ClassAgree(id.Manly, id.true)
```

---

# Manly.Kmeans *k-means algorithm with Manly transformation*

---

## Description

Runs the CEM algorithm for k-means clustering with specified initial membership and transformation parameters.

## Usage

```
Manly.Kmeans(X, id = NULL, la = NULL, Mu = NULL, S = NULL,
initial = "k-means", K = NULL, nstart = 100, method = "ward.D",
tol = 1e-5, max.iter = 1000)
```

## Arguments

| | |
|---|---|
| X | dataset matrix (n x p) |
| id | initial membership vector (length n) |
| la | initial transformation parameters (K x p) |
| Mu | initial matrix of mean vectors (K x p) |
| S | initial vector of variances (K) |
| initial | initialization strategy of the EM algorithm ("k-means" - partition obtained by k-means clustering, "hierarchical" - partition obtained by hierarchical clustering) |
| K | number of clusters for the k-means initialization |
| nstart | number of random starts for the k-means initialization |
| method | linkage method for the hierarchical initialization |
| tol | tolerance level |
| max.iter | maximum number of iterations |

## Details

Runs the CEM algorithm for k-means clustering with Manly transformation for a provided dataset. The model assumes that a multivariate Manly transformation applied to each component allows to reach near-normality. A user has a choice to specify either initial id vector 'id' and transformation parameters 'la' or initial mode parameters 'la', 'Mu', and 'S'. In the case when transformation parameters are not provided, the function runs the EM algorithm without any transformations, i.e., it is equivalent to the EM algorithm for a k-means model. If some transformation parameters have to be excluded from the consideration, in the corresponding positions of matrix 'la', the user has to specify value 0. Notation: n - sample size, p - dimensionality of the dataset X, K - number of mixture components.

## Value

| | |
|---|---|
| la | matrix of the estimated transformation parameters (K x p) |
| Mu | matrix of the estimated mean vectors (K x p) |
| S | array of the estimated covariance matrices (K) |
| id | estimated membership vector (length n) |
| iter | number of EM iterations run |
| flag | convergence flag (0 - success, 1 - failure) |

## See Also

Manly.EM

## Examples

```
set.seed(123)

K <- 3; p <- 4
X <- as.matrix(iris[,-5])
id.true <- rep(1:K, each = 50)

# Obtain initial memberships based on the traditional K-means algorithm
id.km <- kmeans(X, K)$cluster

# Run the CEM algorithm for k-means with Manly transformation based on traditional k-means solution
la <- matrix(0.1, K, p)
B <- Manly.Kmeans(X, id.km, la)
id.Manly <- B$id

ClassAgree(id.Manly, id.true)
```

---

`Manly.model` *Manly mixture model*

---

## Description

Runs all the functionality of a Manly mixture model.

## Usage

```
Manly.model(X, K = 1:5, Gaussian = FALSE, initial = "k-means",
nstart = 100, method = "ward.D",  short.iter = 5,
select = "none", silent = TRUE, plot = FALSE, var1 = NULL,
var2 = NULL, VarAssess = FALSE, conf.CI = NULL, overlap = FALSE, N = 1000,
tol = 1e-5, max.iter = 1000, ...)
```

## Arguments

| | |
|---|---|
| `X` | dataset matrix (n x p) |
| `K` | number of components tested |
| `Gaussian` | whether Gaussian mixture models are run or not |
| `initial` | initialization strategy of the EM algorithm ("k-means" - partition obtained by k-means clustering, "hierarchical" - partition obtained by hierarchical clustering, "emEM" - parameters estimated by the emEM algorithm) |
| `nstart` | number of random starts for the k-means or the emEM initialization |
| `method` | linkage method for the hierarchical initialization |
| `short.iter` | number of short emEM iterations to run |
| `select` | control to run Manly.select or not ("none" - do not run Manly.select , "forward" - run forward selection, "backward" - run backward selection) |

| | |
|---|---|
| silent | control the output from Manly.select |
| plot | control to construct the density or contour plot or not |
| var1 | x-axis variable for contour plot or variable for density plot |
| var2 | y-axis variable for contour plot |
| VarAssess | run the variability assessment of the Manly mixture model or not |
| conf.CI | specify the confidence level of parameter estimates |
| overlap | estimate the overlap of Manly mixture components or not |
| N | number of Monte Carlo simulations to run in the Manly.overlap function |
| tol | tolerance level |
| max.iter | maximum number of iterations |
| ... | further arguments related to Manly.plot |

## Details

Wrapper function that incorporates all functionality associated with Manly mixture modeling.

## Value

| | |
|---|---|
| Model | best mixture model obtained |
| VarAssess | estimated variance-covariance matrix for model parameter estimates |
| Overlap | estimated overlap of Manly mixture components |

## See Also

Manly.EM

## Examples

