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1 **Title**

2 Searching for the origins of bere barley: a geometric morphometric
3 approach to cereal landrace recognition in archaeology

4 **Authors**

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8 **Abstract**

9 Bere is a landrace of barley, adapted to the marginal conditions of northern
10 Scotland, especially those of the Northern and Western Isles. The history of
11 bere on these islands is long and, in an era of diminishing landrace
12 cultivation, bere now represents one of the oldest cereal landraces in Europe
13 still grown commercially. The longevity of bere raises the possibility of using
14 grain characteristics of present-day specimens to identify bere in the
15 archaeological record. Geometric modern morphometric (GMM) analysis of
16 grains from bere and other barley landraces is conducted to determine
17 whether landraces can be differentiated on grain morphology. Results
18 indicate that there are morphological differences between bere and other
19 British and Scandinavian landraces, and between bere from Orkney and the
20 Western Isles, both of which are apparent in genetic analysis. This finding
21 paves the way for the identification of bere archaeologically, helping to
22 establish its status as living heritage and securing its commercial future.
23 More broadly, this work indicates the potential of grain GMM for the
24 recognition of cereal landraces, permitting the ancestry and exchange of
25 landraces to be traced in the archaeological record.

26 **Keywords**

27 Barley; cereals; landraces; archaeology; archaeobotany; agriculture;
28 genetics; geometric morphometrics.

29 **Introduction**

30 The spread of agriculture beyond the regions of cereal domestication in the
31 fertile crescent of southwest Asia, was a lengthy process crossing
32 biogeographic boundaries. Following initial expansion through Anatolia and
33 to Cyprus, domesticated crops reached southeast Europe c.8,500 yrs BP, and
34 from there were dispersed along two main routes: a southern route along
35 the Mediterranean, reaching the Iberian peninsula c.7500 yrs BP, and a
36 northwards route passing through central Europe by c.7,500 yrs BP and
37 eventually reaching northern Scotland c.6,000 yrs BP (Bocquet-Appel et al.
38 2009; Fort 2015). The continued viability of agriculture as it spread across
39 Europe, especially along the latter northwards trajectory, required crops to
40 adapt to environmental conditions starkly different to those under which
41 they were first domesticated (Bogucki 2000; Bonsall et al. 2002; Halstead
42 1989). This is exemplified by adaptations in responsiveness to daylength
43 with the northwards spread of agriculture (Jones et al. 2012) and observed
44 adaptation to specific abiotic stresses (George et al. 2014; Schmidt et al. in
45 prep.). Adaptation in crop species would have come about through periods
46 of stable cultivation on the edges of new environments, leading to the
47 emergence of new, locally-adapted landraces.

48 Landraces are distinguished from modern varieties by their genetic
49 diversity, long history of cultivation in specific regions and lack of formal
50 breeding (Camacho Villa et al. 2006). While modern plant breeding
51 programmes have successfully produced high yielding varieties well-suited
52 to intensive agriculture, this has been accompanied by a large decline in
53 farmed landraces. Although landraces have previously been of importance
54 to many local farming communities, they are 'invisible' to traditional
55 archaeobotanical methods based on identification by eye (e.g. Pearsall 1989;
56 Jacomet and Kreuz 1999). For example, most grains of domesticated barley
57 preserved on archaeological sites are identified to the level of species
58 (*Hordeum vulgare* L.). The presence of two-row (*H. vulgare* var. *distichum*)
59 and six-row (*H. vulgare* var. *hexasticum*) forms can be inferred, at the
60 assemblage level, by the ratio of straight (central) and twisted (lateral)
61 grains, and naked forms (*H. vulgare* var. *nudum*) by the absence of hulls on
62 grains, but further identification to the level of landrace is not attempted.

