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FlexMix: Flexible fitting of finite mixtures with the EM algorithm

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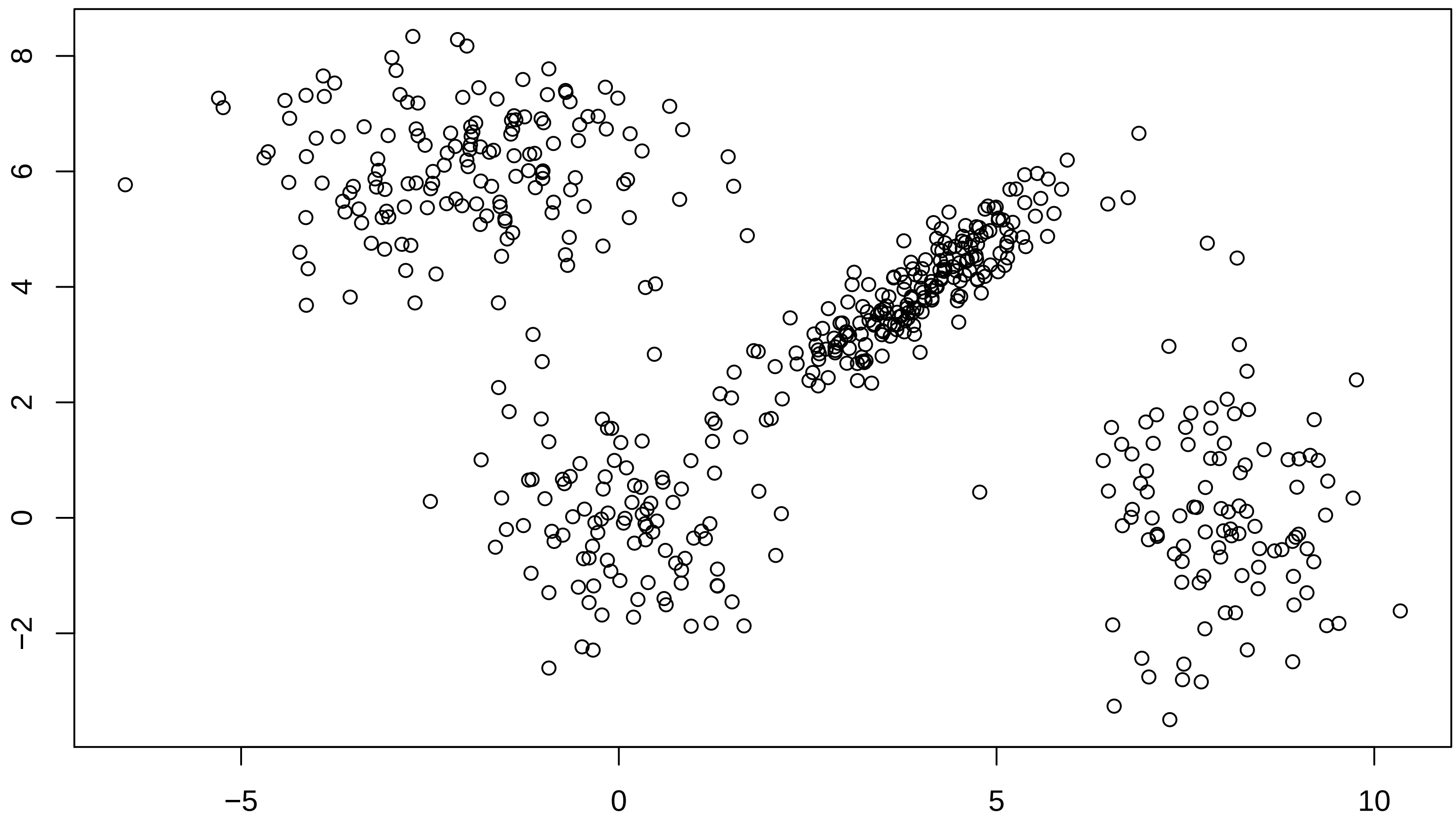
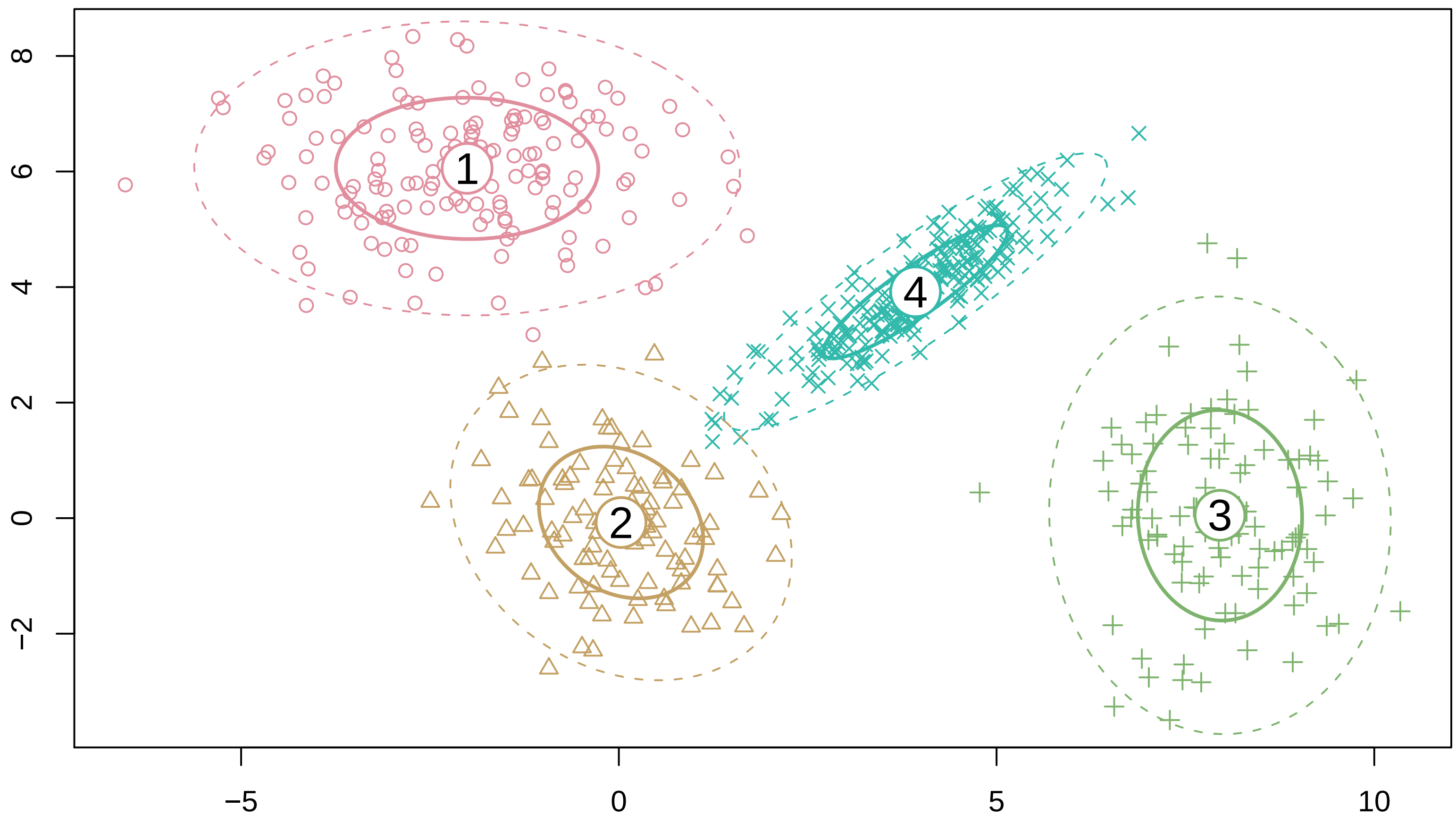
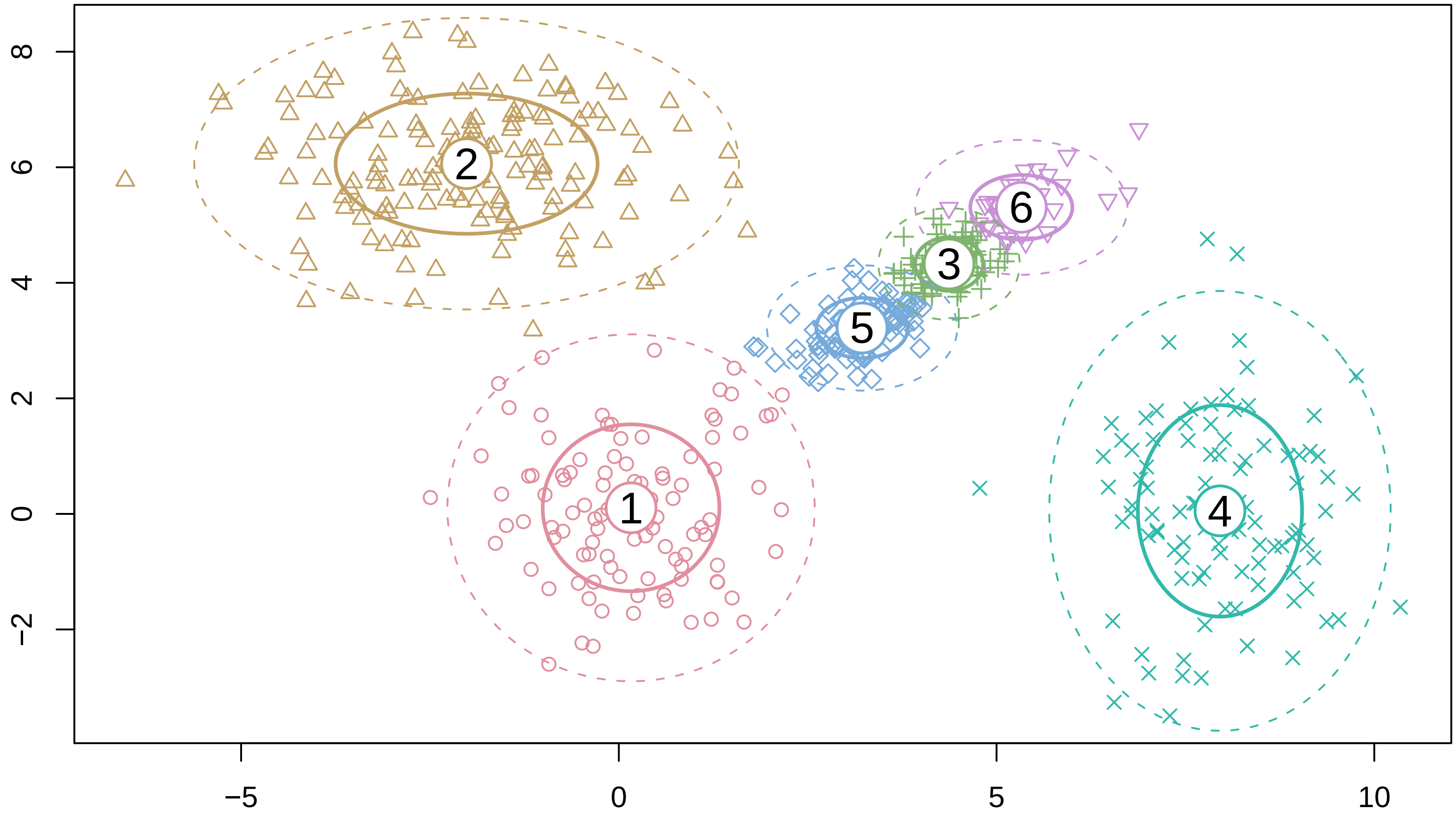
Finite mixture models