```
set.seed(123)

K <- 3; p <- 4
X <- as.matrix(iris[,-5])
id.true <- rep(1:K, each = 50)

Obj <- Manly.model(X, K = 1:5, initial = "emEM", nstart = 1, short.iter = 5)
```

`Manly.overlap` *Estimates the overlap for a Manly mixture*

## Description

Estimates the pairwise overlap matrix for a Manly mixture by simulating samples based on user-specified parameters.

## Usage

```
Manly.overlap(tau, Mu, S, la, N = 1000)
```

## Arguments

| | |
|---|---|
| `la` | matrix of transformation parameters (K x p) |
| `tau` | vector of mixing proportions (length K) |
| `Mu` | matrix of mean vectors (K x p) |
| `S` | array of covariance matrices (p x p x K) |
| `N` | number of samples simulated |

## Details

Estimates the pairwise overlap matrix for a Manly mixture. Overlap is defined as sum of two misclassification probabilities.

## Value

| | |
|---|---|
| `OmegaMap` | matrix of misclassification probabilities (K x K); OmegaMap[i,j] is the probability that X coming from the i-th component is classified to the j-th component. |
| `BarOmega` | value of average overlap. |
| `MaxOmega` | value of maximum overlap. |

## References

Maitra, R. and Melnykov, V. (2010) "Simulating data to study performance of finite mixture modeling and clustering algorithms", *Journal of Computational and Graphical Statistics*, 2:19, 354-376.

Melnykov, V., Chen, W.-C., and Maitra, R. (2012) "MixSim: An R Package for Simulating Data to Study Performance of Clustering Algorithms", *Journal of Statistical Software*, 51:12, 1-25.

## Examples

```
set.seed(123)
#sets the number of components, dimensionality and sample size
K <- 3
p <- 2

#sets the mixture parameters
tau <- c(0.25, 0.3, 0.45)
Mu <- matrix(c(4.5,4,5,7,8,5.5),3)
la <- matrix(c(0.2,0.5,0.3,0.25,0.35,0.4),3)
S <- array(NA, dim = c(p,p,K))
S[,,1] <- matrix(c(0.4,0,0,0.4),2)
S[,,2] <- matrix(c(1,-0.2,-0.2,0.6),2)
S[,,3] <- matrix(c(2,-1,-1,2),2)

#computes the overlap
A <- Manly.overlap(tau, Mu, S, la)
print(A)
```

---

# Manly.plot *Density plot or contour plot for Manly mixture model*

---

## Description

Provides a contour plot or a density plot for the fitted data with Manly mixture model.

## Usage