63 Information about ancient landraces can be inferred through ancient DNA
64 (aDNA) analysis of preserved plant remains (Brown et al. 2015). Analysis of
65 aDNA from barley grains has revealed new insights into the past use of the
66 crop, including millennium-long landrace fidelity (Hagenblad et al. 2017)
67 and the maintenance of local crop populations despite major human
68 demographic change (Mascher et al. 2016; Palmer et al. 2009). These studies
69 are restricted to grains preserved through desiccation, very rare in the
70 archaeological record, or relatively recent deposits (up to c.3000 yrs BP) of
71 charred grain, owing to the poor preservation of DNA following charring
72 (e.g. Bunning et al. 2012). As charring is the most common mode of
73 archaeobotanical preservation, new approaches are required to broaden our
74 knowledge of the role of landraces in ancient agriculture.

75 ***Geometric morphometrics as a new approach to landrace*** 76 ***recognition***

77 The recognition of landraces archaeologically requires the capture of
78 information from preserved plant remains that is diagnostic between
79 landraces. Subtle variations in grain shape, that cannot be quantified
80 through identification-by-eye, may prove informative. Shape variation can
81 be quantified using morphometrics, and in particular the analytically
82 powerful field of geometric modern morphometrics (GMM). GMM gathers an
83 array of highly versatile mathematical descriptors of shapes that turns
84 homologous landmarks (two- or three-dimensionally arranged), outlines
85 (open or closed) or surfaces into quantitative variables that can be analysed
86 in multivariate statistical framework. GMM has additional merit for
87 archaeological application in that it is non-destructive and low-cost.

88 GMM is widely used, especially in the field of evolutionary biology (Cope et
89 al. 2012; Mitteroecker and Gunz 2009; Adams et al. 2004; Zelditch et al.
90 2012), but also increasingly in archaeology, on both material culture (e.g.
91 Lycett and von Cramon-Taubadel 2013) and biological remains (e.g. Perez et
92 al. 2006; Ottoni et al. 2013). In archaeobotany, GMM has proven successful
93 in identifying fruit crop varieties from the shape of pips of grapevine (*Vitis*
94 *vinifera* L.) (Ucchesu et al. 2016; Pagnoux et al. 2015; Bouby et al. 2013;
95 Terral et al. 2010; Orrù et al. 2013), and fruit stones of date palm (*Phoenix*
96 *dactylifera* L.) (Terral et al. 2012), cherry (*Prunus avium* L.) (Burger et al.

97 2011) and olive (*Olea europaea* L.) (C. Newton et al. 2014; C. Newton et al.
98 2006; Terral et al. 2004). The identification of varieties for these taxa is not
99 possible using traditional archaeobotanical techniques, and so variety
100 recognition using GMM permits a re-evaluation of the economic and social
101 role of these past crops (e.g. Pagnoux et al. 2015).

102 Large-seeded cereals were amongst the first domesticated crops, and were
103 throughout much of prehistory the main calorie source, and continue to be
104 of central importance in modern agricultural production. The use of GMM to
105 investigate these important crops has been limited. Ros *et al.* (2014)
106 demonstrated that GMM can be used to differentiate grains of two-row
107 barley from those of six-row barley, across ten cultivars grown in the same
108 conditions. Bonhomme *et al.* (2017) also demonstrated that the grains from
109 three different samples can be differentiated for barley, as well as for
110 einkorn (*Triticum monococcum* L.) and emmer (*T. dicocum* Schübl.). Both of
111 these studies considered the effects of charring on grain morphology, and
112 show that the greatest effect of charring on grain is in terms of size, with
113 grains typically shrinking by around 10% (Charles et al. 2015). As size
114 information can be discarded by the normalisation of outlines or landmarks
115 in GMM, this aspect of charring is inconsequential. Charring also alters grain
116 shape, however, resulting in rounder grains, but since the effect is consistent
117 and predictable, it has been demonstrated to be of limited detriment to grain
118 analysis. Ros *et al.* (2014) classified grains to their row type following linear
119 discriminant analysis (LDA) and found that the leave-one-out (LOO)
120 reclassification rate only reduced from 91% to 86% following charring at
121 250°C. In the Bonhomme *et al.* (2017) study, the more challenging
122 reclassification to within-species samples was reduced from 67% to 50%
123 correct. These results indicate that there is good reason to expect GMM
124 results based on the morphology of uncharred grain to be robust to the
125 effects of charring.

