Using **asremlPlus**, in conjunction with **asreml**, to do the analysis of a wheat experiment that includes choosing a local spatial variation model using AICs

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This vignette shows how to use **asremlPlus** (Brien, 2024), in conjunction with **asreml** (Butler et al., 2023), to select the terms to be included in a mixed model for an experiment that involves spatial variation by comparing of information criteria. It also illustrates diagnostic checking and prediction production and presentation for this experiment. Here, **asremlPlus** and **asreml** are packages for the R Statistical Computing environment (R Core Team, 2024).

It is divided into the following main sections:

1. Set up the initial model for this experiment
2. Compare a series of information criteria to select a linear mixed model for the data
3. Diagnostic checking using residual plots and variofaces
4. Prediction production and presentation

### 1. Set up the initial model for this experiment

```r
library(asreml, quietly=TRUE)

## Offline License checked out Wed Jun 19 15:38:08 2024

## Loading ASReml-R version 4.2

library(asremlPlus)
library(parallel)
library(doParallel)

## Loading required package: foreach

## Loading required package: iterators

library(foreach)
suppressMessages(library(qqplotr, quietly=TRUE))
options(width = 100)
```
Get data available in asremlPlus

The data are from a 1976 spring wheat experiment and are taken from Gilmour et al. (1995). An analysis is presented in the asreml manual by Butler et al. (2023, Section 7.6), although they suggest that it is a barley experiment.

```r
data(Wheat.dat)
```

Add row and column covariates for the spatial modelling

```r
tmp.dat <- within(Wheat.dat, {
    cColumn <- dae::as.numfac(Column)
    cColumn <- cColumn - mean(unique(cColumn))
    cRow <- dae::as.numfac(Row)
    cRow <- cRow - mean(unique(cRow))
})
```

Fit an initial model - Row and column random

In the following, an initial model is fitted that has the terms that would be included for a balanced lattice. In addition, a term WithinColPairs has been included to allow for extraneous variation arising between pairs of adjacent lanes.

```r
current.asr <- do.call(asreml, 
    list(yield ~ Rep + WithinColPairs + Variety, 
         random = ~ Row + Column, 
         residual = ~ Row:Column, 
         data = tmp.dat))
```

```
## ASReml Version 4.2 19/06/2024 15:38:09
## LogLik Sigma2 DF wall
## 1 -702.7015 26232.20 119 15:38:09
## 2 -700.4838 24394.12 119 15:38:09
## 3 -698.4908 22487.75 119 15:38:09
## 4 -697.5842 21242.11 119 15:38:09
## 5 -697.3673 20590.05 119 15:38:09
## 6 -697.3595 20477.28 119 15:38:09
```

Inititalize a model sequence by loading the current fit into an asrtests object

In creating the asrtests object, IClikelihood is set to full so that the full Restricted Maximum Likelihood (full REML) of Verbyla, 2019 is incorporated into the tests.summary of the asrtests object.

```r
current.asrt <- as.asrtests(current.asr, NULL, NULL, IClikelihood = "full", 
                           label = "Initial model")
```

```
## Warning in (function (fixed = -1, random = -NULL, sparse = -NULL, residual = -NULL, : 
## Log-likelihood not converged
```
Check for and remove any boundary terms and print a summary of the fit in the asrtests object

```r
current.asrt <- rmboundary(current.asrt)
print(current.asrt)
```

```r
##
## #### Summary of the fitted variance parameters
##
## component std.error z.ratio bound %ch
## Row 5943.898 3815.514 1.557824 P 0.0
## Column 12380.527 6323.542 1.957847 P 0.3
## Row:Column!R 20477.280 2896.642 7.069316 P 0.0
##
## #### Pseudo-anova table for fixed terms
##
## Wald tests for fixed effects.
## Response: yield
##
## Df denDF F.inc Pr
## (Intercept) 1 14.9 1390.00 0.0000
## Rep 5 25.3 6.04 0.0008
## WithinColPairs 1 10.4 0.49 0.4998
## Variety 24 104.8 4.71 0.0000
##
## #### Sequence of model investigations
##
## (If a row has NA for p but not denDF, DF and denDF relate to fixed and variance parameter numbers)
##
## terms DF denDF p AIC BIC action
## 1 Initial model 31 3 NA 1720.891 1823.253 Starting model
```

The test.summary output shows that no changes have been made to the model loaded using as.asrtests. The pseudo-anova table shows that Varieties are highly significant ($p < 0.001$)

2. Compare a series of information criteria to select a linear mixed model for the data

In this section, models are compared using Akaike Information Criterion (AICs) based on the full REML.

