Shall we use the F_R-test or the simple parametric bootstrap test?

Twelve Working Seminar on Statistical Methods in Variety Testing
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Multi-environment trial of rapeseed

Means of $R = 4$ replicates

$J = 9$ environments

$I = 6$ varieties

	TGA	NC	GGA	SC	VA	TN	NY	WA	ID	Mean
Dwarf	0.00	1.35	1.50	0.86	1.59	2.61	3.57	3.11	5.95	2.28
Jet	0.32	0.70	1.65	0.90	1.81	2.78	3.16	3.12	5.86	2.26
Cascade	1.48	1.10	1.73	2.77	1.46	1.93	2.51	3.94	5.48	2.49
Bridger	1.76	1.61	1.30	2.85	1.65	2.41	3.06	4.05	4.15	2.54
Glacier	0.53	1.39	2.10	1.69	1.91	2.19	3.23	2.79	5.56	2.38
Bienvenu	0.45	1.38	1.85	1.82	1.68	2.89	2.86	1.73	5.35	2.22
Mean	0.76	1.25	1.69	1.81	1.69	2.47	3.07	3.12	0.76	2.36

Shafii and Price (1989)

Outline of the presentation

1. Statistical models
2. Hypothesis tests
3. Simulation study
4. Practical advice

1. Statistical models

Linear fixed-effects models

$$y_{ijr} = \mu + \alpha_i + \xi_j + \eta_{jr} + \theta_{ij} + e_{ijr}$$

- μ is an intercept,
- α_i is a fixed effect of the ith variety,
- ξ_j is a fixed effect of the jth environment,
- η_{jr} is a fixed effect of the rth complete block,
- θ_{ij} is a fixed effect of variety-by-environment interaction,
- $e_{ijr} \sim N(0, \sigma_E^2)$.

Linear fixed-effects models

$$y_{ijr} = \mu + \alpha_i + \xi_j + \eta_{jr} + \theta_{ij} + e_{ijr}$$

Let $\bar{y}_{ij\cdot} = \sum_{r=1}^{R} y_{ijr}/R$. Then,

$$\bar{y}_{ij\cdot} = \mu + \alpha_i + \beta_j + \theta_{ij} + \bar{e}_{ij\cdot}$$

where $\beta_j = \xi_j + \sum_{r=1}^{R} \eta_{jr}/R$ and $\bar{e}_{ij\cdot} = \sum_{r=1}^{R} e_{ijr}/R$.

Linear mixed-effects models

Random effects of **environments**

$$\bar{y}_{ij.} = \mu + \alpha_i + b_j + s_{ij} + \bar{e}_{ij.}$$

where $b_i \sim N(0, \sigma_B^2)$, $s_{ij} \sim N(0, \sigma_S^2)$

(Shukla, 1972; Patterson, 1978).

- If some varieties are missing in some environments, this model might be preferred to the fixed-effects model.
- Inter-environment information is often small (Piepho and Möhring, 2006).

Linear mixed-effects models

Random effects of **varieties**

$$\bar{y}_{ij.} = \mu + a_i + \beta_j + s_{ij} + \bar{e}_{ij.}$$

where $a_i \sim N(0, \sigma_A^2)$, $s_{ij} \sim N(0, \sigma_S^2)$ (Smith, Cullis and Gilmour, 2001).

- Good for prediction of variety effects.
- Popular in plant breeding, where genotypes are correlated according to some genomic relationship matrix (Montesinos-López et al., 2018).

Linear mixed-effects models

Random effects of variety-by-environment **interaction only**

$$\bar{y}_{ij.} = \mu + \alpha_i + \beta_j + s_{ij} + \bar{e}_{ij.}$$

- Random main effects imply random interaction, but not the other way around.
- This model is commonly used in meta-analysis (Piepho, Williams and Madden, 2012).

Bilinear models

The Finlay-Wilkinson (1963) regression model

$$\bar{y}_{ij\cdot} = \mu + \alpha_i + \phi_i w_j + s_{ij} + \bar{e}_{ij\cdot}$$

where ϕ_i is the sensitivity of the ith variety to a latent environmental variable w_j (Piepho, 1999).

- Environment means are often used as estimates of w_j, even though these are not the least-squares estimates (Digby, 1979; Mandel, 1995).
- Models with multiplicative terms, such as $\phi_i w_j$, are known as bilinear models (Gabriel, 1978).

