Package: BinaryReplicates (via r-universe)

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Title Dealing with Binary Replicates

Version 1.0.0

Description Statistical methods for analyzing binary replicates, which are noisy binary measurements of latent binary states. Provides scoring functions (average, median, likelihood-based, and Bayesian) to estimate the probability that an individual is in the positive state. Includes maximum a posteriori estimation via the EM algorithm and full Bayesian inference via Stan. Supports classification with inconclusive decisions and prevalence estimation.

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URL https://github.com/pierrepudlo/BinaryReplicates

BugReports https://github.com/pierrepudlo/BinaryReplicates/issues

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`bayesian_computations` *Bayesian computations*

Description

Get credible intervals, Bayesian scores, and prevalence estimate from the `stanfit` object returned by BayesianFit.

Usage

```
credint(fit, level = 0.9)

bayesian_scoring(ni, si, fit)

bayesian_prevalence_estimate(fit)
```

Arguments

`fit`	The `stanfit` object returned by BayesianFit
`level`	Posterior probability of the credible intervals
`ni`	Numeric vector of n_i's, the total numbers of replicates for each individual
`si`	Numeric vector of s_i's, the numbers of replicates equal to 1 for each individual

Details

See BayesianFit for details on the Bayesian model.

Value

The `credint` function returns the credible interval bounds for the fixed parameters of the Bayesian model. The default posterior probability is 90%.

The `bayesian_scoring` function returns the Bayesian scores. These scores are the posterior probabilities that the true latent T_i's are equal to 1.

The `bayesian_prevalence_estimate` function returns the posterior mean of the posterior distribution on the prevalence of $T_i = 1$.

See Also

`classify_with_scores`, `BayesianFit`

Examples

```
data("periodontal")
theta <- mean(periodontal$ti)
fit <- BayesianFit(periodontal$ni, periodontal$si, chains = 2, iter = 5000)
credint(fit)
Y_B <- bayesian_scoring(periodontal$ni, periodontal$si, fit)
T_B <- classify_with_scores(Y_B, .4, .6)
theta_B <- bayesian_prevalence_estimate(fit)
cat("The Bayesian prevalence estimate is ", theta_B, "\n")
cat("The prevalence in the data is ", theta, "\n")
```

BayesianFit *Fit the Bayesian model for Binary Replicates*

Description

Fit the Bayesian model for Binary Replicates

Usage

```
BayesianFit(
  ni,
  si,
  prior = list(a_FP = 2, b_FP = 2, a_FN = 2, b_FN = 2, a_T = 0.5, b_T = 0.5),
  ...
)
```

Arguments

`ni`	Numeric vector of n_i's, the total numbers of replicates for each individual
`si`	Numeric vector of s_i's, the numbers of replicates equal to 1 for each individual
`prior`	A list of prior parameters for the model, see Details.
`...`	Arguments passed to `rstan::sampling` (e.g. iter, chains).

Details

The model is a Bayesian model for binary replicates. The prior distribution is as follows:

- The false positive rate: $p \sim \text{Beta}(a_{FP}, b_{FP})$
- The false negative rate: $q \sim \text{Beta}(a_{FN}, b_{FN})$
- The prevalence: $\theta \sim \text{Beta}(a_T, b_T)$

The statistical model considers that the true statuses are the latent

$$T_i \sim \text{Bernoulli}(\theta).$$

And, given the true status T_i, the number of positive replicates is

$$S_i \sim \text{Binomial}(n_i, T_i(1-q) + (1-T_i)p).$$

Value

An object of class `stanfit` returned by `rstan::sampling`.

The Stan model samples the posterior distribution of the fixed parameters p, q and θ. It also generates the latent variables T_i according to their predictive distribution.

See Also

credint, bayesian_scoring, classify_with_scores, bayesian_prevalence_estimate

---

`classify_with_scores` *Classification based on a thresholding of the scores*

Description

Classification based on a thresholding of the scores

Usage

```
classify_with_scores(scores, vL, vU)
```

Arguments

`scores`	Numeric vector of the scores, computed with average_scoring, median_scoring, MAP_scoring or bayesian_scoring
`vL`	The lower threshold
`vU`	The upper threshold

Details

Each decision $\hat{t}_i$ is taken according to the following rule:

$$\hat{t}_i = \begin{cases} 0 & \text{if } y_i < v_L, \\ 1/2 & \text{if } v_L \leq y_i \leq v_U, \\ 1 & \text{if } y_i > v_U, \end{cases}$$

where y_i is the score for individual i.