Check the need for the term for within Column pairs (a post hoc factor)

```r
current.asrt <- changeModelOnIC(current.asrt, dropFixed = "WithinColPairs",
                   label = "Try dropping withinColPairs", IClikelihood = "full")
```
It is clear in the call to `changeModelOnIC` that the model is being changed by dropping the `withinColPairs` term, which could also be achieved using `update.asreml`. However, an `asremlPlus` model-changing function operates on an `asrtests` object, that includes an `asreml` object, and, except for `changeTerms.asrtests`, results in an `asrtests` object that may contain the changed model or the supplied model depending on the results of hypothesis tests or comparisons of information criteria. In addition, the result of the test or comparison will be added to a `test.summary` data.frame stored in the new `asrtests` object and, if the model was changed, the `wald.tab` in the new `asrtests` object will have been updated for the new model.

In this case, as can be seen from the summary of `current.asrt` after the call, the model without `withinColPairs` had a smaller AIC and so now the model stored in `current.asrt` does not include `withinColPairs`. The `wald.tab` has been updated for the new model.
Choose a model for local spatial variation from several potential models

This example has been analyzed using a model for the local spatial variation based on a separable auto-
correlation process of order one (Butler et al., 2023). The need for this model can be assessed using the
function `addSpatialModelOnIC` from `asremlPlus` that uses a forward selection strategy for fitting a corre-
lation model (see output below). For this function, the spatial model to be fitted, the centred covariates
for the two dimensions of the grid, and the factors corresponding to the covariates must be specified. Also,
`IClikelihood` is set to `full` so that the likelihood will be based on the full REML. Because the model that
incorporates the spatial model has a smaller AIC, it is the model returned in `spatial.ar1.asrt`.

The print of `spatial.ar1.asrt` shows that an `ar1` model for Row was tried first and was found to reduce
the AIC by 11.898 and so became the current model. Next a model that incorporates an `ar1` function for
Column was similarly tried and became the current model. This model includes a nugget variance, unless
either the variance for Row:Column term or the Residual is bound or fixed. The Residual is the nugget term
and represents non-spatial variance, such as measurement error. An appraisal of the need for a nugget term
was made by comparing the fits with the residual variance unfixed and fixed at one. The model with the
unfixed residual variance was chosen and is the model to be returned. That is, this model includes a term
for nugget variance.

```r
spatial.ar1.asrt <- addSpatialModelOnIC(current.asrt, spatial.model = "corr",
  row.covar = "cRow", col.covar = "cColumn",
  row.factor = "Row", col.factor = "Column",
  IClikelihood = "full")
```

## Warning in (function (fixed = ~1, random = ~NULL, sparse = ~NULL, residual = ~NULL, : Some
## components changed by more than 1% on the last iteration
## Warning in (function (fixed = ~1, random = ~NULL, sparse = ~NULL, residual = ~NULL, : Some
## components changed by more than 1% on the last iteration

## Warning in infoCriteria.asreml(asreml.obj, IClikelihood = ic.lik, bound.exclusions = bound.exclusions)
## Column

## Warning in infoCriteria.asreml(asreml.obj, IClikelihood = ic.lik): The following bound terms were dis
## Column

## Warning in (function (fixed = ~1, random = ~NULL, sparse = ~NULL, residual = ~NULL, : Warning :
## Oscillating parameter(s) reset to average value (iteration 7)
## Warning in (function (fixed = ~1, random = ~NULL, sparse = ~NULL, residual = ~NULL, : Warning :
## Oscillating parameter(s) reset to average value (iteration 7)

## Warning in (function (fixed = ~1, random = ~NULL, sparse = ~NULL, residual = ~NULL, :
## Log-likelihood not converged

## Warning in (function (fixed = ~1, random = ~NULL, sparse = ~NULL, residual = ~NULL, : Some
## components changed by more than 1% on the last iteration