Bilinear models

Mandel (1971) partitioned the interaction term into a sum of multiplicative terms:

$$\bar{y}_{ij\cdot} = \mu + \alpha_i + \beta_j + \sum_{m=1}^{M+1} \gamma_{im}\lambda_m\delta_{jm} + p_{ij}$$

where $p_{ij} \sim N(0, \sigma_P^2)$ and $\sum_{m=1}^{M+1} \gamma_{im}\lambda_m\delta_{jm}$ is the singular value decomposition of the $I \times J$ matrix $\mathbf{\Theta} = \{\bar{y}_{ij\cdot} - \mu - \alpha_i - \beta_j - p_{ij}\}$.

- In variety testing, this model is known as the AMMI model (Gauch, 1988).

- If main effects of varieties, α_i, are omitted, this models is known as the GGE model (Yan et al., 2000).

Bilinear models

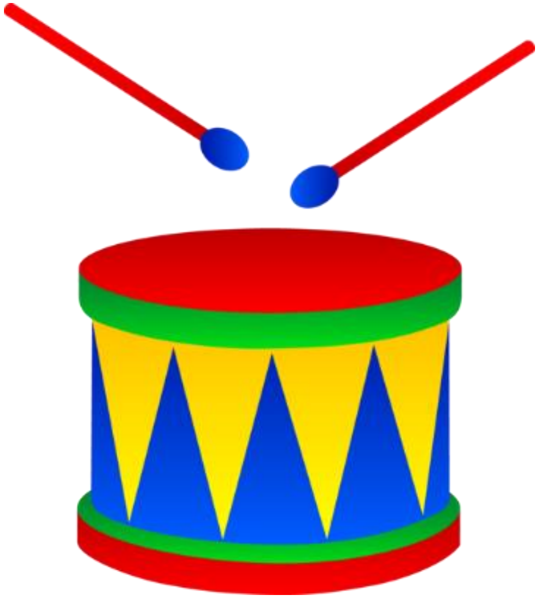
In the bilinear model:

$$\bar{y}_{ij\cdot} = \mu + \alpha_i + \beta_j + \sum_{m=1}^{M+1} \gamma_{im}\lambda_m\delta_{jm} + p_{ij}$$

Let $p_{ij} = s_{ij} + \sum_{r=1}^{R} e_{ijr}/R$,

where $s_{ij} \sim N(0, \sigma_S^2)$ and $e_{ijr} \sim N(0, \sigma_E^2)$.

Then $\sigma_P^2 = \sigma_S^2 + \sigma_E^2/R$, and we have...



... the mixed-interaction model!

The mixed-interaction model

$$\bar{y}_{ij\cdot} = \mu + \alpha_i + \beta_j + \theta_{ij} + s_{ij} + \bar{e}_{ij\cdot}$$

where $\theta_{ij} = \sum_{m=1}^{M+1} \gamma_{im}\lambda_m\delta_{jm}$ and $\bar{e}_{ij\cdot} = \sum_{r=1}^{R} e_{ijr}/R$

- This model is essentially the AMMI model for replicated data (Gauch, 1988), but with the addition of the explicit assumptions that $s_{ij} \sim N(0, \sigma_S^2)$ and $\bar{e}_{ij\cdot} \sim N(0, \sigma_E^2/R)$.

The mixed-interaction model

$$\bar{y}_{ij.} = \mu + \alpha_i + \beta_j + \theta_{ij} + s_{ij} + \bar{e}_{ij.}$$

deviation from a regression
on latent predictor variables

Generalization of the Finlay-Wilkinson regression model

$$\bar{y}_{ij.} = \mu + \alpha_i + \phi_i w_j + s_{ij} + \bar{e}_{ij.}$$

deviation from a regression
on a latent predictor variable

The mixed-interaction model is general

$$\bar{y}_{ij\cdot} = \mu + \alpha_i + \beta_j + \theta_{ij} + s_{ij} + \bar{e}_{ij\cdot}$$

When $s_{ij} > 0$, then $\theta_{ij} + s_{ij} = \sum_{m=1}^{M+1} \gamma'_{im}\lambda'_m\delta'_{jm}$, so that

$$\bar{y}_{ij\cdot} = \mu + \alpha_i + \beta_j + \sum_{m=1}^{M+1} \gamma'_{im}\lambda'_m\delta'_{jm} + \bar{e}_{ij\cdot}$$

When $s_{ij} = 0$, then

$$\bar{y}_{ij\cdot} = \mu + \alpha_i + \beta_j + \sum_{m=1}^{M+1} \gamma_{im}\lambda_m\delta_{jm} + \bar{e}_{ij\cdot}$$

When $\theta_{ij} = 0$, then

$$\bar{y}_{ij\cdot} = \mu + \alpha_i + \beta_j + s_{ij} + \bar{e}_{ij\cdot}$$

2. Hypothesis tests

Multi-environment trial of rapeseed

Means of $R = 4$ replicates

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Shafii and Price (1989)