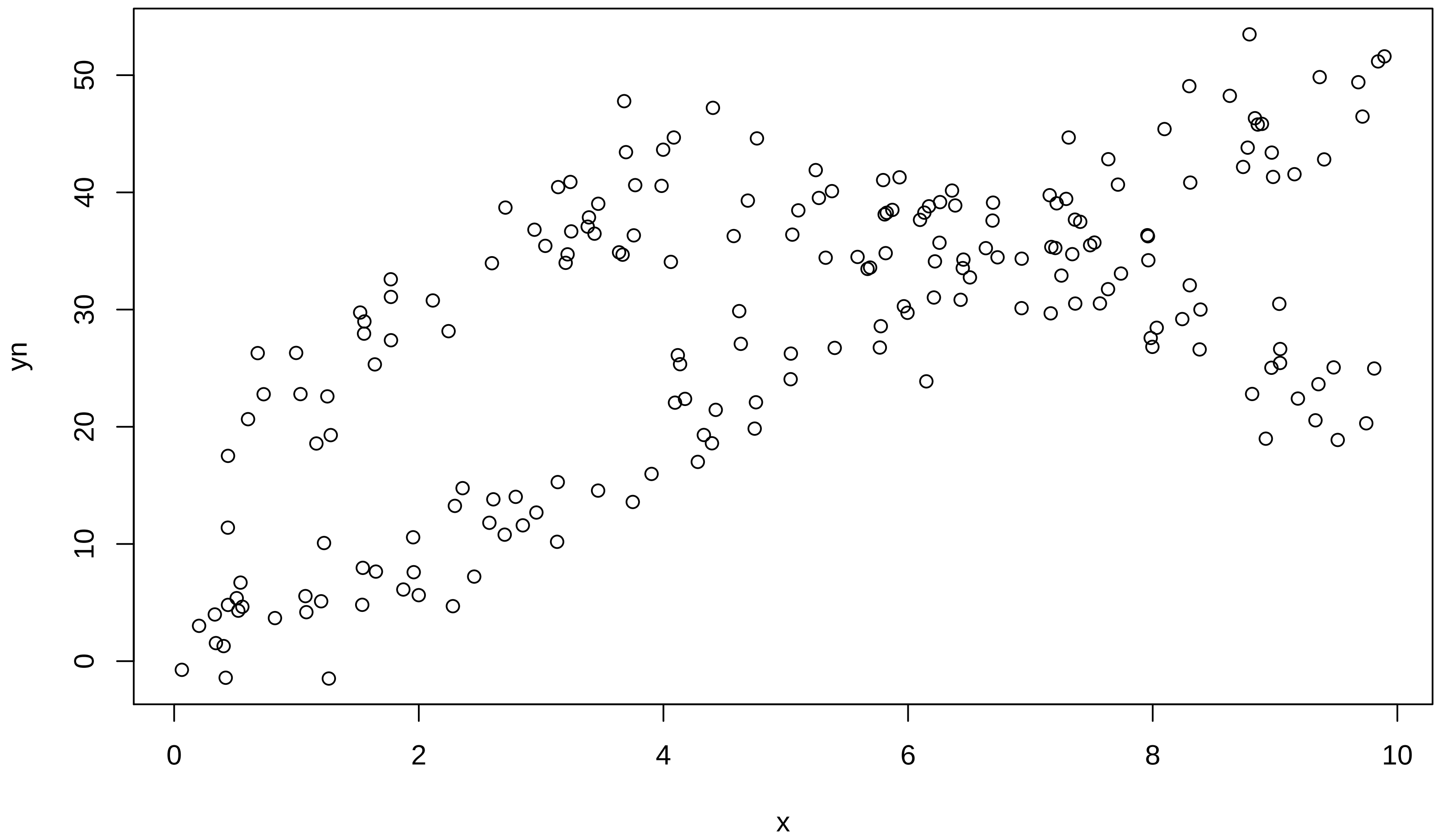
Finite mixture models



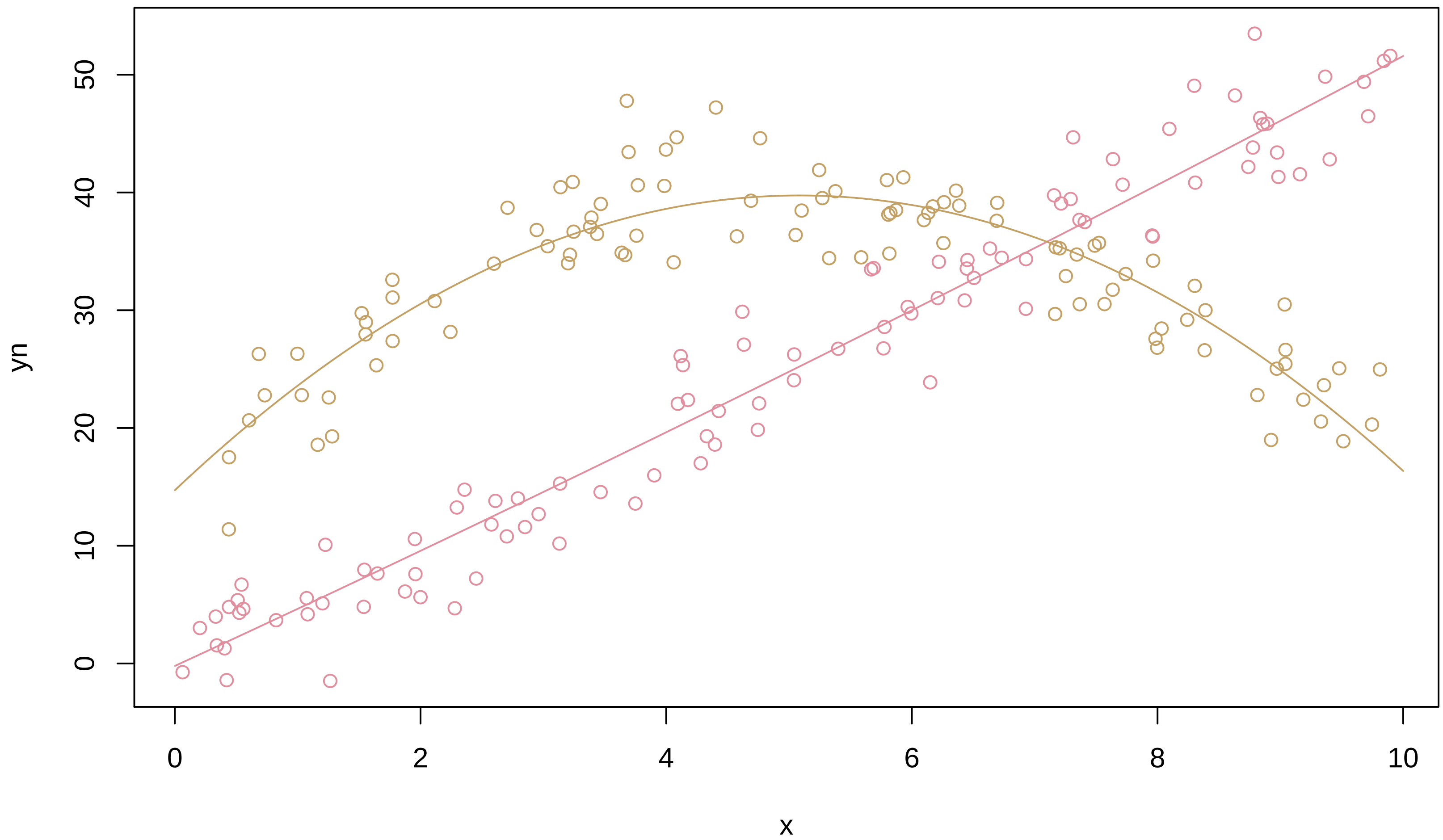
Finite mixture models



Finite mixture models



Finite mixture models



Finite mixture models

The finite mixture density is given by

$$
\begin{aligned}
h(y|x, w, \psi) &= \sum_{k=1}^{K} \pi_k(w, \alpha) f_k(y|x, \theta_k) \\
&= \sum_{k=1}^{K} \pi_k(w, \alpha) \prod_{d=1}^{D} f_{kd}(y_d|x_d, \theta_{kd}),
\end{aligned}
$$

with

$$
\forall w : \sum_{k=1}^{K} \pi_k(w, \alpha) = 1 \quad \wedge \quad \pi_k(w, \alpha) > 0 \, \forall k.
$$

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
  $\longrightarrow$ component membership
- Iterates between

  E-step: determines the a-posteriori probabilities

  M-step: maximizes the complete likelihood where the missing component memberships are replaced
  $\longrightarrow$ weighted ML problem of the component specific model and the concomitant variable model
- Likelihood is increased in each step
  $\longrightarrow$ 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 `flexmix()`

- `flexmix()` takes the following arguments:

  formula: A symbolic description of the model to be fit. The general form is `y~x|g` where `y` is the response, `x` the set of predictors and `g` an optional grouping factor for repeated measurements.

  data: An optional data frame containing the variables in the model.

  k: Number of clusters (not needed if `cluster` is specified).

