Smoothing and extraction of traits in the growth analysis of noninvasive phenotypic data

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Additional File 2: A comparison of the results from separate and joint analyses of per-cart traits

Joint analysis of the per-cart traits

In the proposed analysis of the per-cart traits, each trait is analysed separately by fitting a mixed model to it. However, such an analysis does not take into account the correlation between the measurements of the same trait at different times. To address this a joint analysis was performed, the object of which was to identify a model that described the correlations between the times.

The mixed models for the analysis

The fixed-effects vector $\boldsymbol{\beta}$ is partitioned as $\boldsymbol{\beta}^\top = \left[\mu\ \boldsymbol{\beta}_{\mathrm{B}}^\top\ \boldsymbol{\beta}_{\mathrm{Z}}^\top\ \boldsymbol{\beta}_{\mathrm{A}}^\top\ \boldsymbol{\beta}_{\mathrm{ZA}}^\top\ \boldsymbol{\beta}_{\mathrm{T}}^\top\ \boldsymbol{\beta}_{\mathrm{TB}}^\top\ \boldsymbol{\beta}_{\mathrm{TZ}}^\top\ \boldsymbol{\beta}_{\mathrm{TA}}^\top\ \boldsymbol{\beta}_{\mathrm{TZA}}^\top\right]$, where (i) μ is the overall mean parameter, (ii) $\boldsymbol{\beta}_{\mathrm{Z}}$, $\boldsymbol{\beta}_{\mathrm{A}}$ and $\boldsymbol{\beta}_{\mathrm{ZA}}$ are the Zn main effects, AMF main effects and Zn-AMF interactions effects, (iii) $\boldsymbol{\beta}_{\mathrm{T}}$ is the Time main effects (either DAP of observation or DAP interval midpoint), and (iv) $\boldsymbol{\beta}_{\mathrm{TZ}}$, $\boldsymbol{\beta}_{\mathrm{TA}}$ and $\boldsymbol{\beta}_{\mathrm{TZA}}$ are the Time interactions with Zn and AMF.

The random-effects vector $\mathbf{u}$ is equal to $\mathbf{u}_{\mathrm{BC}}$, a vector of Block-Cart random effects.

The residual effects $\mathbf{e}$ are assumed to be normally distributed with mean vector $\mathbf{0}$ and variance matrix $\boldsymbol{\Sigma}_{32t}$, where t is the number of times per-cart traits were extracted for the primary response being analyzed. For PSA, sPSA was extracted for seven DAPs; for PSA AGR and PSA RGR, six time intervals were calculated for each of sPSA AGR and sPSA AGR. A factor Time will be used to index these different times of observation, with the time of observation of the GRs taken as being for the mid-point of the time intervals i.e. the mean of the two endpoints of each time interval. For $\mathbf{y}$ ordered for Block-Cart then Time, $\boldsymbol{\Sigma}_{32t} = \mathbf{J}_{32} \bigotimes \boldsymbol{\Sigma}_{\mathrm{T}}$, where $\mathbf{J}_{32}$ is a 32×32 matrix of ones and $\boldsymbol{\Sigma}_{\mathrm{T}}$ is a $t \times t$ times matrix specifying the variances and covariances between the times. This implies that $\boldsymbol{\Sigma}_{32t}$ is split into 32×32 blocks each of which consists of $\boldsymbol{\Sigma}_{\mathrm{T}}$. The general form of $\boldsymbol{\Sigma}_{\mathrm{T}}$ is:

$$\boldsymbol{\Sigma}_{\mathrm{T}} = \begin{bmatrix} \sigma_1 & 0 & \cdots & 0 \\ 0 & \sigma_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \sigma_t \end{bmatrix} \begin{bmatrix} 1 & \rho_{12} & \cdots & \rho_{1t} \\ \rho_{21} & 1 & \cdots & \rho_{2t} \\ \vdots & \vdots & \ddots & \vdots \\ \rho_{t1} & \rho_{t2} & \cdots & 1 \end{bmatrix} \begin{bmatrix} \sigma_1 & 0 & \cdots & 0 \\ 0 & \sigma_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \sigma_t \end{bmatrix}$$

where σ_i is the variance for the ith time and ρ_{ij} is the correlation between the ith and jth times. Four different models are considered for $\boldsymbol{\Sigma}_{\mathrm{T}}$:

Heterogeneous, independent times (idh): all σ_is are allowed to differ, $\rho_{ij} = 0$.