Two-way analysis of variance

$$\bar{y}_{ij.} = \mu + \alpha_i + \beta_j + \theta_{ij} + \bar{e}_{ij.}$$

	Df	Sum Sq	Mean Sq	F value	Pr(>F)	
var	5	3.05	0.609	2.9586	0.014	*
env	8	367.01	45.876	222.8078	< 0.001	***
var:env	40	53.68	1.342	6.5173	< 0.001	***
Residuals	162	33.36	0.206			

Remove the main effects

$$\hat{\boldsymbol{\Theta}} = \{\bar{y}_{ij.} - \bar{y}_{i..} - \bar{y}_{.j.} + \bar{y}_{...}\} =$$

	TGA	NC	GGA	SC	VA	TN	NY	WA	ID	Mean
Dwarf	-0.68	0.17	-0.11	-0.87	-0.02	0.22	0.58	0.07	0.64	0
Jet	-0.33	-0.45	0.07	-0.81	0.23	0.41	0.20	0.10	0.58	0
Cascade	0.59	-0.29	-0.08	0.82	-0.35	-0.67	-0.68	0.69	-0.04	0
Bridger	0.83	0.18	-0.57	0.86	-0.21	-0.24	-0.19	0.75	-1.42	0
Glacier	-0.24	0.12	0.40	-0.14	0.21	-0.29	0.15	-0.35	0.15	0
Bienvenu	-0.17	0.26	0.30	0.14	0.14	0.56	-0.07	-1.26	0.09	0
Mean	0	0	0	0	0	0	0	0	0	0

Decompose the interaction

Through singular value decomposition, this matrix can be written as a sum of multiplicative terms:

$$\widehat{\boldsymbol{\Theta}} = \{\bar{y}_{ij.} - \bar{y}_{i..} - \bar{y}_{.j.} + \bar{y}_{...}\} =$$

$$= \{\hat{\gamma}_{i1}\hat{\lambda}_1\hat{\delta}_{j1} + \hat{\gamma}_{i2}\hat{\lambda}_2\hat{\delta}_{j2} + \cdots + \hat{\gamma}_{iM}\hat{\lambda}_M\hat{\delta}_{jM}\}$$

where $M = \min(I-1, J-1) = 5$

Keep the leading terms! 

Singular values

$\hat{\lambda}_1$	3.00	?
$\hat{\lambda}_2$	1.57	?
$\hat{\lambda}_3$	1.14	?
$\hat{\lambda}_4$	0.68	
$\hat{\lambda}_5$	0.46	

Bilinear models

If a single term is retained: $\mu + \alpha_i + \beta_j + \gamma_{i1}\lambda_1\delta_{j1}$

If two terms are retained: $\mu + \alpha_i + \beta_j + \gamma_{i1}\lambda_1\delta_{j1} + \gamma_{i2}\lambda_2\delta_{j2}$

If three terms are retained: $\mu + \alpha_i + \beta_j + \gamma_{i1}\lambda_1\delta_{j1} + \gamma_{i2}\lambda_2\delta_{j2} + \gamma_{i3}\lambda_3\delta_{j3}$

A *bilinear model* is linear with respect to rows and columns.

How many multiplicative terms should be retained?

Two significance tests:

- Simple parametric bootstrap (SPB) test

  Forkman and Piepho (2014)

- F_R-test

  Piepho (1995)

Simple parametric bootstrap (SPB) test

Model: $$\bar{y}_{ij\cdot} = \mu + \alpha_i + \beta_j + \sum_m \gamma_{im}\lambda_m\delta_{jm} + p_{ij}$$

where $p_{ij} \sim \mathrm{N}(0, \sigma_P^2)$

Null hypotheses: $H_0\colon \lambda_{\kappa+1} = 0, \qquad \kappa = 0, 1, 2, \ldots$

Test statistic: $$T = \frac{\hat{\lambda}_{\kappa+1}^2}{\sum_{m=\kappa+1}^{M} \hat{\lambda}_m^2}$$

Simple parametric bootstrap (SPB) test

1. Do the following a large number of times:

   i. Sample an $(I - 1 - \kappa) \times (J - 1 - \kappa)$ matrix of $\mathrm{N}(0,1)$ values.

   ii. For this matrix, compute $T_b = \hat{\lambda}_1^2 / \sum_m \hat{\lambda}_m^2$.

2. Estimate the p-value as the frequency of T_b larger than T.

The simple parametric bootstrap (SPB) test

H_0	*p*-value
$\lambda_1 = 0$	0.006
$\lambda_2 = 0$	0.377

A single multiplicative term is retained.