## Warning in (function (fixed = ~1, random = ~NULL, sparse = ~NULL, residual = ~NULL, : Warning :
## Oscillating parameter(s) reset to average value (iteration 7)
## Warning in (function (fixed = ~1, random = ~NULL, sparse = ~NULL, residual = ~NULL, : Warning :
## Oscillating parameter(s) reset to average value (iteration 7)

## Warning in (function (fixed = ~1, random = ~NULL, sparse = ~NULL, residual = ~NULL, :
## Log-likelihood not converged
## Warning in (function (fixed = ~1, random = ~NULL, sparse = ~NULL, residual = ~NULL, : Some components changed by more than 1% on the last iteration

## Warning in newfit.asreml(asreml.obj, random = mod.ran, trace = trace, update = update, :

## Warning in changeTerms.asrtests(asrtests.obj, dropFixed = dropFixed, addFixed = addFixed, : In analysing yield, boundary terms removed

## Warning in (function (fixed = ~1, random = ~NULL, sparse = ~NULL, residual = ~NULL, : Some components changed by more than 1% on the last iteration

## Warning in (function (fixed = ~1, random = ~NULL, sparse = ~NULL, residual = ~NULL, : Some components changed by more than 1% on the last iteration

## Warning in (function (fixed = ~1, random = ~NULL, sparse = ~NULL, residual = ~NULL, : Some components changed by more than 1% on the last iteration

## Warning in infoCriteria.asreml(asreml.obj, IClikelihood = ic.lik, bound.exclusions = bound.exclusions):
## Row:Column!R

## Warning in infoCriteria.asreml(new.asrtests.obj$asreml.obj, IClikelihood = ic.lik, : The following bound
## Row:Column!R

spatial.ar1.asrt <- rmboundary(spatial.ar1.asrt)
infoCriteria(list(nonspatial = current.asrt$asreml.obj, ar1 = spatial.ar1.asrt$asreml.obj))

## fixedDF varDF NBound AIC BIC loglik
## nonspatial 0 3 0 1409.023 1417.386 -701.5117
## ar1 0 5 0 1353.762 1367.700 -671.8811

print(spatial.ar1.asrt)

## Summary of the fitted variance parameters
##
## #### Summary of the fitted variance parameters
##
## component std.error z.ratio bound %ch
## Row 2.202326e+03 8.222412e+03 0.2678443 P 0.3
## Row:Column 5.181864e+04 3.381226e+04 1.5325399 P 0.0
## Row:Column!Row!cor 7.121302e-01 9.570910e-02 7.4405694 U 0.0
## Row:Column!Column!cor 8.599232e-01 1.103950e-01 7.7895102 U 0.0
## Row:Column!R 4.821622e+03 1.717158e+03 2.8079077 P 0.0

## Wald tests for fixed effects.
## Response: yield
##
## Df denDF  F.inc Pr
However, the spatial models that are available in \textit{asremlPlus} also include those based on two-dimensional tensor-product natural cubic smoothing splines (TPNCSS), as described by Verbyla et al. (2018), and on two-dimensional tensor-product P-splines (TPPS), as described by Rodriguez-Alvarez et al. (2018) and Piepho, Boer and Williams (2022). The P-splines have been implemented using functions from the \textit{R} package \textit{TPSbits} authored by Sue Welham (2022).

The \textit{asremlPlus} function \texttt{chooseSpatialModelOnIC} allows one to select the best model from amongst these spatial correlation models using the AIC or the BIC, the AIC being the default. The four models from which it selects are (i) a separable autocorrelation model on both row and column dimensions (\texttt{corr}), (ii) a two-dimensional tensor-product natural cubic smoothing spline (TPNCSS), (ii) a two-dimensional tensor-product cubic P-spline with second-difference penalties (TPPSC2), and (iii) a tensor-product two-dimensional linear P-spline with first-difference penalties (TPPSL1). By default all four are fitted and compared, but the \texttt{trySpatial} argument can be used to specify a subset of them.