Value

A numeric vector of the classification (where 0.5 = inconclusive)

---

classify_with_scores_cvEM

Perform classification on the scores for each fold of a cvEM object

---

Description

Note that if t_i is provided, the empirical risk is estimated with $a = v_L$.

Usage

```
classify_with_scores_cvEM(object, ti = NULL, vL = 0.5, vU = 0.5)
```

Arguments

object	An object of class cvEM
ti	Numeric vector of t_i's, the true values of the binary variable for each individual. If NULL, the risk is not computed. Defaults to NULL.
vL	The lower threshold for classification. Defaults to 0.5.
vU	The upper threshold for classification. Defaults to 0.5.

Value

A cvEM object with the following components:

predictions A list of the predictions for each fold

risk The empirical risk if t_i is provided

Examples

```
data(periodontal)
modelCV <- cvEM(periodontal$ni, periodontal$si)
modelCV2 <- classify_with_scores_cvEM(modelCV, vL = 0.4)
```

`cvEM` *Cross-validation for the EM algorithm*

Description

Cross-validation for the EM algorithm

Usage

```
cvEM(
  ni,
  si,
  ti = NULL,
  N_cv = NULL,
  N_init = 20,
  maxIter = 1000,
  errorMin = 1e-07,
  prior = list(a_FP = 2, b_FP = 2, a_FN = 2, b_FN = 2)
)
```

Arguments

`ni`	Numeric vector of n_i's, the total numbers of replicates for each individual
`si`	Numeric vector of s_i's, the numbers of replicates equal to 1 for each individual
`ti`	Numeric vector of t_i's, the true values of the binary variable for each individual. If `NULL`, the EM algorithm is used to estimate the parameters. Defaults to `NULL`. See details.
`N_cv`	The number of folds. Defaults to 20.
`N_init`	The number of initializations if `ti` is not provided. Defaults to 20.
`maxIter`	The maximum number of iterations if the EM algorithm is used. Defaults to 1e3.
`errorMin`	The minimum error for convergence if the EM algorithm is used. Defaults to 1e-7.
`prior`	A list of prior parameters for the model.

Details

This function chooses its algorithm according to what is provided in the `ti` argument:

`ti` **is fully provided** The function computes the *Maximum-A-Posteriori* estimate, with an explicit formula.

`ti` **is not provided** The function uses the EM algorithm to estimate the parameters.

`ti` **is partially provided** The function uses the EM algorithm to estimate the parameters.

Value

A list with the following components:

models A list of the models for each fold

predictions A list of the predictions for each fold

See Also

classify_with_scores, EMFit

Examples

```
data("periodontal")
modelCV <- cvEM(periodontal$ni, periodontal$si)
```

`EMFit` *Compute the* Maximum-A-Posteriori *estimate with the EM algorithm*

Description

Compute the *Maximum-A-Posteriori* estimate with the EM algorithm

Usage

```
EMFit(
  ni,
  si,
  ti = NULL,
  prior = list(a_FP = 2, b_FP = 2, a_FN = 2, b_FN = 2),
  N_init = 20,
  maxIter = 1000,
  errorMin = 1e-07
)
```

Arguments

`ni`	Numeric vector of n_i's, the total numbers of replicates for each individual
`si`	Numeric vector of s_i's, the numbers of replicates equal to 1 for each individual
`ti`	Numeric vector of t_i's, the true values of the binary variable for each individual. If `NULL`, the EM algorithm is used to estimate the parameters. Defaults to `NULL`. See details.
`prior`	A list of prior parameters for the model. The prior distribution is as follows: • The false positive rate: $p \sim \text{Beta}(a_{FP}, b_{FP})$ • The false negative rate: $q \sim \text{Beta}(a_{FN}, b_{FN})$

`N_init`	The number of initializations if `ti` is not provided. Defaults to 20.
`maxIter`	The maximum number of iterations if the EM algorithm is used. Defaults to 1e3.
`errorMin`	The minimum error for convergence if the EM algorithm is used. Defaults to 1e-7.

