FlexMix: Flexible fitting of finite mixtures with the EM algorithm

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Finite mixture models
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The finite mixture density is given by

\[
h(y|x, w, \psi) = \sum_{k=1}^{K} \pi_k(w, \alpha) f_k(y|x, \theta_k)
\]

\[
= \sum_{k=1}^{K} \pi_k(w, \alpha) \prod_{d=1}^{D} f_{kd}(y_d|x_d, \theta_{kd}),
\]

with

\[
\forall w : \sum_{k=1}^{K} \pi_k(w, \alpha) = 1 \land \pi_k(w, \alpha) > 0 \forall k.
\]

The posterior probabilities are given by

\[
\tau_k(y|x, \psi) = \frac{\pi_k(w, \alpha) f_k(y|x, \theta_k)}{\sum_{l=1}^{K} \pi_l(w, \alpha) f_l(y|x, \theta_l)}.
\]
**EM algorithm**

- General method for ML estimation in a missing data setting
  → component membership
- Iterates between
  - **E-step:** determines the a-posteriori probabilities
  - **M-step:** maximizes the complete likelihood where the missing component memberships are replaced
    → weighted ML problem of the component specific model and the concomitant variable model
- Likelihood is increased in each step
  → converges to a local optimum if the likelihood is bounded
- Variants: additional step between E- and M-step
  - **Stochastic EM (SEM):** assigns each observation to one component by drawing from the multinomial distribution induced by the a-posteriori probabilities
  - **Classification EM (CEM):** assigns each observation to the component with the maximum a-posteriori probability
FlexMix Design

- Primary goal is extensibility: ideal for trying out new mixture models
- No replacement of specialized mixture packages like `mclust`, but complement
- Usage of S4 classes and methods
- Formula-based interface
- Multivariate responses:
  - **Combination of univariate families**: assumption of independence (given \(x\)), each response may have its own model formula, i.e., a different set of regressors
  - **multivariate families**: if family handles multivariate response directly, then arbitrary multivariate response distributions are possible
Fit function \texttt{flexmix()}

- \texttt{flexmix()} takes the following arguments:
  - \texttt{formula}: A symbolic description of the model to be fit. The general form is \( y \sim x | g \) where \( y \) is the response, \( x \) the set of predictors and \( g \) an optional grouping factor for repeated measurements.
  - \texttt{data}: An optional data frame containing the variables in the model.
  - \texttt{k}: Number of clusters (not needed if \texttt{cluster} is specified).
  - \texttt{cluster}: Either a matrix with \( k \) columns of initial cluster membership probabilities for each observation; or a factor or integer vector with the initial cluster assignments of observations.
  - \texttt{model}: Object of class "FLXM" or list of these objects.
  - \texttt{concomitant}: Object of class "FLXP".
  - \texttt{control}: Object of class "FLXcontrol" or a named list.
    - repeated calls of \texttt{flexmix()} with \texttt{stepFlexmix()}
    - returns an object of class "flexmix"
Controlling the EM algorithm

- "FLXcontrol": for the overall behaviour of the EM algorithm:
  - iter.max: Maximum number of iterations
  - minprior: Minimum prior probability for components
  - verbose: If larger than zero, then `flexmix()` gives status messages each verbose iterations.
  - classify: One of “auto”, “weighted”, “CEM” (or “hard”), “SEM” (or “random”).

For convenience `flexmix()` also accepts a named list of control parameters with argument name completion, e.g.

```
flexmix(..., control=list(class="r"))
```
Variants of mixture models

Component specific models: \texttt{FLXMxxx()}

- Model-based clustering: \texttt{FLXMCxxx()}
  - \texttt{FLXMCmvnorm()}
  - \texttt{FLXMCmvbinary()}
  - \texttt{FLXMCmvpois()}
  - ...
- Clusterwise regression: \texttt{FLXMRxxx()}
  - \texttt{FLXMRglm()}
  - \texttt{FLXMRglmfix()}
  - \texttt{FLXMRziglm()}
  - ...