Homogeneous, power correlation for times (exp): $\sigma_i = \sigma$ and $\rho_{ij} = \rho^{|i-j|}$.

Heterogeneous, power correlation for times (exph): all σ_is are allowed to differ, $\rho_{ij} = \rho^{|i-j|}$.

Unstructured (us): all σ_is are allowed to differ, as are all ρ_{ij}s.

All four forms of $\boldsymbol{\Sigma}_{\mathrm{T}}$ were fitted to the data and REMLRT tests conducted to compare models. Firstly, us and exph models were compared and if significantly different, the us model was selected as required to describe the data. If not significant, exph was compared with both idh and exp models. If both are significant, then the exph models was selected; if only one if idh and exp is significant, then the significant model is selected.

Results of the analysis

For all three primary responses, the unstructured model was selected because it was significantly different ($p < 0.001$) from the heterogeneous power correlation model. The estimated values of $\mathbf{\Sigma}_{\mathrm{T}}$ are given in Tables S1–S3.

Table S1: Estimated $\mathbf{\Sigma}_{\mathrm{T}}$ for sPSA

1.000	0.958	0.851	0.743	0.596	0.339	-0.093
0.958	1.000	0.955	0.851	0.714	0.449	-0.045
0.851	0.955	1.000	0.940	0.815	0.575	0.028
0.743	0.851	0.940	1.000	0.948	0.768	0.222
0.596	0.714	0.815	0.948	1.000	0.900	0.407
0.339	0.449	0.575	0.768	0.900	1.000	0.723
-0.093	-0.045	0.028	0.222	0.407	0.723	1.000

Table S2: Estimated $\mathbf{\Sigma}_{\mathrm{T}}$ for sPSA AGR

1.000	0.921	0.499	-0.435	-0.561	-0.368
0.921	1.000	0.672	-0.428	-0.450	-0.345
0.499	0.672	1.000	0.142	-0.089	0.022
-0.435	-0.428	0.142	1.000	0.580	0.515
-0.561	-0.450	-0.089	0.580	1.000	0.816
-0.368	-0.345	0.022	0.515	0.816	1.000

Table S3: Estimated $\mathbf{\Sigma}_{\mathrm{T}}$ for sPSA RGR

1.000	0.725	0.377	0.424	0.298	0.198
0.725	1.000	0.757	0.586	0.490	0.156
0.377	0.757	1.000	0.860	0.545	0.297
0.424	0.586	0.860	1.000	0.644	0.421
0.298	0.490	0.545	0.644	1.000	0.798
0.198	0.156	0.297	0.421	0.798	1.000

They demonstrate that the assumption of equal correlation for times the same distance apart is not tenable.

Comparison of results from separate and joint analyses

Firstly, we compare, in Tables S4–S6, the means of the LSDs calculated from the separate and joint analyses for comparing the difference between Zn-AMF combinations with a time. The LSD values for one time are not all in equal, because the removal of a plant means that the treatments are not equally replicated; however, the differences are small. The differences between the two analyses are less than 2%.

Table S4: Mean LSDs from separate and joint analyses for sPSA

	Separate analyses	Joint analysis	Difference (%)
Area.smooth.18	3.3	3.3	-1.19
Area.smooth.22	5.7	5.6	-1.19
Area.smooth.27	10.9	10.8	-1.19
Area.smooth.33	15.7	15.5	-1.19
Area.smooth.39	15.1	14.9	-1.19
Area.smooth.43	14.9	14.8	-1.19
Area.smooth.51	28.1	27.8	-1.19