  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.

  model: Object of class `"FLXM"` or list of these objects.

  concomitant: Object of class `"FLXP"`.

  control: Object of class `"FLXcontrol"` or a named list.

  - repeated calls of `flexmix()` with `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: `FLXMxxx()`

- Model-based clustering: `FLXMCxxx()`
  - `FLXMCmvnorm()`
  - `FLXMCmvbinary()`
  - `FLXMCmvpois()`
  - ...
- Clusterwise regression: `FLXMRxxx()`
  - `FLXMRglm()`
  - `FLXMRglmfix()`
  - `FLXMRziglm()`
  - ...

Concomitant variable models: `FLXPxxx()`

- `FLXPconstant()`
- `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

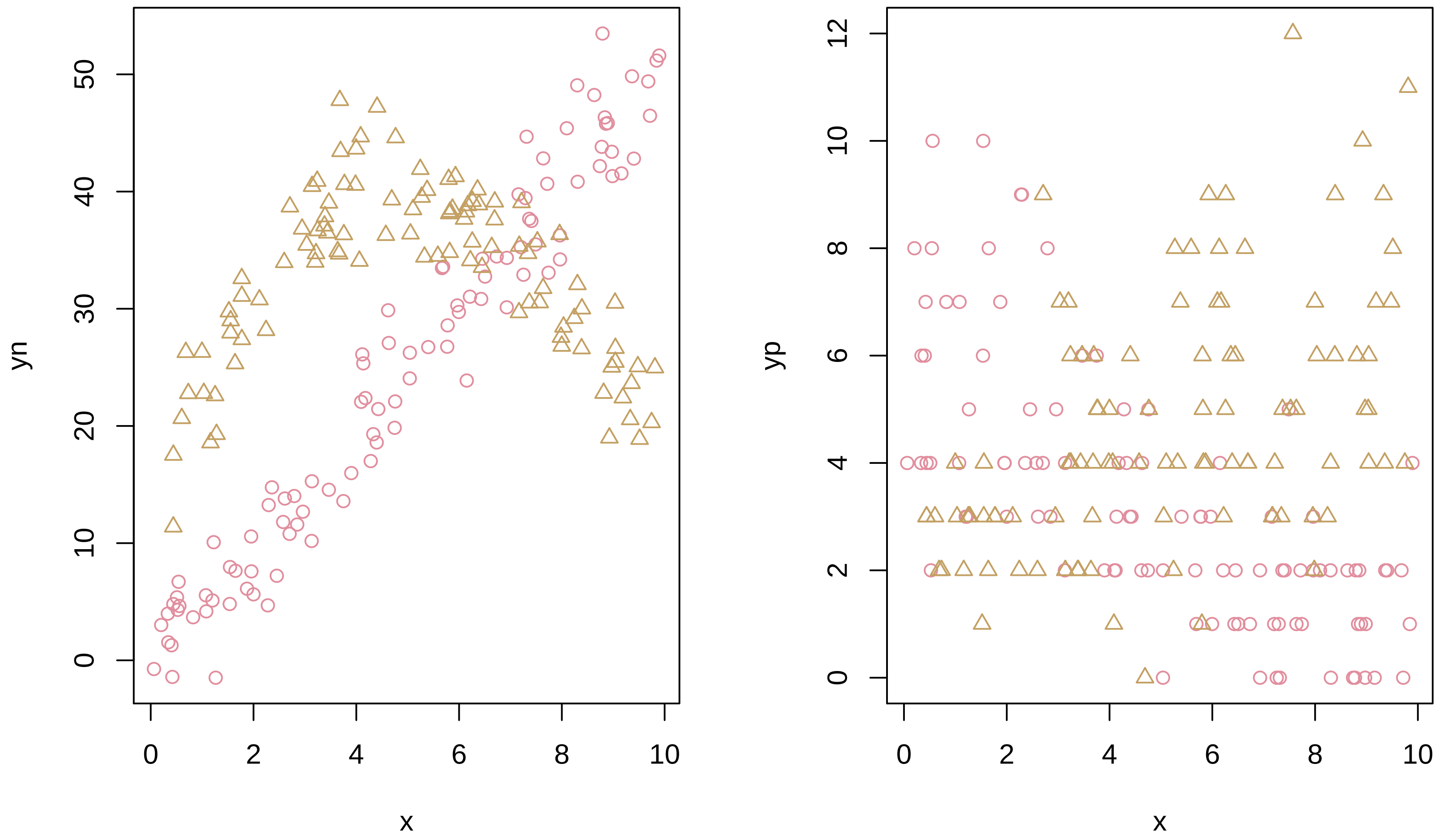
Example: artificial data

- 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 Normal$(y|\mu, \sigma^2)$ is the Gaussian distribution and Poi$(y|\lambda)$ the Poisson distribution.

Example: artificial data



Example: artificial data

```
> 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(verbose = 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(verbose = 10))

Cluster sizes:
  1   2
 96 104

convergence after 11 iterations
```

