Matlab Documentation

Table of Contents

Fluorescence correction and calibration model.

biasanalysis

Description

Bias analysis for a given pair of predicted and observed values. Fits a linear regression model of the prediction error, returning the table with the information of the coefficients and a figure with the bias at each level of the predicted variable.

Inputs

`xobs`: vector with observed values.

`xpred`: vector with predicted values.

`varproc`: matrix with process variability (2nd column) for each concentration level (1st column).

`biasnorm`: number indicating the regresor of the bias analysis. Possible values are `0` (x, dafault value) and `1` (1/x).

`basemodel`: number indicating if the bias and linearity terms should be referred to the fitted model (0) or to the basic linear model (1).

`xlab`: optional label for the horizontal axis. Default value set to `" "`.

Outputs

`mdl`: LinearModel object with the information of the bias regression model.

|contlin!: contribution of the linear term from the bias regression model to the total variability of the bias.

`meanbias`: mean contribution of the bias to the total variability.

blkcorr

Description

Returns fluorescence values corrected by the blank noise.

Inputs

`yflu`: vector with fluorescence values (F read).

`yblk`: vector with blank values (F BLK).

`scale`: optional input with the scale of the output. Options: " "(default)||"log"|

Outputs

`ycorr`: vector with corrected values (F reporter).

checkblk

Description

Checks blank fluorescence values and returns average F BLK for each gain level.

Inputs

`fblk`: vector with blank fluorescence values (F BLK).

`gblk`: vector with gain at which each fblk value was measured (G)

`blkdata`: optional table with information about the F BLK values from the plate reader. Only necessary if the user asks for the report.

`report`: optional input indicating if user wants a report about the exluded blank values, printed in the command window. Possible values are `1` (report) and `0` (w.o. report). Default value set to `0`.

`alpha`: type I risk (false positive rate) assumed. Default value set to `0.01`.

`plottype`: char indicating the tpye of data representation, with possible values 'boxplot' or 'points'. Default set to boxplot.

Outputs

`blk`: struct with blank values for each gain level. Fields:

- `Gain`: vector with Gain levels.

- `mFread`: vector with mean F BLK value for each Gain level.

- `sFread`: vector with standard deviation of F BLK values for each Gain level.

ciplots

Description

Plot the confidence intervals with a layout distinguishing between concentration levels and samples.

Inputs

`datatbl`: table with the data containing the predicted and the true values.

`sterror`: value of the estimated error standard deviation.

`edf`: value of the error degrees of fredom.

`cicol`: char or RGB color of the shadowed area for the confidence intervals. Default set to 'b'.

Outputs

Figure with as many subplots as concentration levels, with the known concentration values and the estimated confidence interval for the predictions. Subplots present divided regions for each sample.

cipred

Description

Calculates lower and upper extremes of confidence intervals for the predictions in xpred, at a type I risk of alpha, assuming given values of the mean squared error and error degrees of freedom.

Inputs

`xpred`: vector with predicted values.

`se`: value of the estimated standard deviation of the error.

`edf`: value of the error degrees of freedom (edf).

`alpha`: optional input indicating the type I risk used to calculate the confidence intervals. Default value set to `0.05`. Must be between `0` and `1`.

Outputs

`LowCI`: vector with the lower limit of the confidence interval for each observation from xpred.

`UpCI`: vector with the upper limit of the confidence interval for each observation from xpred.

cvsplit

Description

Provides partition of the data set into a calibration and a validation data sub sets. The selection is done on the wells variable, keeping all the gains and repetitions of a certain well as part of the training or the validation. Both subsets are exluding (they do not repeat wells). The calibration percentage is applied stratifying in each concentration.

Inputs

`dataset`: table with complete data set.

`calpctge`: percentage (0 to 1) of observations to be part of the calibration data set.

Outputs

`data_cal`: table with calibration data set.

`data_val`: table with validation data set.

`idcal`: index of calibration observations, referred to the original data set.

fitfc

Description

Fits the coefficients of the f_C function with the conversion from corrected fluorescence to concentration.

Inputs

`flu`: vector with corrected fluorescence values (F real).

`c_pattern`: vector with fluorescein pattern concentration values (Concentration).

`intercept`: optional input indicating if the intercept term of the model should be considered or not. Possible values are 1 (with intercept term) and 0 (w.o. intercept). Default value set to 0.

Outputs

`c`: coefficients of the units conversion model.