Concomitant variable models: \texttt{FLXPxxx()}

- \texttt{FLXPconstant()}
- \texttt{FLXPmultinom()}
Methods for "flexmix" objects

- `show()`, `summary()`: some information on the fitted model
- `plot()`: rootogram of posterior probabilities
- `refit()`: refits an estimated mixture model to obtain other additional information, such as for example the variance-covariance matrix
- `logLik()`, `BIC()`, ...: obtain log-likelihood and model fit criteria
- `parameters()`, `priors()`: obtain component specific or concomitant variable model parameters and prior class probabilities/component weights
- `posteriors()`, `clusters()`: obtain a-posteriori probabilities and assignments to the maximum a-posteriori probability
- `fitted()`, `predict()`: fitted and predicted (component-specific) values
Example: artificial data

- 200 observations from a mixture given by

\[
h(y|x, \psi) = \frac{1}{2}\text{Normal}(yn|15 + 10x - x^2, 9)\text{Poi}(yp|e^{1+0.1x}) + \\
+ \frac{1}{2}\text{Normal}(yn|5x, 9)\text{Poi}(yp|e^{2-0.2x})
\]

where \(\text{Normal}(y|\mu, \sigma^2)\) is the Gaussian distribution and \(\text{Poi}(y|\lambda)\) the Poisson distribution.
Example: artificial data
Example: artificial data

```r
> set.seed(1802)
> library("flexmix")
> data("NPreg")
> Model_n <- FLXMRglm(yn ~ . + I(x^2))
> Model_p <- FLXMRglm(yp ~ ., family = "poisson")
> m1 <- flexmix(. ~ x, data = NPreg, k = 2, model = list(Model_n, Model_p),
+                control = list(verbos...e = 10))

Classification: weighted
   10 Log-likelihood :  -1044.7688
   11 Log-likelihood :  -1044.7678
converged
> m1
Call:
  flexmix(formula = . ~ x, data = NPreg, k = 2, model = list(Model_n,
                 Model_p), control = list(verbos...e = 10))

Cluster sizes:
   1  2
   96 104

convergence after 11 iterations
```
Example: artificial data

```r
> summary(m1)
Call:
flexmix(formula = . ~ x, data = NPreg, k = 2, model = list(Model_n,
   Model_p), control = list(verbse = 10))

prior size post>0 ratio
Comp.1 0.493 96   139 0.691
Comp.2 0.507 104  137 0.759

'log Lik.' -1044.768 (df=13)
AIC: 2115.536    BIC: 2158.414
> plot(m1)
```
Example: artificial data

Rootogram of posterior probabilities $> 1e^{-04}$

Comp. 1

Comp. 2
Example: artificial data

```r
> m1_refit <- refit(m1)
> summary(m1_refit, which = "model", model = 1)

$Comp.1

|                | Estimate | Std. Error | z value | Pr(>|z|) |
|----------------|----------|------------|---------|----------|
| (Intercept)    | 14.58965 | 1.24635    | 11.706  | < 2.2e-16 *** |
| x              | 9.91572  | 0.55294    | 17.933  | < 2.2e-16 *** |
| I(x^2)         | -0.97578 | 0.05201    | -18.762 | < 2.2e-16 *** |

---

Signif. codes:  0 *** 0.001 ** 0.01 * 0.05 . 0.1 1

$Comp.2

|                | Estimate | Std. Error | z value | Pr(>|z|) |
|----------------|----------|------------|---------|----------|
| (Intercept)    | -0.140549| 0.961868   | -0.1461 | 0.8838   |
| x              | 4.732610 | 0.474428   | 9.9754  | < 2e-16 *** |
| I(x^2)         | 0.042722 | 0.046890   | 0.9111  | 0.3622   |

---

Signif. codes:  0 *** 0.001 ** 0.01 * 0.05 . 0.1 1

> plot(m1_refit, bycluster = FALSE)
```
Example: artificial data
Example: artificial data

> summary(m1_refit, which = "model", model = 2)

$Comp.1

        Estimate Std. Error z value  Pr(>|z|)  
(Intercept) 1.037805   0.113005  9.1837 < 2.2e-16 ***
x          0.091034   0.017994  5.0592  4.21e-07 ***
---
Signif. codes:  0 *** 0.001 ** 0.01 * 0.05 . 0.1  1

$Comp.2

        Estimate Std. Error z value  Pr(>|z|)  
(Intercept) 1.939213   0.088046 22.0249 < 2.2e-16 ***
x       -0.180959   0.020856 -8.6767 < 2.2e-16 ***
---
Signif. codes:  0 *** 0.001 ** 0.01 * 0.05 . 0.1  1