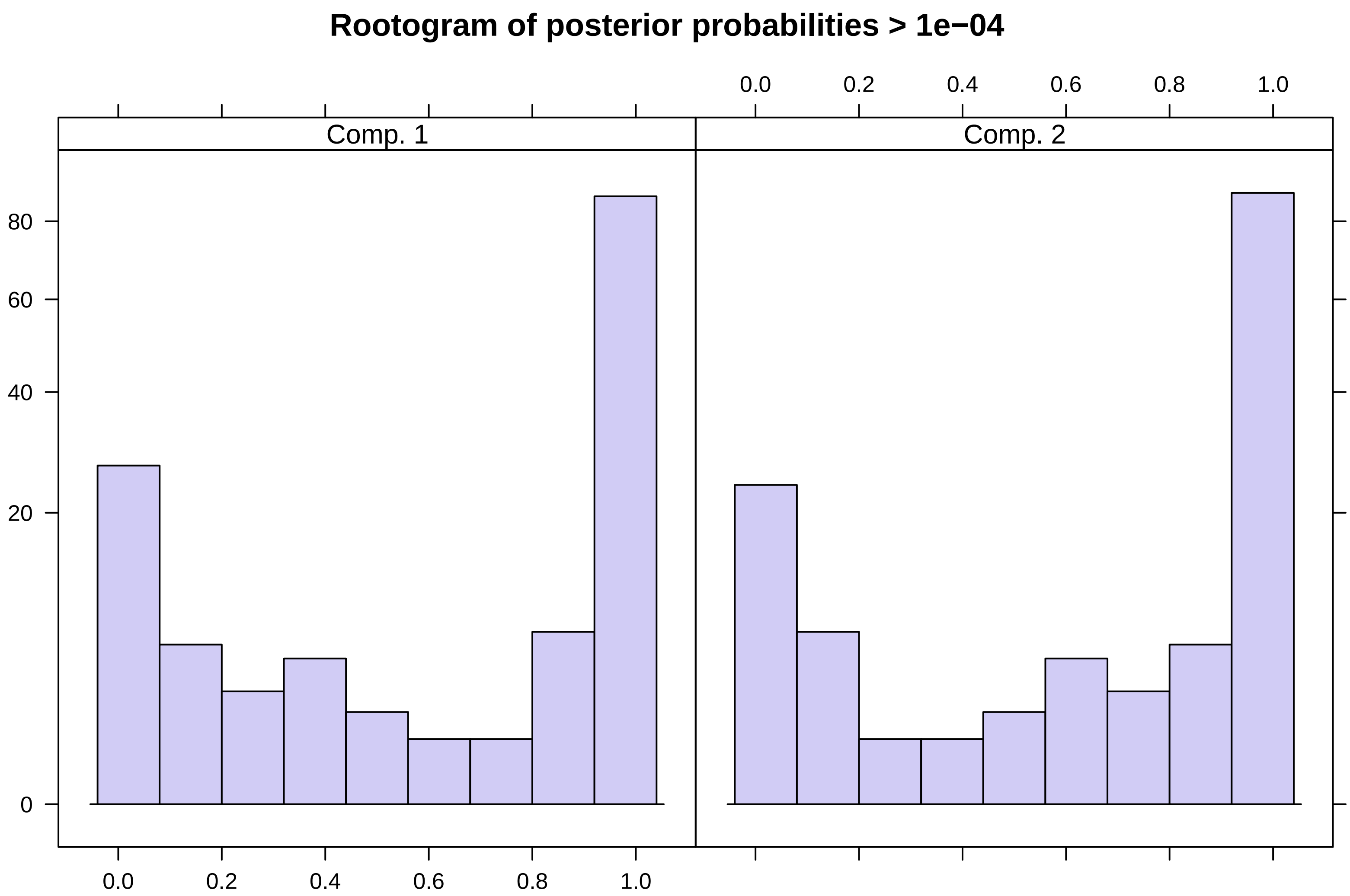
Example: artificial data

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

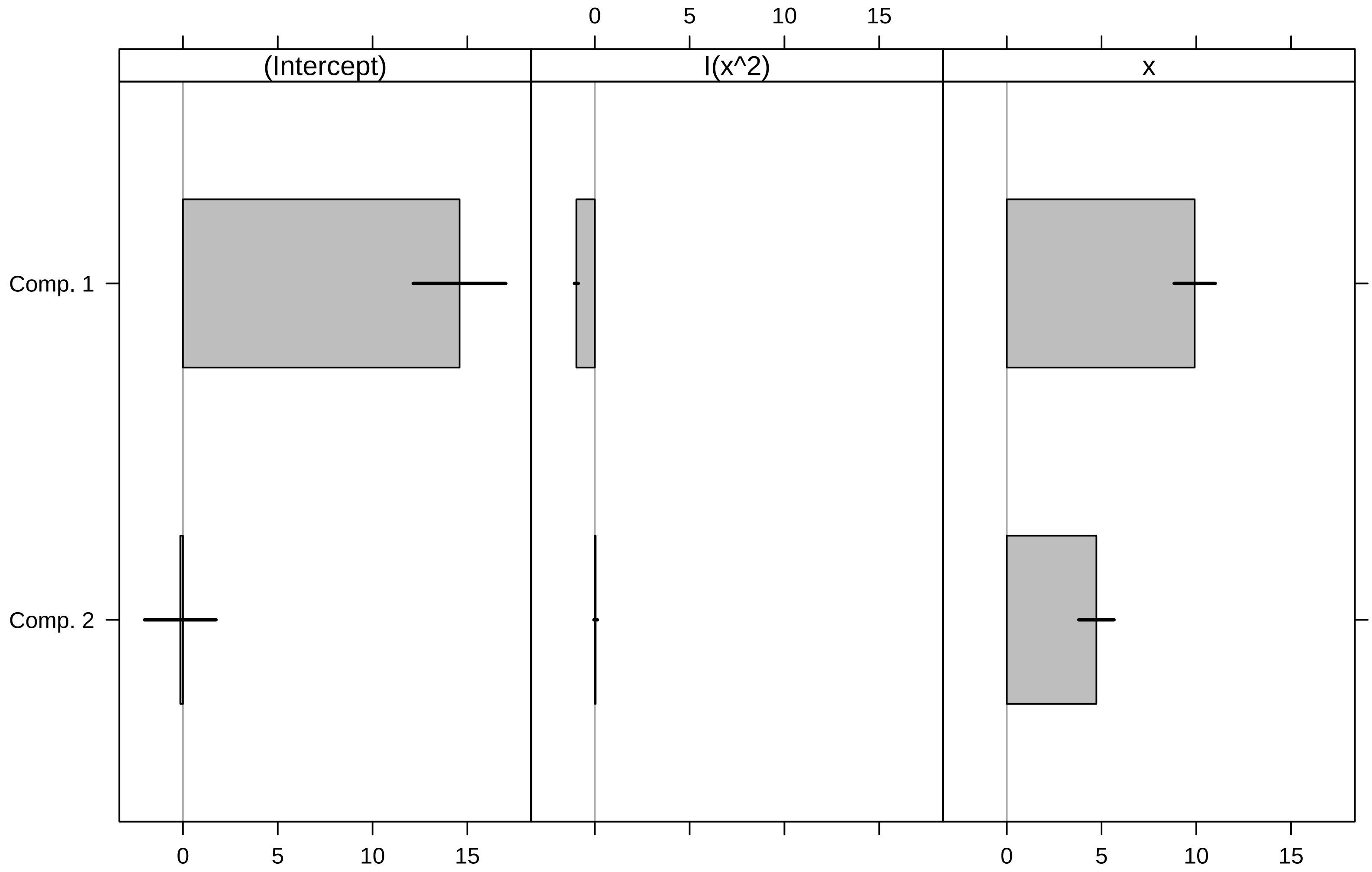