`mdl`: LinearModel object with the information of the calibration Fluorescence-Concentration model.

fitfg

Description

Fits the terms of the f_G function with the effect of the gain on the fluorescence measurements. It assumes the following exponential gain effect: $F_{real} = (F_{obs} - F_{BLK})\exp(b_1 \cdot G + b_2 \cdot G^2)$. It fits the aforementioned expression using 4 data points of the same well and repetition, obtainining `size(gfpdata,1)/gain_levels` models. In order to prove the assumptions on the coefficients' consistency, an ANOVA test is carried out on b1 and b2, studying statistically significant differcens between concentrations and wells.

Inputs

`blkdata`:table with the fluorescence measured from empty wells (F_BLK).

`gfpdata`: table with the fluorescence measured from wells with fluorescein.

Outputs

`model_parameters`: table with coefficients of the model (F_BLK for each gain, b1 and b2).

gfpdata: gfp table with two additional columns. One is the F_BLK value used with each F_obs value to correct the aditive noise effect of the medium. The other column is the F_reporter value, but still with the gain effect.

gmtable: table used for the ANOVA on the b1 and b2 coefficients of f_G.

fgtest: results of the ANOVA.

flu2conc

Description

Predicts concentration from corrected fluorescence data.

Inputs

f: vector with corrected fluorescence vlaues (F real).

c0: intercept term of the units conversion model.

c1: slope term of the units conversion model.

Outputs

conchat: vector with predicted values of the concentration ($\hat{C}$).

gaincfs

Description

Fits gain effect correction model. Applicable to each group of measurements of the same well and repetition at different gain levels.

Inputs

y: vector with fluorescence (F reporter) values already without the F BLK.

g: vector with gain values at which each observation in y was acquired.

order: optioanl argument with the order of the expression in the exponent term of the gain effect correction model. Default value set to 2.

Outputs

B: array with coefficients of the gain effect correction model.

gaincorrect

Description

Corrects the fluorescence values (F read) eliminating the blank (F BLK) and the gain effect.

Inputs

ymeas: vector with fluorescence (F read) values.

`yblk`: vector with fluorescence blank (F BLK) values.

`gain`: vector with gain (G) values.

`b1`: linear term of the gain effect correction model.

`b2`: quadratic term of the gain effect correction model

`scale`: optional string or char indicating the scale of the output fector. Possible values are `" "`(default)||"log"|.

Outputs

`ycorr`: vector with the corrected falue of fluorescence (F real) for each observation.

normalout

Description

Eliminates outlying observations assuming a normal distribution of the variable and a type I risk level of alpha.

Inputs

`x`: vector observations.

`alpha`: optional argument with the type I risk level assumed to compute the threshold value based on the normal distrbution (i.e.: the false positive rate). Default value set to `0.05`.

Outputs

`xclean`: vector with clean observation.

`outids`: logical vector indicating outyling observations

plotbyfactor

Description

Fits gain effect correction model.

Inputs

`x`: vector with values in the horizontal axis.

`y`: vector with values in the vertical axis.

`g`: vector with group of each observation.

`xdiscrete`: optional argument indicating if the x variable is discrete. If it is (value set to `1`), jitter will be added to the plot in this axis. Default value is set to `0`.

`ydiscrete`: optional argument indicating if the y variable is discrete. If it is (value set to `1`), jitter will be added to the plot in this axis. Default value is set to `0`.

`disp`: optional argument indicating the dispersion to be considered when adding the jitter to the points. Default value set to `0.01*min(abs(x))`.

`xlab`: optional string with the horizontal label. Default value set to `""`.

`ylab`: optional string with the vertical label. Default value set to `""`.

`titlab`: optional string with the title. Default value set to `""`.

Outputs

Displays the scatter plot.

plotcalib

Description

Returns a plot with the calibration model obtained between variables in the horizontal and vertical axis.

Inputs

`x`: vector with variable in the horizontal axis.

`y`: vector with variable in the vertical axis.

`c0`: intercept term of the calibration model.

`c1`: linear term of the calibration model.

`scalex`: optional input indicaint the scale in the horizontal axis. Possible values are `""`(default)||"log"|.

`scaley`: optional input indicaint the scale in the vertical axis. Possible values are `""`(default)||"log"|.

Outputs

Displays plot with the points from x and y and the calibration curve.

quantifyuncertainty

Description

Quantifies uncertainty according to the prediction error. Returns normal probability plots for the error considering it in normal scale and scaling it by the observed values of the variable. If the later option presents a better normal probability plot, then this option should be considered to estimate the uncertainty in the predictions.