> plot(m1_refit, model = 2, bycluster = FALSE)
Example: artificial data
Example: artificial data

```r
> Model_n2 <- FLXMRglmfix(yn ~ . + 0, nested = list(k = c(1, 1),
+ formula = c(~ 1 + I(x^2), ~ 0)))
> m2 <- flexmix(. ~ x, data = NPreg, cluster = posterior(m1),
+ model = list(Model_n2, Model_p))
> m2
Call:
flexmix(formula = . ~ x, data = NPreg, cluster = posterior(m1),
    model = list(Model_n2, Model_p))

Cluster sizes:
  1  2
 96 104

convergence after 3 iterations

> c(BIC(m1), BIC(m2))
[1] 2158.414 2149.956
```
Example: artificial data
**Example: patent data**

given in Wang, Cockburn and Puterman (1998)

- 70 observations from pharmaceutical and biomedical companies in 1976 taken from the National Bureau of Economic Research R&D Masterfile
- Variables:
  - number of patent applications
  - R&D spending
  - sales in millions

\[
h(\text{Patents} \mid \text{lgRD}, \text{RDS}, \psi) = \sum_{s=1}^{S} \pi_s(\text{RDS}, \alpha) \text{Poi}(\text{Patents} \mid \lambda_s) \\
\log(\lambda_s) = \beta_1^s + \text{lgRD} \cdot \beta_2^s
\]
Example: patent data
Example: `patent data`

```r
> data("patent")
> Conc <- FLXPmultinom(~ RDS)
> (m_step <- stepFlexmix(Patents ~ lgRD, k = 2:5, nrep = 5,
+                      concomitant = Conc, data = patent,
+                      model = FLXMRglm(family = "poisson")))
2 : * * * * *
3 : * * * * *
4 : * * * * *
5 : * * * * *

Call:
stepFlexmix(Patents ~ lgRD, concomitant = Conc, data = patent,
model = FLXMRglm(family = "poisson"), k = 2:5, nrep = 5)

iter converged k k0 logLik  AIC   BIC    ICL
 2   26      TRUE  2   2  -218.4911 448.9822 462.4731 473.6855
 3   29      TRUE  3   3  -197.6752 415.3504 437.8354 453.5647
 4   39      TRUE  4   4  -193.8785 415.7571 447.2360 471.2140
 5   37      TRUE  5   5  -192.6904 421.3808 461.8537 512.0378
```
Example: patent data

> (m1 <- getModel(m_step, "BIC"))
Call:
stepFlexmix(Patents ~ lgRD, concomitant = Conc, data = patent,
    model = FLXMRglm(family = "poisson"), k = 3, nrep = 5)

Cluster sizes:
  1  2  3
13 45 12

corvergence after 29 iterations
Example: patent data
Example: patent data

```r
> m1_refit <- refit(m1)
> summary(m1_refit, which = "concomitant")

$Comp.2

| Estimate | Std. Error | z value | Pr(>|z|) |
|----------|------------|---------|----------|
| (Intercept) | 3.10653 | 0.87491 | 3.5507 | 0.0003842 *** |
| RDS | -40.99625 | 16.09568 | -2.5470 | 0.0108642 * |

---

Signif. codes: 0 *** 0.001 ** 0.01 * 0.05 . 0.1 1

$Comp.3

| Estimate | Std. Error | z value | Pr(>|z|) |
|----------|------------|---------|----------|
| (Intercept) | 0.21385 | 0.52411 | 0.4080 | 0.6833 |
| RDS | -0.74566 | 1.01832 | -0.7322 | 0.4640 |

> plot(m1_refit, which = "concomitant")
```
Example: *patent data*
Summary

- **FlexMix** offers an easy and extensible way of EM-based estimation of finite mixture models in R.
  ⇒ Users are able to write their own model drivers to fit new variants of mixture models.
- **FlexMix** currently contains only interpreted code.
  ⇒ An efficient M-step is crucial to fit large models in reasonable time.
  ⇒ Popular models are re-implemented in C by Arijit Das as a “Google Summer of Code 2008” project.

For more information see

http://cran.r-project.org/package=flexmix.