The call to \texttt{chooseSpatialModelOnIC}, in addition to the arguments specifying covariates and factors, has further arguments: (i) \texttt{dropFixed} and \texttt{dropRandom} that are relevant to fitting P-splines and are used here to remove the random, overall Row and Column terms that were included in the original model so that the fitted P-spline model will be compared to a model including them and because the code for fitting P-splines also automatically includes these terms so that they would be included twice in the model to be fitted resulting in model singularities, (ii) \texttt{rotateX} and \texttt{ngridangles} so that the angles in both row and column directions for rotating the eigenvectors of the penalty matrix for the linear component of the P-splines is optimized (setting \texttt{ngridangles} to \texttt{NULL} causes the \texttt{R} function \texttt{nloptr::bobyqa} to be invoked for finding the optimal angles), (iii) an \texttt{asreml.option} argument to specify that the \texttt{grp} method be used in fitting the P-spline terms, this being safer because the data.frame needed for any post-fitting computation is available in the \texttt{asreml} object, and (iv) \texttt{return.asrts} to specify which \texttt{asrtests} objects are to be returned. Here we specify all so that \texttt{asrtests} objects for the best fits between the model supplied in the \texttt{current.asrt} and each of the spatial models is returned for all four spatial models. In this case, neither the \texttt{checkboundaryonly} nor the \texttt{IClikelihood} arguments were set because their defaults for \texttt{chooseSpatialModelOnIC} are appropriate.

```r
suppressWarnings(
  spatial.asrts <- chooseSpatialModelOnIC(current.asrt,
    row.covar = "cRow", col.covar = "cColumn", row.factor = "Row", col.factor = "Column",
    dropRandom = "Row + Column", rotateX = TRUE, ngridangles = NULL,
    asreml.option = "grp", return.asrts = "all")
)
```

## Notice : Spline design points closer than .000900 have been merged
## Notice: Spline design points closer than .001400 have been merged
## Notice: Spline design points closer than .000900 have been merged
## Notice: Spline design points closer than .001400 have been merged
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## Notice: Spline design points closer than .001400 have been merged
## Notice: Spline design points closer than .000900 have been merged
## Notice: Spline design points closer than .001400 have been merged
## Warning: Spline design points closer than .000900 have been merged
## elapsed time for bobyqa: 15.76 seconds

## #### Optimal thetas: 20.2026926907242, 64.9728898361927 with criterion 1659.433

## Notice: Spline design points closer than .000900 have been merged
## Notice: Spline design points closer than .001400 have been merged
## Notice: Spline design points closer than .000900 have been merged
## Notice: Spline design points closer than .001400 have been merged
## Notice: Spline design points closer than .000900 have been merged
## Notice: Spline design points closer than .001400 have been merged
## Notice: Spline design points closer than .000900 have been merged
## Notice: Spline design points closer than .001400 have been merged

Output the results

```r
print(spatial.asrts$spatial.IC)
```

```r
table <- read.table(text = "fixedDF varDF AIC  BIC  loglik
nonspatial 30 3 1718.609 1817.960 -826.3047
corr 30 5 1651.317 1756.689 -790.6583
TPNCSS 33 6 1639.489 1756.904 -780.7445
TPPS2 33 7 1642.838 1763.263 -781.4190
TPPSL1 30 3 1708.443 1807.794 -821.2214

print(R2adj(spatial.asrts$asrts$TPNCSS$asreml.obj, include.which.random = ~ .))
```

```r
## ASReml Version 4.2 19/06/2024 15:39:05
## LogLik Sigma2 DF wall
## 1 -662.1988 7657.986 117 15:39:05
```
print(spatial.asrts$best.spatial.mod)

## [1] "TPNCS"

print(spatial.asrts$asrts$TPNCS)

##
## Summary of the fitted variance parameters
##
## component std.error  z.ratio bound %ch
## spl(cRow):cColumn  523.2004  372.8016  1.403429 P  0
## dev(cRow)  7664.0211  4442.0646  1.725329 P  0
## spl(cColumn) 13338.7348  9236.0511  1.444203 P  0
## spl(cColumn):cRow  366.7707  322.7484  1.136399 P  0
## spl(cRow):spl(cColumn) 3630.2187  2186.1497  1.660554 P  0
## Row:Column!R  7658.0113  1312.2026  5.835998 P  0

##
## Pseudo-anova table for fixed terms
##
## Wald tests for fixed effects.
## Response: yield
##
## (Intercept)  1  6.8 2645.00  0.0000
## Rep  5  41.3  20.45  0.0000
## Variety 24  86.5  10.15  0.0000
## cRow  1  7.0  0.07  0.7954
## cColumn  1 30.1  20.30  0.0001
## cRow:cColumn  1 64.3  22.00  0.0000