Fitted values: $\hat{\mu} + \hat{\alpha}_i + \hat{\beta}_j + \hat{\gamma}_{i1}\hat{\lambda}_1\hat{\delta}_{j1}$

F_R test

Model: $$\bar{y}_{ij.} = \mu + \alpha_i + \beta_j + \sum_{m=1}^{M+1} \gamma'_{im}\lambda'_m\delta'_{jm} + \bar{e}_{ij.}$$

where $\bar{e}_{ij.} \sim \mathrm{N}(0, \sigma_E^2/R)$

Null hypotheses: $H_0\colon \lambda'_{\kappa+1} = 0, \qquad \kappa = 0, 1, 2, \ldots$

Test statistic: $$F = \frac{\mathrm{MSR}}{\mathrm{MSE}}$$

$$\mathrm{MSR} = R\sum_{m=\kappa+1}^{M} \hat{\lambda}_m^2 \Big/ \big((I-1-\kappa)(J-1-\kappa)\big)$$

$$\mathrm{MSE} = \sum_{i=1}^{I}\sum_{j=1}^{J}\sum_{\mathrm{r}=1}^{R}\left(y_{ijr} - \bar{y}_{ij.} - \bar{y}_{.jr} + \bar{y}_{.j.}\right)^2 \Big/ \big(J(I-1)(K-1)\big)$$

Compare with an $\mathrm{F}_{(I-1-\kappa)(J-1-\kappa),\, I(J-1)(K-1)}$ distribution.

The F_R test

H_0	p-value
$\lambda_1 = 0$	0.000
$\lambda_2 = 0$	0.000
$\lambda_3 = 0$	0.009
$\lambda_4 = 0$	0.237

Three multiplicative terms are retained.

Fitted values: $\hat{\mu} + \hat{\alpha}_i + \hat{\beta}_j + \hat{\gamma}_{i1}\hat{\lambda}_1\hat{\delta}_{j1} + \hat{\gamma}_{i2}\hat{\lambda}_2\hat{\delta}_{j2} + \hat{\gamma}_{i3}\hat{\lambda}_3\hat{\delta}_{j3}$

The results of the two tests differ

The SPB test

H_0	*p*-value
$\lambda_1 = 0$	0.006
$\lambda_2 = 0$	0.377

The F_R test

H_0	*p*-value
$\lambda_1 = 0$	0.000
$\lambda_2 = 0$	0.000
$\lambda_3 = 0$	0.009
$\lambda_4 = 0$	0.237

Conclusions differ

The SPB test:

$$\hat{\mu} + \hat{\alpha}_i + \hat{\beta}_j + \hat{\gamma}_{i1}\hat{\lambda}_1\hat{\delta}_{j1}$$

Dwarf is the best variety for Georgia.

The F_R test:

$$\hat{\mu} + \hat{\alpha}_i + \hat{\beta}_j + \hat{\gamma}_{i1}\hat{\lambda}_1\hat{\delta}_{j1} + \hat{\gamma}_{i2}\hat{\lambda}_2\hat{\delta}_{j2} + \hat{\gamma}_{i3}\hat{\lambda}_3\hat{\delta}_{j3}$$

Bienvenu is the best variety for Georgia.

How many multiplicative terms should be retained?

Two significance tests:

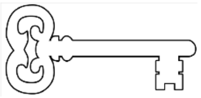
Test	Replicates
Simple parametric bootstrap (SPB) test Forkman and Piepho (2014)	Does not require replicates
F_R-test Piepho (1995)	Requires replicates

SPB test

$$\bar{y}_{ij.} = \mu + \alpha_i + \beta_j + \sum_m \gamma_{im}\lambda_m\delta_{jm} + p_{ij}$$

F_R-test

$$\bar{y}_{ij.} = \mu + \alpha_i + \beta_j + \boxed{\sum_m \gamma'_{im}\lambda'_m\delta'_{jm}} + \bar{e}_{ij.}$$



$p_{ij} = s_{ij} + \bar{e}_{ij.}$ where $s_{ij} \sim \mathrm{N}(0, \sigma_s^2)$, $\bar{e}_{ij.} \sim \mathrm{N}(0, \sigma_E^2/R)$

$$\bar{y}_{ij.} = \mu + \alpha_i + \beta_j + \boxed{\sum_m \gamma_{im}\lambda_m\delta_{jm} + s_{ij}} + \bar{e}_{ij.}$$

The SPB and F_R tests are used for different null hypotheses

$$\bar{y}_{ij.} = \mu + \alpha_i + \beta_j + \sum_m \gamma_{im}\lambda_m\delta_{jm} + s_{ij} + \bar{e}_{ij.}$$

$$= \mu + \alpha_i + \beta_j + \sum_m \gamma'_{im}\lambda'_m\delta'_{jm} + \bar{e}_{ij.}$$

SPB test

$H_0: \lambda_{\kappa+1} = 0$

F_R-test

$H_0: \lambda'_{\kappa+1} = 0$

3. Simulation study

Simulation study setup

$$y_{ijr} = \gamma_{i1}\lambda_1\delta_{j1} + \gamma_{i2}\lambda_2\delta_{j2} + s_{ij} + e_{ijr}$$

where $i = 1, 2, \ldots, 15$; $j = 1, 2, \ldots, 10$; $r = 1, 2, 3, 4$

and $\sigma_E^2 = 1$.