Table S5: Mean LSDs from separate and joint analyses for sPSA AGR

	Separate analyses	Joint analysis	Difference (%)
Area.smooth.AGR.18to22	0.67	0.66	-1.36
Area.smooth.AGR.22to27	1.15	1.13	-1.36
Area.smooth.AGR.27to33	1.10	1.09	-1.36
Area.smooth.AGR.33to39	0.84	0.83	-1.36
Area.smooth.AGR.39to43	1.68	1.66	-1.36
Area.smooth.AGR.43to51	2.52	2.48	-1.36

Table S6: Mean LSDs from separate and joint analyses for sPSA RGR

	Separate analyses	Joint analysis	Difference (%)
Area.smooth.RGR.18to22	0.046	0.045	-1.36
Area.smooth.RGR.22to27	0.029	0.028	-1.36
Area.smooth.RGR.27to33	0.023	0.022	-1.36
Area.smooth.RGR.33to39	0.017	0.017	-1.36
Area.smooth.RGR.39to43	0.016	0.016	-1.36
Area.smooth.RGR.43to51	0.020	0.020	-1.36

Secondly, we compare the predictions and LSDs obtained from the separate and joint analyses in Tables S7–S9. The LSDs are the mean LSD for a time. There is very little difference between the values obtained from the two analyses.

Table S7: Comparison of predictions and mean LSDs for sPSA

			Separate analyses		Joint analyses	
DAP	AMF	Zn	Prediction	LSD (5%)	Prediction	LSD (5%)
18	-	0	7.48349	3.3258	7.48349	3.2864
18	-	10	7.23739	3.3258	7.23739	3.2864
18	-	40	6.04026	3.3258	6.04026	3.2864
18	-	90	4.12758	3.3258	4.12758	3.2864
18	+	0	9.08390	3.3258	9.08390	3.2864
18	+	10	7.94306	3.3258	7.94306	3.2864
18	+	40	5.88241	3.3258	5.88241	3.2864
18	+	90	5.09575	3.3258	5.09575	3.2864
22	-	0	17.86788	5.6949	17.86788	5.6274
22	-	10	16.62808	5.6949	16.62808	5.6274
22	-	40	12.93739	5.6949	12.93739	5.6274
22	-	90	7.21250	5.6949	7.21250	5.6274
22	+	0	18.37357	5.6949	18.37357	5.6274
22	+	10	16.32219	5.6949	16.32219	5.6274
22	+	40	12.11094	5.6949	12.11094	5.6274
22	+	90	11.88015	5.6949	11.88015	5.6274
27	-	0	51.24286	10.9155	51.24286	10.7861
27	-	10	47.93267	10.9155	47.93267	10.7861
27	-	40	36.04308	10.9155	36.04308	10.7861
27	-	90	14.66772	10.9155	14.66772	10.7861
27	+	0	42.74331	10.9155	42.74331	10.7861
27	+	10	40.02209	10.9155	40.02209	10.7861
27	+	40	30.60120	10.9155	30.60120	10.7861
27	+	90	32.34847	10.9155	32.34847	10.7861
33	-	0	112.01847	15.7225	112.01847	15.5361
33	-	10	106.49127	15.7225	106.49127	15.5361
33	-	40	84.11786	15.7225	84.11786	15.5361
33	-	90	29.12448	15.7225	29.12448	15.5361
33	+	0	81.33478	15.7225	81.33478	15.5361
33	+	10	84.19125	15.7225	84.19125	15.5361
33	+	40	66.38026	15.7225	66.38026	15.5361
33	+	90	70.00257	15.7225	70.00257	15.5361
39	-	0	146.14435	15.0862	146.14435	14.9073
39	-	10	142.03229	15.0862	142.03229	14.9073
39	-	40	118.62116	15.0862	118.62116	14.9073
39	-	90	45.60211	15.0862	45.60211	14.9073
39	+	0	106.31225	15.0862	106.31225	14.9073
39	+	10	116.49478	15.0862	116.49478	14.9073
39	+	40	96.35160	15.0862	96.35160	14.9073
39	+	90	98.27789	15.0862	98.27789	14.9073
43	-	0	150.83970	14.9343	150.83970	14.7572
43	-	10	145.86938	14.9343	145.86938	14.7572
43	-	40	130.15988	14.9343	130.15988	14.7572
43	-	90	56.72693	14.9343	56.72693	14.7572
43	+	0	116.06750	14.9343	116.06750	14.7572
43	+	10	128.64563	14.9343	128.64563	14.7572
43	+	40	108.74468	14.9343	108.74468	14.7572
43	+	90	109.77001	14.9343	109.77001	14.7572
51	-	0	151.44971	28.0834	151.44971	27.7505
51	-	10	141.86055	28.0834	141.86055	27.7505
51	-	40	151.35577	28.0834	151.35577	27.7505
51	-	90	78.34587	28.0834	78.34587	27.7505
51	+	0	137.51969	28.0834	137.51969	27.7505
51	+	10	149.93282	28.0834	149.93282	27.7505
51	+	40	128.14947	28.0834	128.14947	27.7505
51	+	90	132.76307	28.0834	132.76307	27.7505