##
## Sequence of model investigations
##
## (If a row has NA for p but not denDF, DF and denDF relate to fixed and variance parameter numbers)
The output shows that the TPNCSS model has the lowest AIC and so is selected as the best model. The adjusted $R^2$ value shows that the fixed and random terms in the fitted model account for 93% of the total variation in the yield. The model fitted for the TPNCSS model has been printed using `printFormulae.asreml`. The fitted model includes the term `dev(cRow)` that is equivalent to a random `Row` term and measures the deviations of the Row trend from a linear trend, the `spl(cRow)` term having been dropped because it was estimated to be zero. The Wald $F$-statistic for `Variety` is now 10.15 with 86.5 denominator degrees of freedom, as compared to 10.56 and 74.3 for the correlation model and 4.71 and 105.3 for the initial nonspatial model.

### 3. Diagnosting checking using residual plots and variofaces

Get current fitted asreml object and update to include standardized residuals

```r
Wheat.dat$res <- residuals(current.asr, type = "stdCond")
Wheat.dat$fit <- fitted(current.asr)
```
Do diagnostic checking

Do residuals-versus-fitted values plot

\texttt{with(Wheat.dat, plot(fit, res))}

Plot variofaces

\texttt{variofaces(current.asr, V=NULL, units="addtores", maxiter=50, update = FALSE, ncores = parallel::detectCores())}
Variogram face of Standardized conditional residuals for Row
The variograms are the lag 1 plots of the sample semivariogram with simulated confidence envelopes (Stefanova et al., 2009).

**Plot normal quantile plot**

The plot is obtained using the `ggplot` function with extensions available from the `qqplotr` package (Almeida et al., 2023).

```r
ggplot(data = Wheat.dat, mapping = aes(sample = res)) +
  stat_qq_band(bandType = "ts") + stat_qq_line() + stat_qq_point() +
  labs(x = "Theoretical Quantiles", y = "Sample Quantiles",
       title = "Normal probability plot") +
  theme(plot.title = element_text(size = 12, face = "bold")) + theme_bw()
```
4. Prediction production and presentation

Get Variety predictions and all pairwise prediction differences and p-values

```r
Var.diffs <- predictPlus(classify = "Variety",
                         asreml.obj=current.asr,
                         error.intervals="halfLeast",
                         wald.tab=current.asrt$wald.tab,
                         sortFactor = "Variety",
                         tables = "predictions")
```

## Notice : Spline design points closer than .001400 have been merged
## Notice : Spline design points closer than .000900 have been merged
##
## #### Predictions for yield from Variety
##
## Notes:
## - The predictions are obtained by averaging across the hypertable
calculated from model terms constructed solely from factors in
the averaging and classify sets.
## Use 'average' to move ignored factors into the averaging set.
## spl(cRow) evaluated at average value of 0.00000
## spl(cColumn) evaluated at average value of 0.00000
## The simple averaging set: Rep