126 ***An old landrace to test archaeobotanical geometric*** 127 ***morphometrics***

128 To determine the ability of GMM to recognise landraces in the archaeological
129 record, testing using present-day landraces is required. An ideal candidate
130 is bere (pronounced *bear*), a six-row hulled barley landrace once widely

131 grown in Scotland. Whilst today largely restricted to Orkney, bere has long
132 been associated with Scotland's island groups and has genotypically distinct
133 forms from Orkney, Shetland and the Western Isles (Southworth 2007).

134 Bere is thought to be one of the oldest surviving cereal landraces in Europe
135 (Jarman 1996). This longevity may be attributed to bere's adaptation to the
136 conditions of northern Scotland, including its suitability for short, cool
137 growing seasons (Chappell et al. 2017) and tolerance of sandy, coastal soils
138 which are deficient in trace elements (George et al. 2014), specifically
139 manganese deficiency (Schmidt et al. in prep.). Bere is, therefore, an
140 important genetic resource for crop breeding (Feuillet et al. 2008; Negri et
141 al. 2009), with conservation on working farms most likely to ensure its
142 continued availability (Green et al. 2009; A. C. Newton et al. 2011). This can
143 be encouraged by developing high provenance food or drink markets for
144 bere products (Martin et al. 2009), based on the landrace's historic (and,
145 potentially, prehistoric) association with the islands.

146 Although the chronology of bere's introduction to northern Scotland is
147 unknown, a Scandinavian introduction to Britain in the 8th Century AD has
148 been suggested (Jarman 1996). This is supported by many historical
149 references in which the crop is often called *bygg*, the Old Norse for barley
150 (Fenton 1978), and by the frequent use of the word *bere*, in Old English, for
151 barley (Cameron et al. 2016). More recent evidence for bere comes from the
152 usage of the terms '*bere*' and '*beare*' for a type of British six-row barley in
153 historical literature dating back to the 16th Century AD (Jarman 1996;
154 Neilson 2016). Such sources are notoriously difficult to interpret, however,
155 as naming conventions change over time. Today the name '*bere*' is restricted
156 to the particular landrace grown in northern Scotland but this may not have
157 always been the case historically. The uncertainties of bere's heritage can be
158 better addressed by the identification of the landrace in the archaeological
159 record.

160 Bere's long history of use in northern Scotland presents an ideal opportunity
161 to test the ability of GMM to differentiate it from other landraces. In order to
162 be relevant for archaeological research, analysis is restricted to shape
163 information of grains (as other characteristics, such as veining or colour,
164 rarely preserve archaeologically). The research presented here goes further

165 than previous studies (Ros et al. 2014; Bonhomme et al. 2017) as it attempts
166 to identify a specific landrace relevant to the archaeological record, and also
167 investigates the influence of growing conditions on grain shape. Specifically,
168 we will determine whether bere can be differentiated from similar barley
169 landraces by grain shape alone and despite differences in growing
170 conditions, between two locations, and the effects of charring.

171 **Materials and methods**

172 ***Growth trials***

173 A series of hulled barleys were grown in two trials, one at Orkney College,
174 Kirkwall (58°59'N and 2°56'W) and the other at the James Hutton Institute
175 (56°29'N and 3°7'W) near Dundee. These barleys were represented by 54
176 accessions (each a specific example of a landrace sourced from a gene bank)
177 grouped in the following categories: bere barley (six-row) of Orkney and
178 Western Isles provenance, Scandinavian landraces (six-row), non-bere
179 Scottish landraces (two-row) and non-Scottish British landraces (two-row)
180 (Table S1). The soil at both sites was a clay loam. Each accession was planted
181 in a single, individual plot (2 × 1 m) at a seed rate giving 365 plants.m⁻².