Example: artificial data

```
> 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

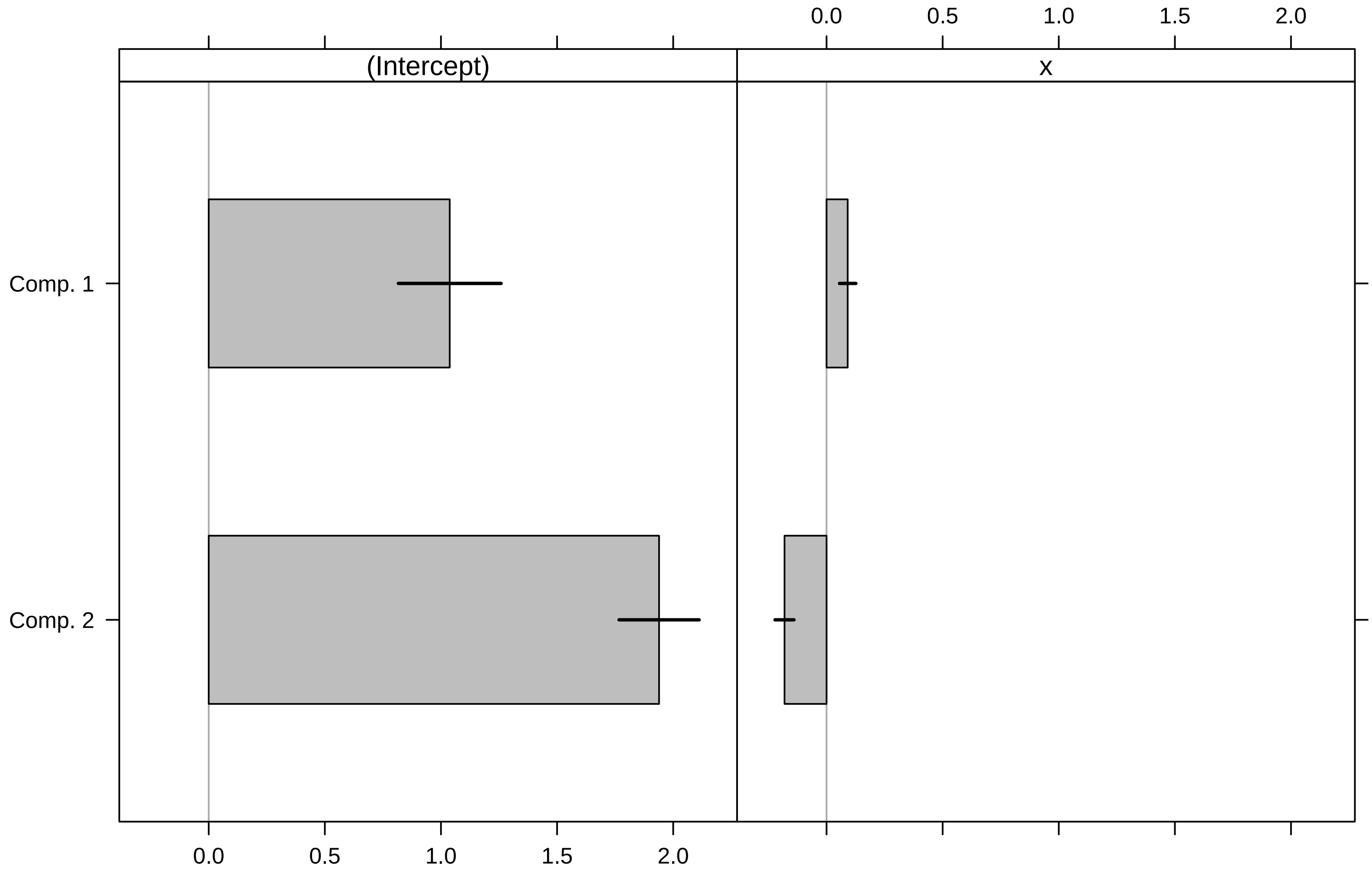


Example: artificial data