Table S8: Comparison of predictions and mean LSDs for sPSA AGR

			Separate analyses		Joint analyses	
DAP	AMF	Zn	Prediction	LSD (5%)	Prediction	LSD (5%)
18–22	-	0	2.59610	0.6714	2.59610	0.6622
18–22	-	10	2.34767	0.6714	2.34767	0.6622
18–22	-	40	1.72428	0.6714	1.72428	0.6622
18–22	-	90	0.77123	0.6714	0.77123	0.6622
18–22	+	0	2.32242	0.6714	2.32242	0.6622
18–22	+	10	2.09478	0.6714	2.09478	0.6622
18–22	+	40	1.55713	0.6714	1.55713	0.6622
18–22	+	90	1.69610	0.6714	1.69610	0.6622
22–27	-	0	6.67500	1.1459	6.67500	1.1303
22–27	-	10	6.26092	1.1459	6.26092	1.1303
22–27	-	40	4.62114	1.1459	4.62114	1.1303
22–27	-	90	1.49104	1.1459	1.49104	1.1303
22–27	+	0	4.87395	1.1459	4.87395	1.1303
22–27	+	10	4.73998	1.1459	4.73998	1.1303
22–27	+	40	3.69805	1.1459	3.69805	1.1303
22–27	+	90	4.09366	1.1459	4.09366	1.1303
27–33	-	0	10.12927	1.1011	10.12927	1.0860
27–33	-	10	9.75977	1.1011	9.75977	1.0860
27–33	-	40	8.01246	1.1011	8.01246	1.0860
27–33	-	90	2.40946	1.1011	2.40946	1.0860
27–33	+	0	6.43191	1.1011	6.43191	1.0860
27–33	+	10	7.36153	1.1011	7.36153	1.0860
27–33	+	40	5.96318	1.1011	5.96318	1.0860
27–33	+	90	6.27568	1.1011	6.27568	1.0860
33–39	-	0	5.68765	0.8368	5.68765	0.8254
33–39	-	10	5.92350	0.8368	5.92350	0.8254
33–39	-	40	5.75055	0.8368	5.75055	0.8254
33–39	-	90	2.74627	0.8368	2.74627	0.8254
33–39	+	0	4.16291	0.8368	4.16291	0.8254
33–39	+	10	5.38392	0.8368	5.38392	0.8254
33–39	+	40	4.99522	0.8368	4.99522	0.8254
33–39	+	90	4.71255	0.8368	4.71255	0.8254
39–43	-	0	1.17384	1.6814	1.17384	1.6585
39–43	-	10	0.95927	1.6814	0.95927	1.6585
39–43	-	40	2.88468	1.6814	2.88468	1.6585
39–43	-	90	2.78121	1.6814	2.78121	1.6585
39–43	+	0	2.43881	1.6814	2.43881	1.6585
39–43	+	10	3.03771	1.6814	3.03771	1.6585
39–43	+	40	3.09827	1.6814	3.09827	1.6585
39–43	+	90	2.87303	1.6814	2.87303	1.6585
43–51	-	0	0.07625	2.5153	0.07625	2.4809
43–51	-	10	-0.50110	2.5153	-0.50110	2.4809
43–51	-	40	2.64949	2.5153	2.64949	2.4809
43–51	-	90	2.70237	2.5153	2.70237	2.4809
43–51	+	0	2.68152	2.5153	2.68152	2.4809
43–51	+	10	2.66090	2.5153	2.66090	2.4809
43–51	+	40	2.42560	2.5153	2.42560	2.4809
43–51	+	90	2.87413	2.5153	2.87413	2.4809