For each case, $100\ 000$ datasets were generated.

Results of the simulation study

Frequencies of significant results when testing at level 0.05

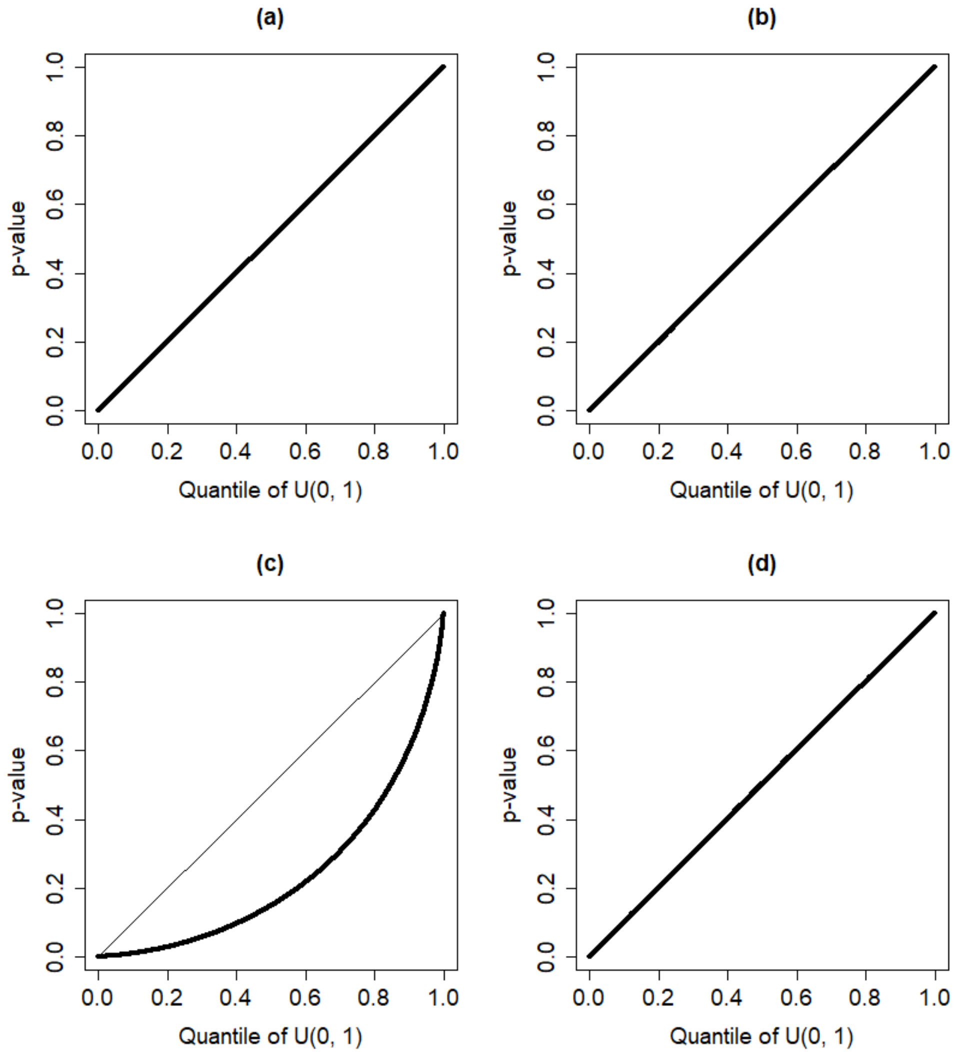
Parameter settings				F_R test		SPB test	
Case	λ_1	λ_2	σ_S^2	Null hypothesis	Freq.	Null hypothesis	Freq.
1	0	0	0	H_0: $\lambda_1' = 0$	0.051 [a]	H_0: $\lambda_1 = 0$	0.051 [a]
2	0	0	0.04	H_0: $\lambda_1' = 0$	0.281 [b]	H_0: $\lambda_1 = 0$	0.050 [a]

a) Frequency of Type I error, b) Power

F_R test SPB test

Case	λ_1	λ_2	σ_S^2
1	0	0	0

Case	λ_1	λ_2	σ_S^2
2	0	0	0.04



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2	0	0	0.04	$H_0\colon \lambda_1' = 0$	0.281 [b]	$H_0\colon \lambda_1 = 0$	0.050 [a]
3	2	0	0	$H_0\colon \lambda_1' = 0$	0.181 [b]	$H_0\colon \lambda_1 = 0$	0.131 [b]
4	2	0	0.04	$H_0\colon \lambda_1' = 0$	0.517 [b]	$H_0\colon \lambda_1 = 0$	0.109 [b]