```
> 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

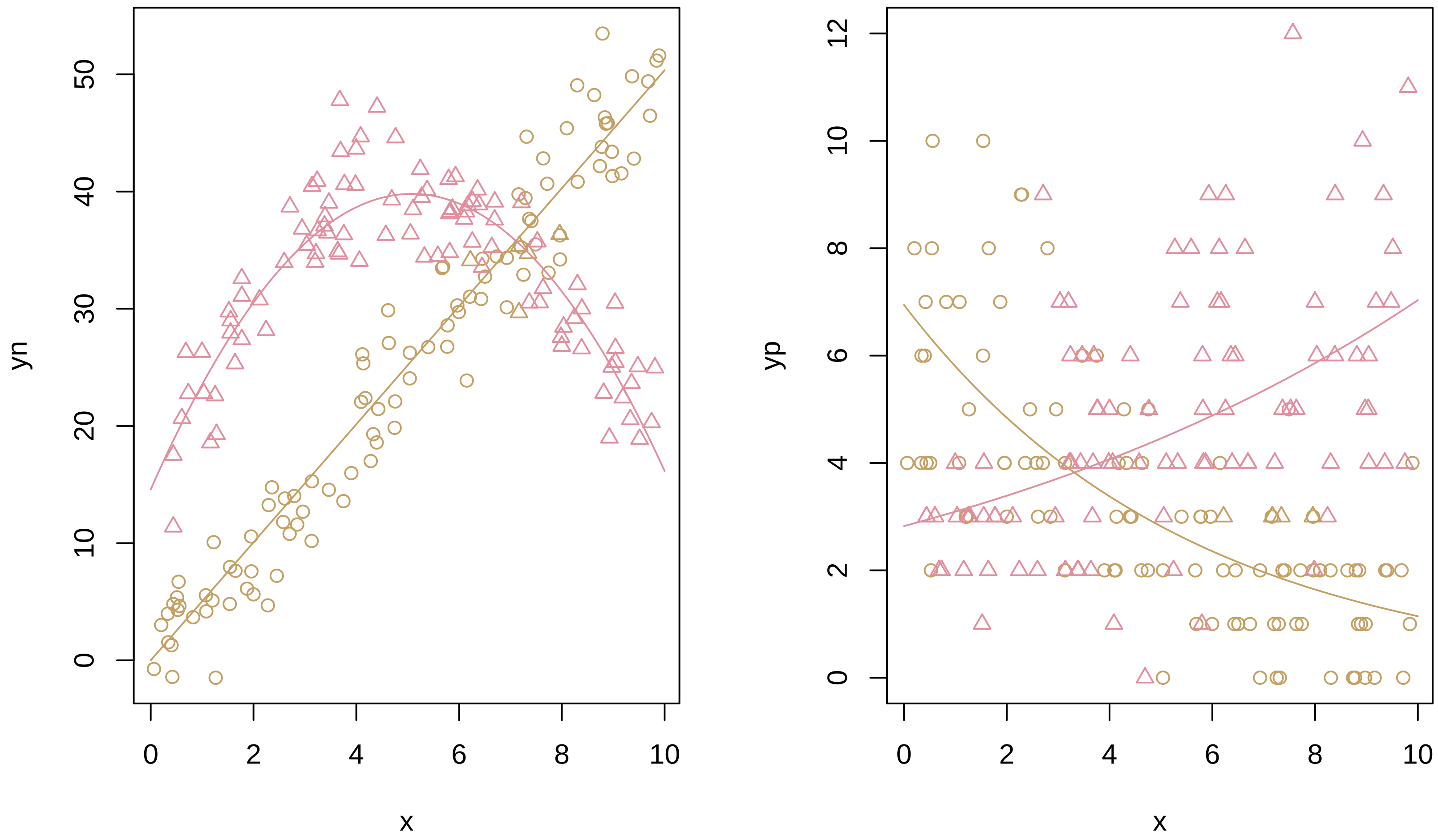
```
> Model_n2 <- FLXMRglmfix(yn ~ . + 0, nested = list(k = c(1, 1),
+                                        formula = c(~ 1 + I(x^2), ~ 0)))
> m2 <- flexmix(. ~ x, data = NPreg, cluster = posterior(m1),
+               model = list(Model_n2, Model_p))
> m2
Call:
flexmix(formula = . ~ x, data = NPreg,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



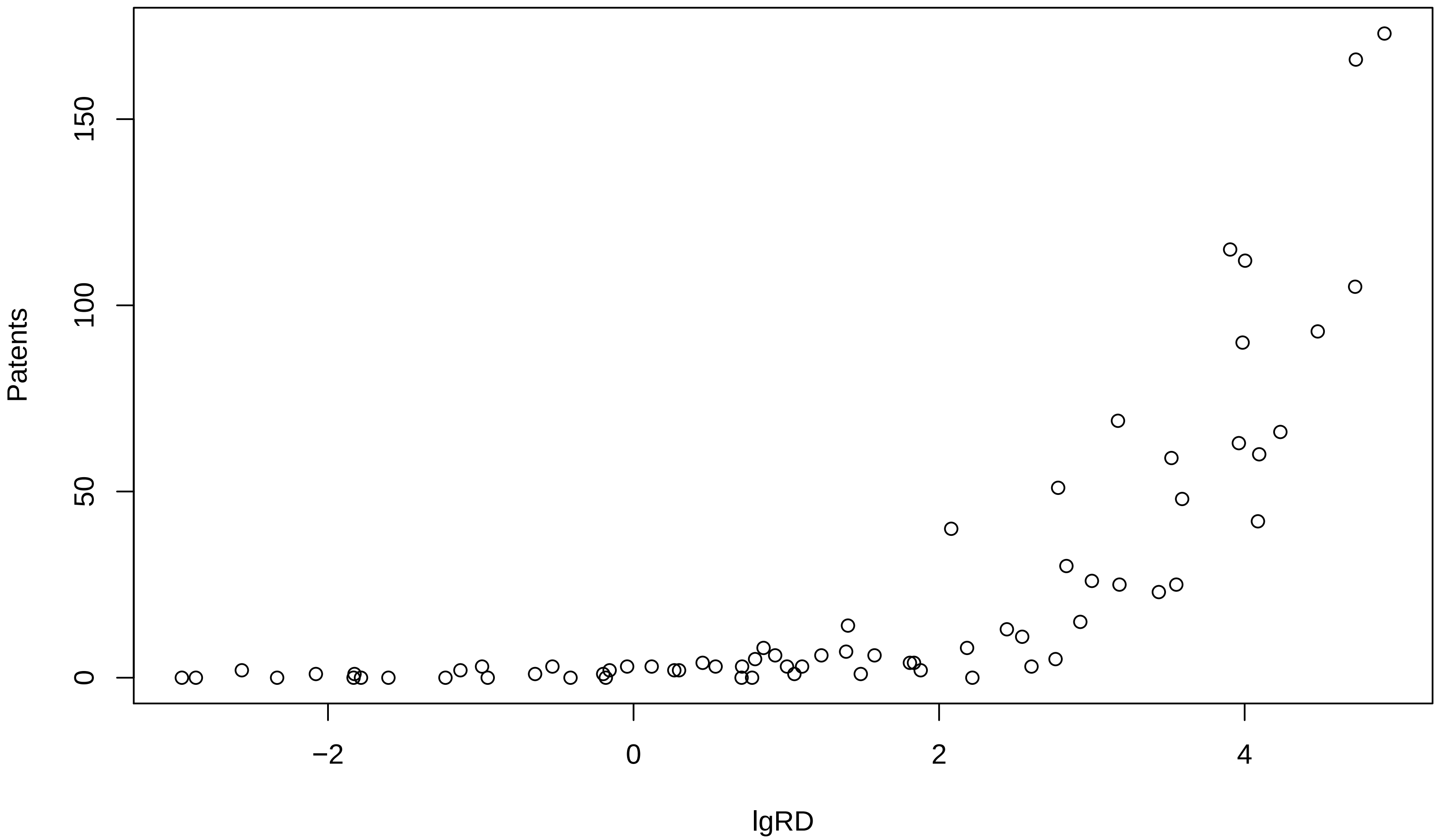
Example: `patent` **data**

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

$$
\begin{aligned}
h(\text{Patents} \mid \text{lgRD}, \text{RDS}, \psi) &= \sum_{s=1}^{S} \pi_s(\text{RDS}, \alpha) \text{Poi}(\text{Patents} \mid \lambda_s) \\
\log(\lambda_s) &= \beta_1^s + \text{lgRD} \cdot \beta_2^s
\end{aligned}
$$

Example: `patent` data



Example: `patent` data

