

## Random cluster generation with known structure of clusters

### Models

#### *Metric data (dataType="m")*

**model=1.** No cluster structure. The observations are simulated from the uniform distribution over the unit hypercube.

**model=2.** The observations are independently drawn from normal distribution with means and covariances are taken from arguments `means` and `cov`.

**model=3.** Two elongated clusters in 2 dimensions. The observations in each of two clusters are independent bivariate normal random variables with means (0, 0), (1, 5), and covariance matrix  $\Sigma$  ( $\sigma_{jj} = 1$ ,  $\sigma_{jl} = -0.9$ ).

**model=4.** Three elongated clusters in 2 dimensions. The observations are independently drawn from bivariate normal distribution with means (0, 0), (1.5, 7), (3, 14) and covariance matrix  $\Sigma$  ( $\sigma_{jj} = 1$ ,  $\sigma_{jl} = -0.9$ ).

**model=5.** Three elongated clusters in 3 dimensions. The observations are independently drawn from multivariate normal distribution with means (1.5, 6, -3), (3, 12, -6), (4.5, 18, -9), and identity covariance matrix  $\Sigma$ , where  $\sigma_{jj} = 1$  ( $1 \leq j \leq 3$ ),  $\sigma_{12} = \sigma_{13} = -0.9$ , and  $\sigma_{23} = 0.9$ .

**model=6.** Five clusters in 2 dimensions that are not well separated. The observations are independently drawn from bivariate normal distribution with means (5, 5), (-3, 3), (3, -3), (0, 0), (-5, -5), and identity covariance matrix  $\Sigma$  ( $\sigma_{jj} = 1$ ,  $\sigma_{jl} = 0.9$ ).

**model=7.** Five clusters in 3 dimensions that are not well separated. The observations are independently drawn from multivariate normal distribution with means (5, 5, 5), (-3, 3, -3), (3, -3, 3), (0, 0, 0), (-5, -5, -5), and covariance matrix  $\Sigma$ , where  $\sigma_{jj} = 1$  ( $1 \leq j \leq 3$ ), and  $\sigma_{jl} = 0.9$  ( $1 \leq j \neq l \leq 3$ ).

**model=8.** Five clusters in 2 dimensions. The observations are independently drawn from bivariate normal distribution with means (0, 0), (0, 10), (5, 5), (10, 0), (10, 10), and identity covariance matrix  $\Sigma$  ( $\sigma_{jj} = 1$ ,  $\sigma_{jl} = 0$ ).

**model=9.** Five clusters in 3 dimensions. The observations are independently drawn from multivariate normal distribution with means (0, 0, 0), (10, 10, 10), (-10, -10, -10), (10, -10, 10), (-10, 10, 10), and identity covariance matrix  $\Sigma$ , where  $\sigma_{jj} = 3$  ( $1 \leq j \leq 3$ ), and  $\sigma_{jl} = 2$  ( $1 \leq j \neq l \leq 3$ ).

**model=10.** Four clusters in 2 dimensions. The observations are independently drawn from bivariate normal distribution with means (-4, 5), (5, 14), (14, 5), (5, -4), and identity covariance matrix  $\Sigma$  ( $\sigma_{jj} = 1$ ,  $\sigma_{jl} = 0$ ).

**model=11.** Four clusters in 3 dimensions. The observations are independently drawn from multivariate normal distribution with means (-4, 5, -4), (5, 14, 5), (14, 5, 14), (5, -4, 5), and identity covariance matrix  $\Sigma$ , where  $\sigma_{jj} = 1$  ( $1 \leq j \leq 3$ ), and  $\sigma_{jl} = 0$  ( $1 \leq j \neq l \leq 3$ ).

**model=12.** Four clusters in 1 dimension. The observations are independently drawn from univariate normal distribution with means -2, 4, 10, 16 respectively, and identity variance  $\sigma_j^2 = 0.5$  ( $1 \leq j \leq 4$ ).

**model=13.** Three elongated clusters in 2 dimensions. The observations are independently drawn from bivariate normal distribution with means (0, 0), (1.5, 7), (3, 14) and covariance matrices  $\Sigma_1 = \begin{bmatrix} 1 & -0.9 \\ -0.9 & 1 \end{bmatrix}$ ,  $\Sigma_2 = \begin{bmatrix} 1.5 & 0 \\ 0 & 1.5 \end{bmatrix}$ ,  $\Sigma_3 = \begin{bmatrix} 1 & 0.5 \\ 0.5 & 1 \end{bmatrix}$ .