```
Manly.plot(X, var1 = NULL, var2 = NULL, model = NULL, x.slice = 100,
y.slice = 100, x.mar = 1, y.mar = 1, col = "lightgrey", ...)
```

## Arguments

| | |
|---|---|
| X | dataset matrix (n x p) |
| var1 | x-axis variable for contour plot or variable for density plot |
| var2 | y-axis variable for contour plot |
| model | fitted Manly mixture model |
| x.slice | number of slices in the first variable sequence in the contour |
| y.slice | number of slices in the second variable sequence in the contour |
| x.mar | value to be subtracted/added to the smallest/largest observation in the x-axis |
| y.mar | value to be subtracted/added to the smallest/largest observation in the y-axis |
| col | color of the contour lines |
| ... | further arguments related to contour and hist |

## Details

Provides the contour plot or density plot for the fitted data by Manly mixture model.

## See Also

Manly.EM

## Examples

```
set.seed(123)

K <- 2; p <- 2
X <- as.matrix(faithful)

# Obtain initial memberships based on the K-means algorithm
id.km <- kmeans(X, K)$cluster

# Run the EM algorithm for a Manly mixture model based on K-means solution
la <- matrix(0.1, K, p)
B <- Manly.EM(X, id.km, la)

Manly.plot(X, model = B, var1 = 1, x.mar = 1, y.mar = 2,
xaxs="i", yaxs="i", xaxt="n", yaxt="n", xlab="",
ylab = "", nlevels = 10, drawlabels = FALSE,
lwd = 3.2, col = "lightgrey", pch = 19)
```

---

# Manly.select *Manly transformation selection*

---

## Description

Runs forward or backward model selection procedures for finding the optimal model in terms of BIC.

## Usage

```
Manly.select(X, model, method, tol = 1e-5, max.iter = 1000, silent = FALSE)
```

## Arguments

| | |
|---|---|
| X | dataset matrix (n x p) |
| model | list containing parameters of the initial model |
| method | model selection method (options 'forward' and 'backward') |
| tol | tolerance level |
| max.iter | maximum number of iterations |
| silent | output control |

## Details

Runs Manly forward and backward model selection procedures for a provided dataset. Forward and backward selection can be started from any ManlyMix object provided in 'model'. Manly transformation parameters are provided in matrix 'model$la'. If some transformations are not needed for specific components, zeros have to be specified in corresponding poisition. When all transformation parameters are set to zero, Manly mixture model degenerates to a Gaussian mixture model. Notation: n - sample size, p - dimensionality of the dataset X, K - number of mixture components.

## Value

| | |
|---|---|
| `la` | matrix of the estimated transformation parameters (K x p) |
| `tau` | vector of mixing proportions (length K) |
| `Mu` | matrix of the estimated mean vectors (K x p) |
| `S` | array of the estimated covariance matrices (p x p x K) |
| `gamma` | matrix of posterior probabilities (n x K) |
| `id` | estimated membership vector (length n) |
| `ll` | log likelihood value |
| `bic` | Bayesian Information Criterion |
| `iter` | number of EM iterations run |
| `flag` | convergence flag (0 - success, 1 - failure) |

## See Also

Manly.EM

## Examples

```
set.seed(123)

K <- 3; p <- 4
X <- as.matrix(iris[,-5])
id.true <- rep(1:K, each = 50)

# Obtain initial memberships based on the K-means algorithm
id.km <- kmeans(X, K)$cluster

# Run the EM algorithm for a Gaussian mixture model based on K-means solution
G <- Manly.EM(X, id = id.km)
id.G <- G$id

# Run FORWARD SELECTION ('silent' is on)
F <- Manly.select(X, model = G, method = "forward", silent = TRUE)

# Run the EM algorithm for a full Manly mixture model based on Gaussian mixture solution
la <- matrix(0.1, K, p)
M <- Manly.EM(X, id = id.G, la = la)

# Run BACKWARD SELECTION ('silent' is off)
```

```
B <- Manly.select(X, model = M, method = "backward")

BICs <- c(G$bic, M$bic, F$bic, B$bic)
names(BICs) <- c("Gaussian", "Manly", "Forward", "Backward")
BICs
```

---

`Manly.sim` *Simulates Manly mixture dataset*

---

## Description

Simulates Manly mixture dataset given the mixture parameters and sample size.

## Usage