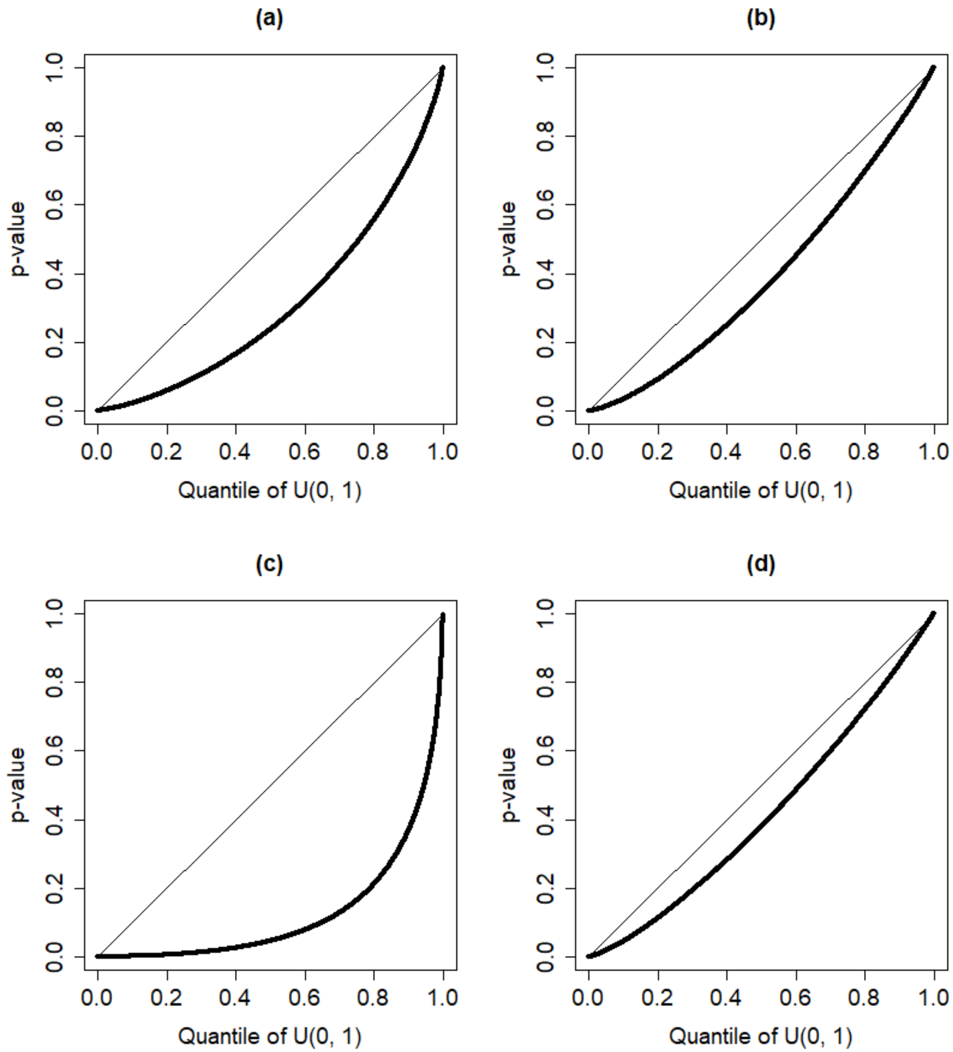
[a)] Frequency of Type I error, [b)] Power

F_R test

SPB test

Case	λ_1	λ_2	σ_S^2
3	2	0	0

Case	λ_1	λ_2	σ_S^2
4	2	0	0.04



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4	2	0	0.04	$H_0\colon \lambda_1' = 0$	0.517 [b]	$H_0\colon \lambda_1 = 0$	0.109 [b]
5	10	0	0	$H_0\colon \lambda_2' = 0$	0.047 [a]	$H_0\colon \lambda_2 = 0$	0.050 [a]
6	10	0	0.04	$H_0\colon \lambda_2' = 0$	0.248 [b]	$H_0\colon \lambda_2 = 0$	0.050 [a]