Details

This function chooses its algorithm according to what is provided in the `ti` argument:

`ti` **is fully provided** The function computes the *Maximum-A-Posteriori* estimate, with an explicit formula.

`ti` **is not provided** The function uses the EM algorithm to estimate the parameters.

`ti` **is partially provided** The function uses the EM algorithm to estimate the parameters.

Value

A list with the following components:

score The estimated values of the scores

parameters_hat The estimated values of the parameters θ, p and q

See Also

classify_with_scores

Examples

```
data("periodontal")
# Get ML estimate knowing the true values of the latent ti's
periodontal_ml <- EMFit(periodontal$ni, periodontal$si, periodontal$ti)
# Get MAP estimate without knowing the true values of the latent ti's
periodontal_EM <- EMFit(periodontal$ni, periodontal$si, ti = NULL)
```

`mammography-datasets` *A mammography dataset*

Description

Data from a mammography screening program. The dataset is not the original dataset, but an imputed dataset based on the summary statistics available publicly.

Usage

```
data(mammography)

data(observed)
```

Format

The data frame mammography has 148 rows and 3 variables

ti True latent state of the individual (1=positive, 0=negative)

ni Number of mammography tests performed for each individual

si Number of positive mammography tests for each individual

The matrix observed is a 110x148 array with the observed replicates, one column for each individual. The rows correspond to the replicates, and the values are either 0 or 1.

Source

Beam C, Conant E, Sickles E. Association of volume and volume-independent factors with accuracy in screening mammogram interpretation. *JNCI.* 2003;95:282-290.

---

non_bayesian_scoring *Non-Bayesian scoring methods*

Description

Compute the average-, median- and likelihood-based scores

Usage

```
average_scoring(ni, si)

median_scoring(ni, si)

likelihood_scoring(ni, si, param)

MAP_scoring(ni, si, fit)
```

Arguments

ni	Numeric vector of n_i's, the total numbers of replicates for each individual
si	Numeric vector of s_i's, the numbers of replicates equal to 1 for each individual
param	A list with 3 entries: theta The probability that $T = 1$, i.e., the prevalence, p The false positive rate, q The false negative rate.
fit	The object returned by EMFit containing the results of the EM algorithm

Value

A numeric vector of the scores

Note

For likelihood-based scores, the values of θ, p and q are required. Consequently, likelihood scoring is not directly applicable in practice without parameter estimates.

See Also

EMFit

Examples

```
data("periodontal")
Y_A <- average_scoring(periodontal$ni, periodontal$si)
Y_M <- median_scoring(periodontal$ni, periodontal$si)
# In order to compute the likelihood-based scores, we need to know theta,
# p and q which can be estimated in this example as follows:
theta_hat <- mean(periodontal$ti)
cat("The prevalence in the data is ", theta_hat, "\n")
p_hat <- with(periodontal, sum(si[ti == 0]) / sum(ni[ti == 0]))
q_hat <- with(periodontal, 1 - sum(si[ti == 1]) / sum(ni[ti == 1]))
Y_L <- likelihood_scoring(periodontal$ni, periodontal$si,
                          list(theta = theta_hat, p = p_hat, q = q_hat))

data("periodontal")
Y_M <- median_scoring(periodontal$ni, periodontal$si)

data("periodontal")
fit <- EMFit(periodontal$ni, periodontal$si)
Y_MAP <- MAP_scoring(periodontal$ni, periodontal$si, fit)
```

---

periodontal *A periodontal dataset*

Description

Data from enzymatic diagnostic tests to detect two organisms Treponema denticola and Bacteroides gingivalis.

Usage

```
data(periodontal)
```

Format

A data frame with 50 rows and 3 variables:

ni Total numbers of sites tested for each individual

si Number of positive tests for each individual

ti Status of the individual (1=infected, 0=non-infected)

References

Hujoel PP, Moulton LH, Loesche WJ. Estimation of sensitivity and specificity of site-specific diagnostic tests. J Periodontal Res. 1990 Jul;25(4):193-6. doi: 10.1111/j.1600-0765.1990.tb00903.x. Erratum in: J Periodontal Res 1990 Nov;25(6):377. PMID: 2197400. Moore et al. (2013) Genetics 195:1077-1086 (PubMed)

Examples

```
data(periodontal)
hat_prevalence <- mean(periodontal$si/periodontal$ni)
hat_prevalence
# should be compared to:
mean(periodontal$ti)
```