Table S9: Comparison of predictions and mean LSDs for sPSA RGR

			Separate analyses		Joint analyses	
DAP	AMF	Zn	Prediction	LSD (5%)	Prediction	LSD (5%)
18–22	-	0	0.22677	0.0456	0.22677	0.0450
18–22	-	10	0.21103	0.0456	0.21103	0.0450
18–22	-	40	0.19333	0.0456	0.19333	0.0450
18–22	-	90	0.14470	0.0456	0.14470	0.0450
18–22	+	0	0.17960	0.0456	0.17960	0.0450
18–22	+	10	0.17964	0.0456	0.17964	0.0450
18–22	+	40	0.19441	0.0456	0.19441	0.0450
18–22	+	90	0.20741	0.0456	0.20741	0.0450
22–27	-	0	0.21272	0.0288	0.21272	0.0284
22–27	-	10	0.21255	0.0288	0.21255	0.0284
22–27	-	40	0.20573	0.0288	0.20573	0.0284
22–27	-	90	0.14503	0.0288	0.14503	0.0284
22–27	+	0	0.17307	0.0288	0.17307	0.0284
22–27	+	10	0.17897	0.0288	0.17897	0.0284
22–27	+	40	0.18944	0.0288	0.18944	0.0284
22–27	+	90	0.19927	0.0288	0.19927	0.0284
27–33	-	0	0.13055	0.0227	0.13055	0.0224
27–33	-	10	0.13338	0.0227	0.13338	0.0224
27–33	-	40	0.14161	0.0227	0.14161	0.0224
27–33	-	90	0.11843	0.0227	0.11843	0.0224
27–33	+	0	0.11069	0.0227	0.11069	0.0224
27–33	+	10	0.12463	0.0227	0.12463	0.0224
27–33	+	40	0.12954	0.0227	0.12954	0.0224
27–33	+	90	0.12956	0.0227	0.12956	0.0224
33–39	-	0	0.04449	0.0170	0.04449	0.0167
33–39	-	10	0.04862	0.0170	0.04862	0.0167
33–39	-	40	0.05724	0.0170	0.05724	0.0167
33–39	-	90	0.07863	0.0170	0.07863	0.0167
33–39	+	0	0.04619	0.0170	0.04619	0.0167
33–39	+	10	0.05471	0.0170	0.05471	0.0167
33–39	+	40	0.06226	0.0170	0.06226	0.0167
33–39	+	90	0.05742	0.0170	0.05742	0.0167
39–43	-	0	0.00774	0.0160	0.00774	0.0158
39–43	-	10	0.00658	0.0160	0.00658	0.0158
39–43	-	40	0.02298	0.0160	0.02298	0.0158
39–43	-	90	0.05721	0.0160	0.05721	0.0158
39–43	+	0	0.02293	0.0160	0.02293	0.0158
39–43	+	10	0.02500	0.0160	0.02500	0.0158
39–43	+	40	0.03022	0.0160	0.03022	0.0158
39–43	+	90	0.02827	0.0160	0.02827	0.0158
43–51	-	0	-0.00026	0.0204	-0.00026	0.0202
43–51	-	10	-0.00610	0.0204	-0.00610	0.0202
43–51	-	40	0.01803	0.0204	0.01803	0.0202
43–51	-	90	0.04243	0.0204	0.04243	0.0202
43–51	+	0	0.02148	0.0204	0.02148	0.0202
43–51	+	10	0.01901	0.0204	0.01901	0.0202
43–51	+	40	0.02051	0.0204	0.02051	0.0202
43–51	+	90	0.02371	0.0204	0.02371	0.0202