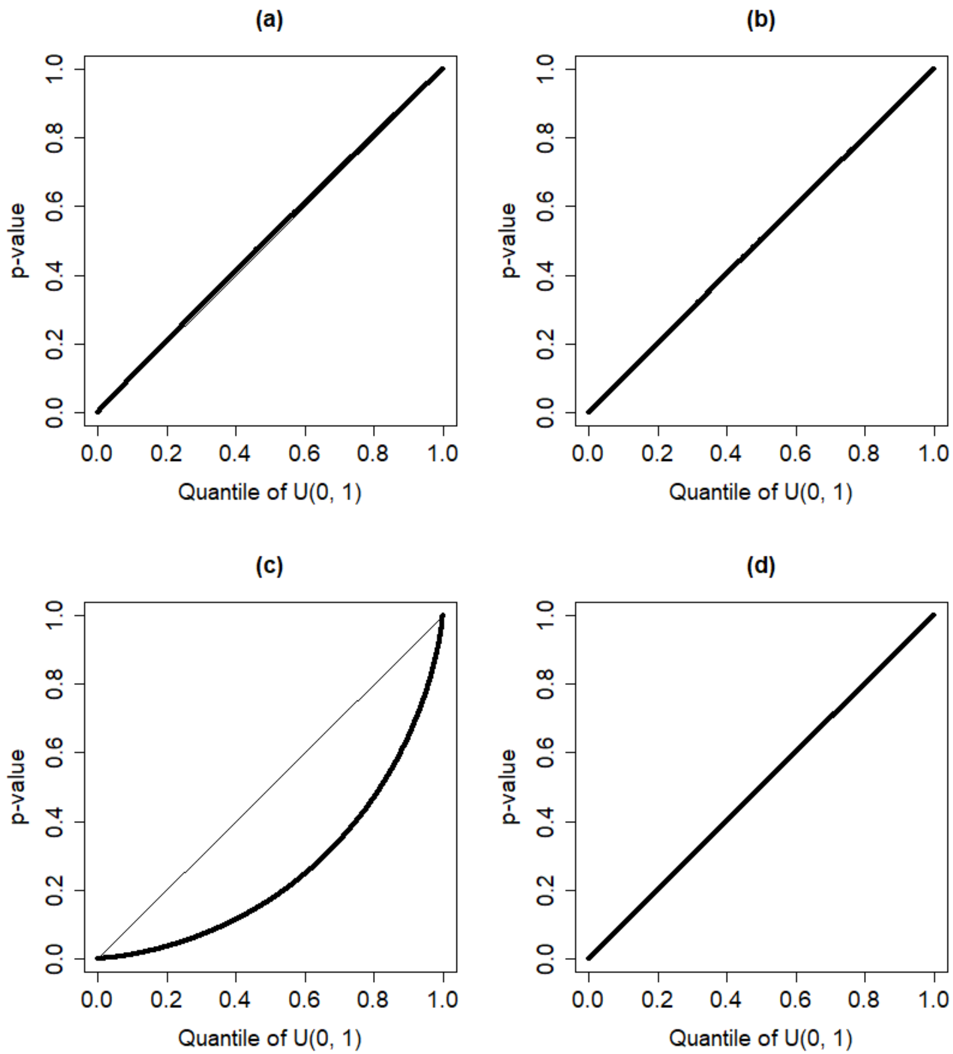
[a)] Frequency of Type I error, [b)] Power