<table>
<thead>
<tr>
<th>Variety</th>
<th>predicted.value</th>
<th>standard.error</th>
<th>upper.halfLeastSignificant.limit</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1196.214</td>
<td>64.11316</td>
<td>1255.028</td>
</tr>
<tr>
<td>2</td>
<td>1266.442</td>
<td>69.62176</td>
<td>1325.255</td>
</tr>
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<td>3</td>
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<td>74.01873</td>
<td>1327.020</td>
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<td>4</td>
<td>1273.794</td>
<td>69.30592</td>
<td>1332.608</td>
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<td>70.75661</td>
<td>1369.620</td>
</tr>
<tr>
<td>6</td>
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<td>73.70238</td>
<td>1387.928</td>
</tr>
<tr>
<td>7</td>
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<td>75.07426</td>
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<td>8</td>
<td>1406.408</td>
<td>76.83336</td>
<td>1465.222</td>
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<tr>
<td>9</td>
<td>1408.543</td>
<td>71.85868</td>
<td>1467.356</td>
</tr>
<tr>
<td>10</td>
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<td>72.23082</td>
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</tr>
<tr>
<td>11</td>
<td>1423.303</td>
<td>71.18629</td>
<td>1482.117</td>
</tr>
<tr>
<td>12</td>
<td>1445.533</td>
<td>75.37805</td>
<td>1504.347</td>
</tr>
<tr>
<td>13</td>
<td>1480.687</td>
<td>70.31499</td>
<td>1539.500</td>
</tr>
<tr>
<td>14</td>
<td>1485.249</td>
<td>74.28025</td>
<td>1544.063</td>
</tr>
<tr>
<td>15</td>
<td>1495.212</td>
<td>71.09930</td>
<td>1554.026</td>
</tr>
<tr>
<td>16</td>
<td>1512.767</td>
<td>72.53109</td>
<td>1571.580</td>
</tr>
<tr>
<td>17</td>
<td>1520.841</td>
<td>72.50721</td>
<td>1579.654</td>
</tr>
<tr>
<td>18</td>
<td>1563.649</td>
<td>65.33308</td>
<td>1622.463</td>
</tr>
<tr>
<td>19</td>
<td>1568.887</td>
<td>71.06200</td>
<td>1627.700</td>
</tr>
<tr>
<td>20</td>
<td>1579.929</td>
<td>70.52509</td>
<td>1638.743</td>
</tr>
<tr>
<td>21</td>
<td>1585.398</td>
<td>74.96623</td>
<td>1644.211</td>
</tr>
<tr>
<td>22</td>
<td>1633.080</td>
<td>71.38265</td>
<td>1691.894</td>
</tr>
<tr>
<td>23</td>
<td>1637.119</td>
<td>66.24775</td>
<td>1695.932</td>
</tr>
<tr>
<td>24</td>
<td>1651.533</td>
<td>74.93686</td>
<td>1710.347</td>
</tr>
<tr>
<td>25</td>
<td>1657.612</td>
<td>68.65452</td>
<td>1716.426</td>
</tr>
</tbody>
</table>

## lower.halfLeastSignificant.limit est.status
| 1       | 1137.400        | Estimable      |
| 2       | 1207.628        | Estimable      |
| 3       | 1209.393        | Estimable      |
| 4       | 1214.980        | Estimable      |
| 5       | 1251.993        | Estimable      |
| 6       | 1270.300        | Estimable      |
| 7       | 1281.854        | Estimable      |
| 8       | 1347.594        | Estimable      |
| 9       | 1349.729        | Estimable      |
| 10      | 1355.657        | Estimable      |
| 11      | 1364.490        | Estimable      |
| 12      | 1386.720        | Estimable      |
| 13      | 1421.873        | Estimable      |
| 14      | 1426.435        | Estimable      |
| 15      | 1436.399        | Estimable      |
| 16      | 1453.953        | Estimable      |
| 17      | 1462.027        | Estimable      |
| 18      | 1504.836        | Estimable      |
| 19      | 1510.073        | Estimable      |
| 20      | 1521.115        | Estimable      |
| 21      | 1526.584        | Estimable      |
| 22      | 1574.266        | Estimable      |
We have set `error.intervals` to `halfLeast` so that the limits for each prediction \( \pm (0.5 \text{ LSD}) \) are calculated. When these are plotted overlapping error bars indicate predictions that are not significant, while those that do not overlap are significantly different (Snee, 1981).

Also set was `sortFactor`, so that the results would be ordered for the values of the predictions for Variety. The function `predictPlus` returns an `alldiffs` object, a list consisting of the following components:

- **predictions**: the predictions, their standard errors and error intervals;
- **vcov**: the variance matrix of the predictions;
- **differences**: all pairwise differences between the predictions;
- **p.differences**: p-values for all pairwise differences between the predictions;
- **sed**: the standard errors of all pairwise differences between the predictions;
- **LSD**: the mean, minimum and maximum of the LSDs.

Plot the Variety predictions, with halfLSD intervals, and the p-values

```r
plotPredictions(Var.diffs$predictions,
                classify = "Variety", y = "predicted.value",
                error.intervals = "half")
```
plotPvalues(Var.diffs)
References


Welham, S. J. (2022) **TPSbits**: Creates Structures to Enable Fitting and Examination of 2D Tensor-Product Splines using ASReml-R. Version 1.0.0 https://mmade.org/tpsbits/