```
Manly.sim(n, la, tau, Mu, S)
```

## Arguments

| | |
|---|---|
| `n` | sample size |
| `la` | matrix of transformation parameters (K x p) |
| `tau` | vector of mixing proportions (length K) |
| `Mu` | matrix of mean vectors (K x p) |
| `S` | array of covariance matrices (p x p x K) |

## Details

Simulates a Manly mixture dataset. Manly mixture data points are computed from back-transforming Gaussian distributed data points using user-specified transformation parameters 'la'.

## Value

| | |
|---|---|
| `X` | the simulated Manly mixture dataset |
| `id` | the simulated membership of the data |

## Examples

```
set.seed(123)

#sets the number of components, dimensionality and sample size
K <- 3
p <- 2
n <- 1000

#sets the parameters to simulate data from
tau <- c(0.25, 0.3, 0.45)
Mu <- matrix(c(12,4,4,12,4,10),3)
```

```
la <- matrix(c(1.2,0.5,1,0.5,0.5,0.7),3)
S <- array(NA, dim = c(p,p,K))
S[,,1] <- matrix(c(4,0,0,4),2)
S[,,2] <- matrix(c(5,-1,-1,3),2)
S[,,3] <- matrix(c(2,-1,-1,2),2)

#use function Manly.sim to simulate dataset with membership
A <- Manly.sim(n, la, tau, Mu, S)

#plot the data
plot(A$X, col = A$id)
```

---

`Manly.var` *Variability assessment of Manly mixture model*

---

## Description

Runs the variability assessment for a Manly mixture model.

## Usage

```
Manly.var(X, model = NULL, conf.CI = NULL)
```

## Arguments

| | |
|---|---|
| `X` | dataset matrix (n x p) |
| `model` | Manly mixture model |
| `conf.CI` | confidence level, say 95 percent confidence |

## Details

Returns the estimated variance-covariance matrix and confidence intervals for model parameter estimates.

## Value

| | |
|---|---|
| `V` | variance-covariance matrix. |
| `CI` | confidence intervals for each parameter. |

## See Also

Manly.EM

## Examples

```
set.seed(123)

#Use iris dataset
K <- 3; p <- 4
X <- as.matrix(iris[,-5])

#Use k-means clustering result
#all skewness parameters set to be 0.1 as the initialization of the EM algorithm
id.km <- kmeans(X, K)$cluster
la <- matrix(0.1, K, p)

#Run the EM algorithm with Manly mixture model
M.EM <- Manly.EM(X, id.km, la)

# Run the variability assessment
Manly.var(X, M.EM, conf.CI = 0.95)
```

---

# seeds *Wheat kernel Data*

---

## Description

The examined group comprised kernels belonging to three different varieties of wheat: Kama, Rosa and Canadian, 70 elements each, randomly selected for the experiment. High quality visualization of the internal kernel structure was detected using a soft X-ray technique. Studies were conducted using combine harvested wheat grain originating from experimental fields, explored at the Institute of Agrophysics of the Polish Academy of Sciences in Lublin.

## Usage

```
data(seeds)
```

## Format

A data frame with 210 observations on the following 7 variables.

**V1** Area A;

**V2** Perimeter P;

**V3** Compactness;

**V4** Length of kernel;

**V5** Width of kernel;

**V6** Asymmetry coefficient;

**V7** Length of kernel groove;

**V8** Seed species: 1, 2, 3

## References

M. Charytanowicz, J. Niewczas, P. Kulczycki, P.A. Kowalski, S. Lukasik, S. Zak (2010), *A Complete Gradient Clustering Algorithm for Features Analysis of X-ray Images*. Information Technologies in Biomedicine, Ewa Pietka, Jacek Kawa, Springer-Verlag, Berlin-Heidelberg.

## Examples

```
data(seeds)
```

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