Inputs

`xobs`: vector with the observed values.

`xpred`: vector with the predicted values.

`vblename`: optional argument with variable name, to be included in the plots. Default set to `""`.

Outputs

`sBias`: standard deviation of the bias.

`sBiasnorm`: standard deviation of the bias scaled by the concentration.

`mdl1`: linear model fitteg for the bias.

`mdl2`: linear model fitteg for the bias scaling by the concentration.

randr

Description

Runs a Repeatability and Reproducibility (R&R) analyis. Obtains the decomposition of total variability in the different sources, as well as bar plots for the variability sources and anova tables for each type of piece considering as factors the different sources of variability.

Inputs

`measurements`: vector with the response variable measurements.

`replicates`: vector or cell indicating the replicates ID for each observation.

`pieces`: vector or cell indicating the piece ID for each observation.

`operary`: vectoror cell indicating the operary ID for each observation.

`repeat`: vector or cell indicating the repetition ID for each observation.

`allinone`: optional number indicating if the bar plots with the different sources of variability for each piece, will be all in the same figure, or separated. Possible values are 0(different figure, default value)||1| (same figure).

Outputs

`s_RandR`: struct with the amount of variability accounted to each source for each type of piece. Contains one struct for each piece. The fields for each piece, are:

- `s2Gain`: variability apported by variations in the operary (gain) term.

- `s2nReplicate`: variability apported by variations in the replicate term.

- `s2Repeat`: variability apported by variations in the repetition term.

- `Gage`: variability apported by the machine (operary + repeat).

- `VarCont.s2Gain`: pctge of variability apported by s2Gain.

- `VarCont.s2nReplicate`: pctge of variability apported by s2nReplicate.

- `VarCont.s2Repeat`: pctge of variability apported by s2Repeat.

- `VarCont.Gage`: pctge of variability apported by Gage.

readexperiment

Description

Re-arragnes table for its further use with the toolbox functions.

```
%
% *Inputs*
```

```
%
% |filename|: name of the excel file with the data.
%
% |datarange|: char with data range in the excel file.
%
% |glevels|: vector with gain levels.
%
% |readvarnames|: boolean indicating if variable names should be read.
% Default set to |'false'|.

% |varnames|: vector with the variable names of the resulting table.
% Recommended to use its default value.

% *Outputs*
%
% |datPRnew|: re-arranged table with plate reader measurements.
```

samplegainmodel

Description

Fits gain effect correction model with each set of values acquired at G_level1,...,G_levelN.

Inputs

`ymeas`: vector with fluorescence (F read) values.

`yblk`: vector with fluorescence blank (F BLK) values.

`g`: vector with gain (G) values.

`sample`: vector indicating the sample to which each observation belongs.

`reps`: vector indicating the repetition to which each observation belongs.

`order`: optional input with the order considered on the epression of the exponential term of the gain effect model. Default value set to 2.

`alpha`: type I risk (false positive rate) assumed. Default value set to 0.01.

`plottype`: char indicating the tpye of data representation, with possible values 'boxplot' or 'points'. Default set to boxplot.

Outputs

`coeffs`: struct with the average coefficients of the gain effect model. Containing fields:

- `b1`: linear term of the gain effect correction model.

- `b2`: quadratic term of the gain effect correction model.

`gfcstable`: table with the fitted terms of the gain effect model for each sample.

studymissing

Description

Provides a descriptive analysis of the presence of missing data in the table.

Inputs

`datatable`: table with the data recorded by the plate reader.

Outputs

Displays barplot with the amount of missing observations for each concentration level.

tableprep

Description

Re-arragnes table for its further use with the toolbox functions.

Inputs

`tableold`: table with information to be rearranged.

`colidsjoin`: vector with indices of the columns in table_old which have to be joined in one varible in the new table.

`colidsrep`: vector with indices of the columns in table_old which have to be repeated in the new table.

`factorlevels`: vector with the Gain levels.

Outputs

`tablenew`: re-arranged table.

validateci

Description

Calculates the pertentage of observations whose confidence interval (C.I.) contains the true observed value.

Inputs

`LowCI`: vector with lower limit of the confidence interval for each observation.

`UpCI`: vector with upper limit of the confidence interval for each observation.

`x`: vector with true observed values of each observation.

Outputs

`Percent_in`: percentage of observations whose C.I. contains the true observed value.

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