Case	λ_1	λ_2	σ_S^2
5	10	0	0

Case	λ_1	λ_2	σ_S^2
6	10	0	0.04

F_R test

SPB test



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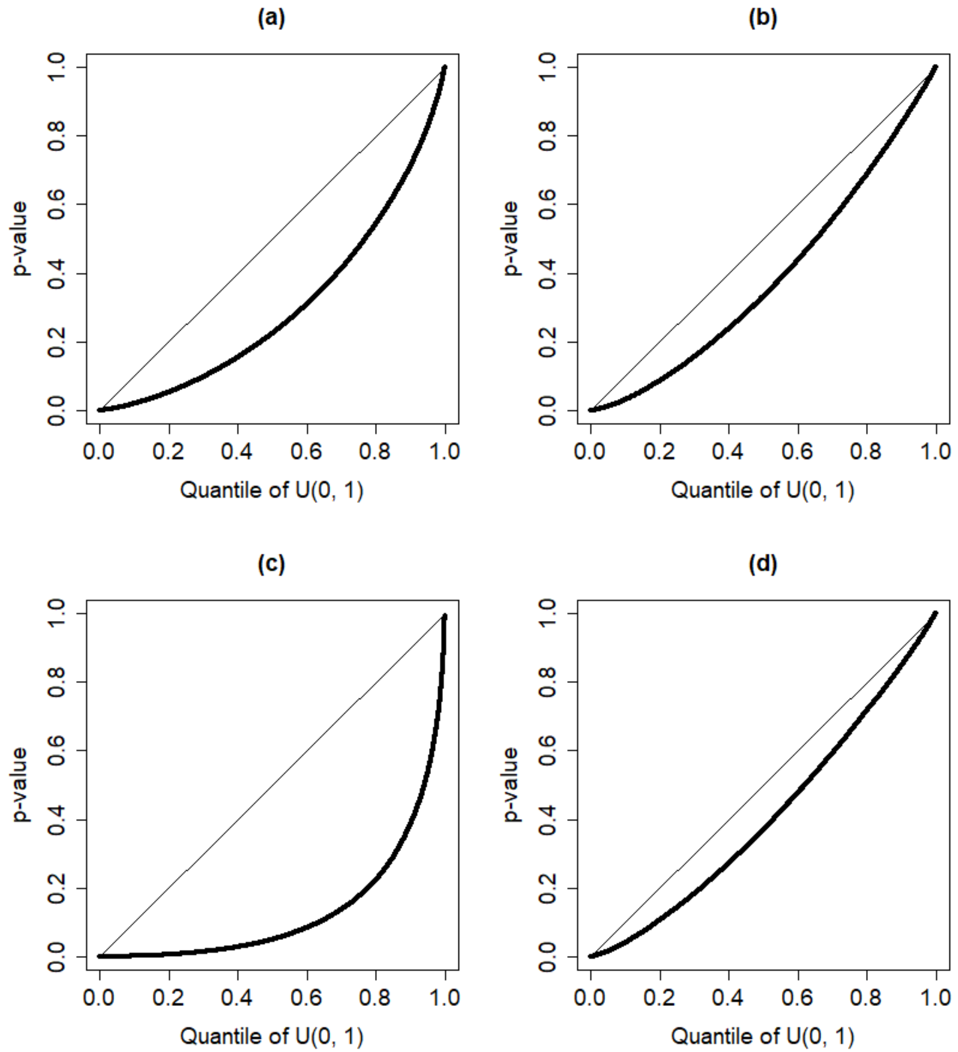
6	10	0	0.04	$H_0\colon \lambda_2' = 0$	0.248 [b]	$H_0\colon \lambda_2 = 0$	0.050 [a]
7	10	2	0	$H_0\colon \lambda_2' = 0$	0.194 [b]	$H_0\colon \lambda_2 = 0$	0.138 [b]
8	10	2	0.04	$H_0\colon \lambda_2' = 0$	0.503 [b]	$H_0\colon \lambda_2 = 0$	0.115 [b]

[a)] Frequency of Type I error, [b)] Power

F_R test SPB test

Case	λ_1	λ_2	σ_S^2
7	10	2	0

Case	λ_1	λ_2	σ_S^2
8	10	2	0.04



Conclusions from the simulation study

- When there is random interaction, the tests aim at different hypotheses.

- When there is no random interaction, the F_R test is more powerful than the SPB test.

4. Practical advice

The tests should be used for different questions

- The SPB test investigates null hypotheses regarding **the fixed-effects part** of the interaction.

- The F_R test explores null hypotheses regarding **the sum of the fixed and the random parts** of the interaction.

The tests should be used for different questions

- The SPB test aims at finding fixed patterns in the interaction that are larger than would be expected by random variety-by-environment interaction.

- The F_R test aims at any interaction in the data, regardless of this interaction being fixed or random.

The effect of replication

In practice, variety-by-environment interaction usually exists. In this case:

- The F_R test gives significant results if the number of repliactes is sufficiently large.

- The SPB test does not necessarily give significant results, even if the number of replicates is large.

Is random interaction signal or noise?

$$\bar{y}_{ij.} = \mu + \alpha_i + \beta_j + \theta_{ij} + s_{ij} + \bar{e}_{ij.}$$

- If the random interaction, s_{ij}, is regarded as **signal**, then use the F_R test.

- If the random interaction, s_{ij}, is regarded as **noise**, then use the SPB test.

The F_R test is useful for these questions:

- Which variety performs best in some specific environment?
- Which environment is best for some specific variety?

Bienvenu is the best variety for Georgia!

The SPB test is useful for:

- ❖ Grouping of environments into mega-environments that will be used for future varieties.

- ❖ Finding out which varieties respond similarly under varying environmental conditions.

Different inference spaces

- The SPB test should be used for **broad** inference, which extends beyond the experiment.

- The F_R test should be used for **narrow** inference, which is confined to the investigated environments and varieties.

Summary

- Multiplicative components of interaction can be tested using the SPB test and the F_R test.
- The mixed-interaction model is the key to understand the differences between the two tests.
- The SPB test looks for fixed patterns in the interaction that are larger than random effects of interaction.
- The F_R test looks for any effects of interaction, fixed or random, that are larger than expected due to inter-plot variability.

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