```
> 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
```

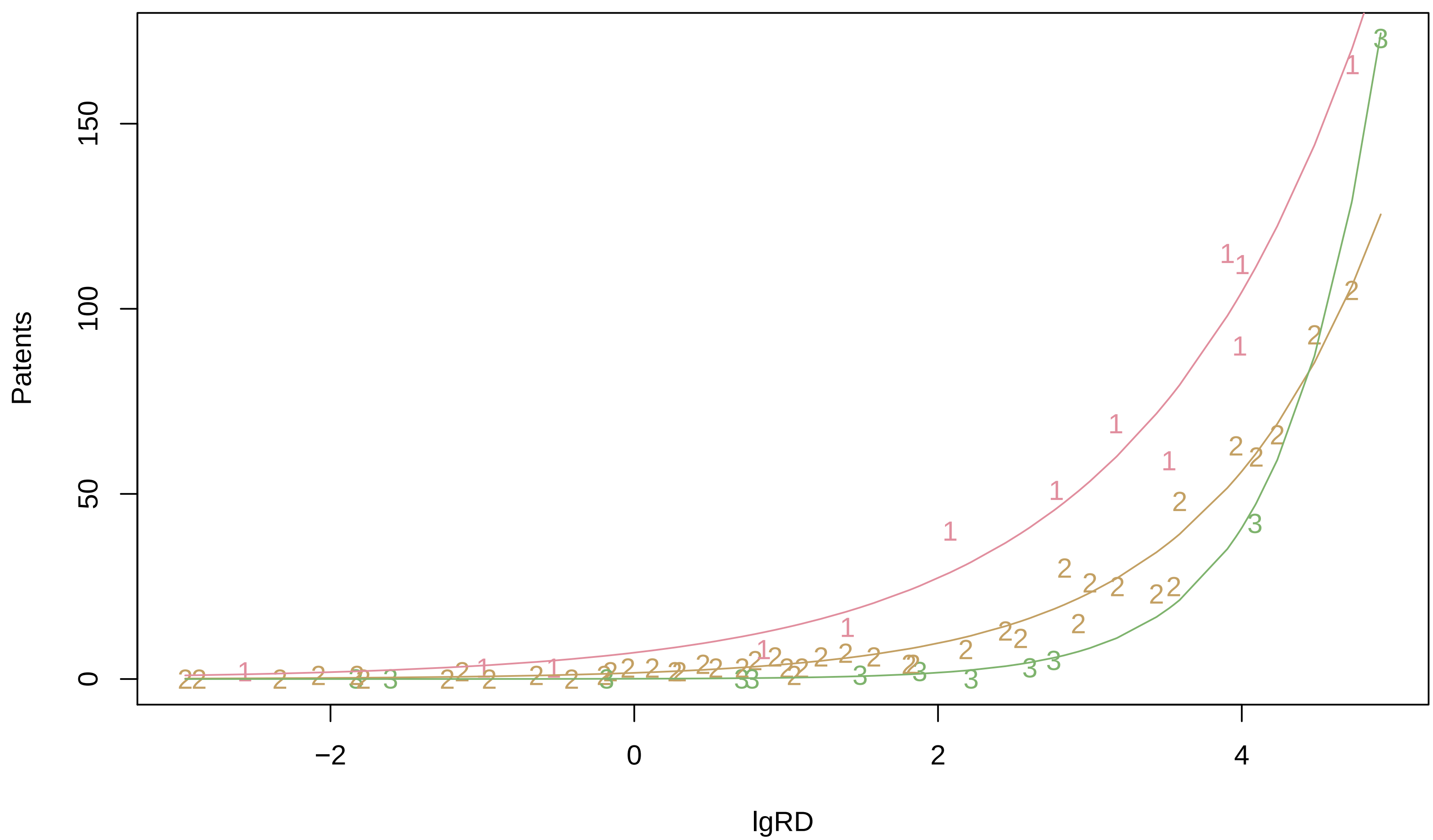
Example: `patent` data

```
> (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

convergence after 29 iterations
```

Example: `patent` data

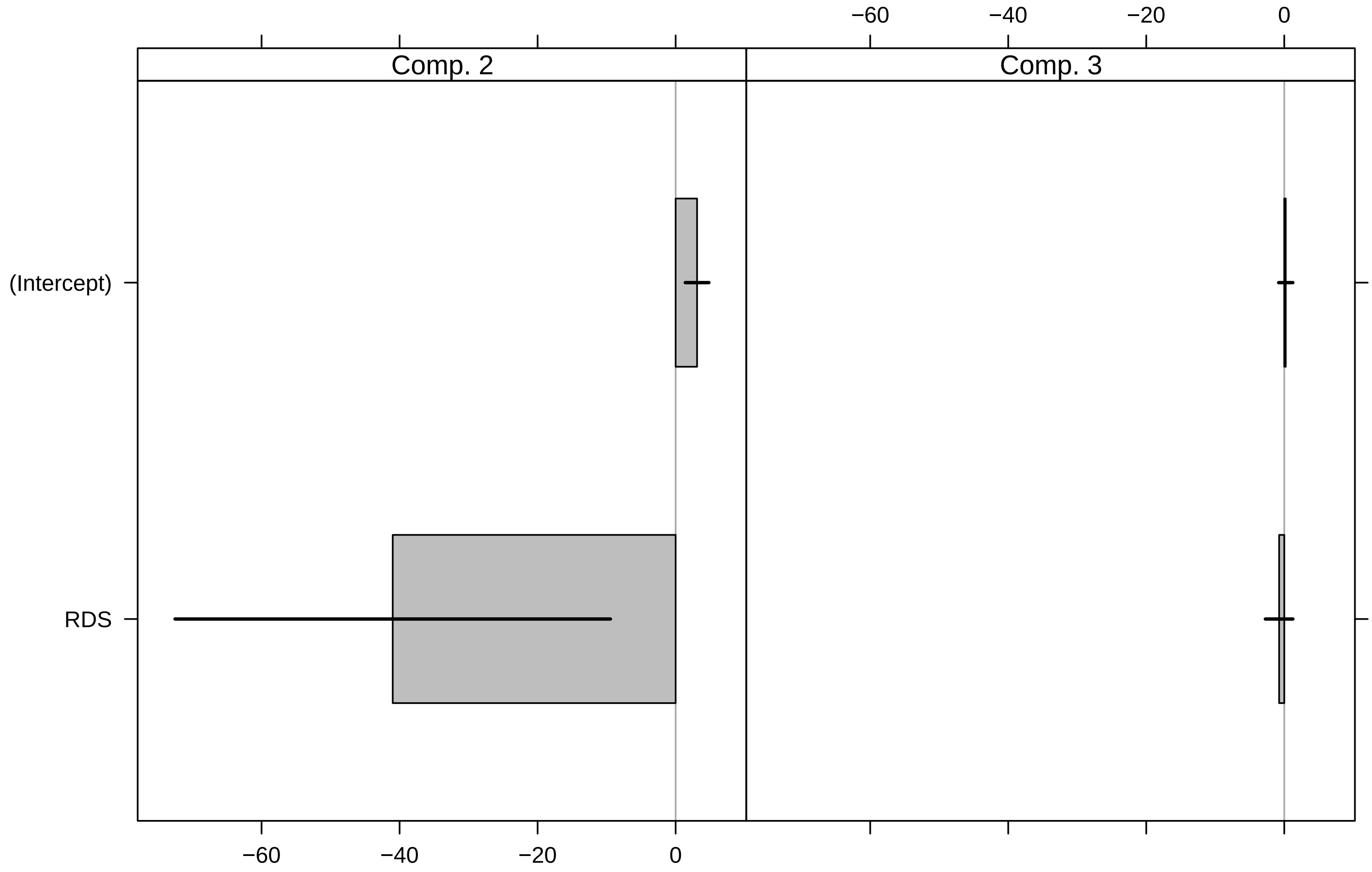


Example: patent data

```
> 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.
  $\Rightarrow$ Users are able to write their own model drivers to fit new variants of mixture models.
- **FlexMix** currently contains only interpreted code.
  $\Rightarrow$ An efficient M-step is crucial to fit large models in reasonable time.
  $\Rightarrow$ 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`.