**model=14.** Four clusters in 3 dimensions. The observations are independently drawn from multivariate normal distribution with means (-4, 5, -4), (5, 14, 5), (14, 5, 14), (5, -4, 5), and covariance matrices  $\Sigma_1 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$ ,  $\Sigma_2 = \begin{bmatrix} 1 & -0.9 & -0.9 \\ -0.9 & 1 & 0.9 \\ -0.9 & 0.9 & 1 \end{bmatrix}$ ,  $\Sigma_3 = \begin{bmatrix} 1 & 0.9 & 0.9 \\ 0.9 & 1 & 0.9 \\ 0.9 & 0.9 & 1 \end{bmatrix}$ ,  $\Sigma_4 = \begin{bmatrix} 3 & 2 & 2 \\ 2 & 3 & 2 \\ 2 & 2 & 3 \end{bmatrix}$ .

**model=15.** Five clusters in 3 dimensions that are not well separated. The observations are independently drawn from multivariate normal distribution with means (5, 5, 5), (-3, 3, -3), (3, -3, 3), (0, 0, 0), (-5, -5, -5), and covariance matrices  $\Sigma_1 = \begin{bmatrix} 1 & -0.9 & -0.9 \\ -0.9 & 1 & 0.9 \\ -0.9 & 0.9 & 1 \end{bmatrix}$ ,  $\Sigma_2 = \begin{bmatrix} 0.5 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{bmatrix}$ ,

$\Sigma_3 = \begin{bmatrix} 1 & 0.9 & 0.9 \\ 0.9 & 1 & 0.9 \\ 0.9 & 0.9 & 1 \end{bmatrix}$ ,  $\Sigma_4 = \begin{bmatrix} 1 & 0.6 & 0.6 \\ 0.6 & 1 & 0.6 \\ 0.6 & 0.6 & 1 \end{bmatrix}$ ,  $\Sigma_5 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$ .

**model=16.** Two elongated clusters in 2 dimensions. The observations in each of two clusters are independent bivariate normal random variables with means (0, 0), (1, 5), and covariance matrices  $\Sigma_1 = \begin{bmatrix} 1 & -0.9 \\ -0.9 & 1 \end{bmatrix}$ ,  $\Sigma_2 = \begin{bmatrix} 1 & 0.5 \\ 0.5 & 1 \end{bmatrix}$ .

**model=21, 22, ...** - if `fixedCov=TRUE` means should be read from `means_<modelName>.csv` and covariance matrix for all clusters should be read from `cov_<modelName>.csv` and if `fixedCov=FALSE` means should be read from `means_<modelName>.csv` and covariance matrices should be read separately for each cluster from `cov_<modelName>_<clusterNumber>.csv`, e.g. (`inputType="csv"`)

<i>means_21.csv</i>	<i>cov_21_1.csv</i>	<i>cov_21_2.csv</i>
"V1", "V2"	"V1", "V2"	"V1", "V2"
"1", 4, 8	"1", 1.0, 0.9	"1", 1.0, -0.9
"2", 0, 4	"2", 0.9, 1.0	"2", -0.9, 1.0

**Ordinal data (dataType="o").** The clusters in models 1, 2, ... contain continuous data and a discretization process is performed on each variable to obtain ordinal data. The number of categories  $k$  determines the width of each class intervals:  $\left\lceil \frac{\max_i \{x_{ij}\} - \min_i \{x_{ij}\}}{k} \right\rceil$ . Independently for each variable each class interval receive category  $1, \dots, k$  and the actual value of variable  $x_{ij}$  is replaced by these categories.

**Symbolic interval data (dataType="s").** To obtain symbolic interval data the data were generated for each model twice into sets  $A$  and  $B$  and minimal (maximal) value of  $\{a_{ij}, b_{ij}\}$  is treated as the beginning (the end) of an interval.

**Noisy variables.** The noisy variables are simulated independently from the uniform distribution. We require that the variations of noisy variables in the generated data are similar to non-noisy variables (see Milligan [1985], Qiu and Joe [2006], p. 322).

**Outliers** (for metric and symbolic interval data only). The outliers are generated independently for each variable for the whole data set from uniform distribution (the default range is [1, 10]). The generated values are randomly added to maximum of  $j$ -th variable or subtracted from minimum of  $j$ -th variable.

## References

- Qiu, W., Joe, H. (2006), *Generation of random clusters with specified degree of separation*, “Journal of Classification”, vol. 23, 315-334.
- Steinley, D., Henson, R. (2005), *OCCLUS: an analytic method for generating clusters with known overlap*, “Journal of Classification”, vol. 22, 221-250.
- Walesiak, M., Dudek, A. (2007), *Identification of noisy variables for nonmetric and symbolic data in cluster analysis*, In: Data Analysis, Machine Learning, and Applications, Springer-Verlag, Berlin, Heidelberg (in press).