`predict_scores` *Compute predictive Bayesian scores*

Description

Compute predictive Bayesian scores

Usage

```
predict_scores(newdata_ni, newdata_si, fit)
```

Arguments

`newdata_ni`	Numeric vector of the total numbers of replicates per individuals
`newdata_si`	Numeric vector of the numbers of positive replicates per individuals
`fit`	The `stanfit` object returned by BayesianFit

Details

The `predict_scores` function computes the predictive Bayesian scores. It computes the empirical estimator, for a new individual $n+1$, of the following integral:

$$Y_{B,n+1} = \int Y_{L,n+1}(\theta_T, p, q)\pi(\theta_T, p, q|S_1, ..., S_n)\mathrm{d}\theta_T\mathrm{d}p\mathrm{d}q$$

where $\pi(\theta, p, q|S_1, ..., S_n)$ is the posterior distribution of the parameters θ, p and q given the data $S_1, ..., S_n$ and $Y_{L,n+1}(\theta_T, p, q)$ is given by the function likelihood_scoring, such as

$$Y_{L,n+1}(\theta_T, p, q) = \boldsymbol{P}(T_{n+1} = 1|S_{n+1} = s_{n+1}) = \frac{\theta_T q^{n_{n+1}-S_{n+1}}(1-q)^{S_{n+1}}}{\theta_T q^{n_{n+1}-S_{n+1}}(1-q)^{S_{n+1}} + (1-\theta_T)p^{S_{n+1}}(1-p)^{n_{n+1}-S_{n+1}}}.$$

Thus the estimator is given by

$$\hat{Y}_{B,n+1} = \frac{1}{K}\sum_{k=1}^{K} Y_{L,n+1}(\theta_{T,k}, p_k, q_k),$$

where each parameter $(\theta_{T,k}, p_k, q_k)_k$ is sampled from the posterior distribution, output of the function BayesianFit. K is the total number of sampled parameters.

Value

The `predict_scores` function returns the predictive Bayesian scores in a numeric vector. The predictive Bayesian scores are the posterior probabilities that the true latent T_i's are equal to 1 on new data, averaged over the posterior distribution.

Examples

```
data("periodontal")
theta <- mean(periodontal$ti)
fitBay <- BayesianFit(periodontal$ni, periodontal$si, chains = 2, iter = 500)
fitMAP <- EMFit(periodontal$ni, periodontal$si)

## Comparison Bayesian <--> MAP
ni <- 200
Ni <- rep(ni,ni+1)
Si <- 0:ni
scores <- cbind(predict_scores(Ni,Si,fitBay),
                likelihood_scoring(Ni,Si,fitMAP$parameters_hat))
matplot(Si,scores,type = "l",lty = 1,col = 1:2,
        ylab = "Scores",xlab = "Number of Successes",main = "")
```

---

prevalence_estimate *Compute the average-/median- or MAP-based prevalence estimates based on the scores*

Description

Compute the average-/median- or MAP-based prevalence estimates based on the scores

Usage

```
prevalence_estimate(scores)
```

Arguments

`scores`	Numeric vector of the scores, computed with average_scoring, median_scoring or MAP_scoring

Value

A numeric value of the prevalence estimate

Note

We have shown that the median-based prevalence estimator is better than the average-based prevalence estimator in terms of bias, except when the prevalence is in an interval J. The length of J is small when the number of replicates is always large.

Examples

```
data("periodontal")
theta <- mean(periodontal$ti)
Y_A <- average_scoring(periodontal$ni, periodontal$si)
Y_M <- median_scoring(periodontal$ni, periodontal$si)
fit <- EMFit(periodontal$ni, periodontal$si)
Y_MAP <- MAP_scoring(periodontal$ni, periodontal$si, fit)
hat_theta_A <- prevalence_estimate(Y_A)
hat_theta_M <- prevalence_estimate(Y_M)
hat_theta_MAP <- prevalence_estimate(Y_MAP)
cat("The average-based prevalence estimate is ", hat_theta_A, "\n")
cat("The median-based prevalence estimate is ", hat_theta_M, "\n")
cat("The MAP-based prevalence estimate is ", hat_theta_MAP, "\n")
cat("The prevalence in the dataset is ", theta, "\n")
```

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