182 Trials were sown at Orkney and Dundee on 21st April and 14th March 2016,
183 respectively, and the inputs applied are detailed in Table S2. During most of
184 the cropping season conditions at Orkney were cooler and wetter (March to
185 August 2016: mean temperature 10.3°C vs. 11.2°C; total rainfall 367 mm vs.
186 327 mm; Table S3). At Orkney, barley was harvested between 16th August
187 and 12th September, upon reaching the hard grain stage (Zadoks growth
188 stage 92). Prior to harvest, a 60 cm length of row was sampled and three
189 representative spikes were selected from this sample to provide grains for
190 morphometric analysis. Spikes were dried at 35°C for 24 hours. Harvesting
191 of the Dundee trial with a small plot combine occurred on 29th August.

192 ***Genotyping***

193 For each sample, five grains were taken for genotyping from the source used
194 to sow each of the field trials. Seeds were germinated in Petri plates on filter
195 paper for five days and DNA was extracted from young leaf material, using
196 Qiagen DNeasy plant mini-preparation kit (Qiagen, Hilden, Germany).
197 Genotyping was undertaken using Illumina GoldenGate BeadArray

198 technology with the BOPA1 and 2 single nucleotide polymorphism (SNP)
199 sets (Close et al. 2009). Genotype data were processed and manually
200 inspected using the BeadStudio 3.1.3.0 software package (Illumina Inc., San
201 Diego, California, USA). Of the 3072 BOPA SNPs, 2312 were reliably called in
202 at least 95% of the individuals and used in the analysis (Table S4). A simple
203 cluster analysis using PAST 1.91 software suite (Hammer et al. 2001) based
204 on Hamming's distance (=1 simple matching) was undertaken, as was
205 Principal Coordinate Analysis (PCoA).

206 ***Morphometrics***

207 Barley was available as whole ears from Orkney and as free grain from
208 Dundee. For the Orkney material, grains were removed individually from
209 ears with only central (untwisted) grains selected from along the ears. Only
210 central grains were included so as to exclude differences in grain shape due
211 to the degree of twisting in lateral grains, and to provide equivalent plant
212 parts from six-row and two-row barley samples. Tail grains exhibiting
213 stunted growth (e.g. Hillman 1984) and grains with any other obvious
214 malformation were avoided because these atypically shaped grains would
215 generate excess variation in the GMM analysis, and they can be excluded also
216 from archaeological samples. Grains from Dundee were selected at random
217 avoiding tail, malformed and visibly twisted grains. At least five grains were
218 selected per accession.

219 Hulls and embryo protrusions, obscuring the grain outline, were removed
220 with forceps. The dorsal plane of grains was photographed using a Leica
221 DFC450 camera attached to a Leica M205 APO microscope. Photographed
222 grains were outlined using Adobe® Photoshop® and converted to binary
223 masks. Landmarks were added to the embryo-end tip and apical-end tip
224 using ImageJ (Schneider et al. 2012). Binary (black-and-white) masks and
225 landmarks coordinates were imported to the R environment version 3.4.2.
226 (R Core Team 2017) and the package Momocs version 1.2.1. (Bonhomme et
227 al. 2014) was used for morphometric analysis.

228 Size and orientation were excluded by Bookstein alignment using the two
229 landmarks, centred and scaled. Elliptical Fourier representations were
230 calculated for the first five harmonics (sufficient to gather 95% harmonic
231 power; Bonhomme et al. 2014: 14). Twenty quantitative variables were

232 generated, of which 13 were non-normally distributed (i.e. Shapiro-Wilks
233 test p-value ≤ 0.05) and the variance between barley groups for 15 was
234 uneven (i.e. Levene's test p-value ≤ 0.05). All variables were analysed using
235 multivariate statistical approaches (Venables and Ripley 2002), including
236 Principal Components Analysis (PCA) and Linear Discriminant Analysis
237 (LDA). LDA was chosen as the primary basis of analysis because LDA, as a
238 supervised classification tool, seeks out the most diagnostic variable
239 combination to separate known groups rather than simply the largest source
240 of variation, as is the case for unsupervised procedures, and is thus
241 appropriate for establishing the diagnostic capabilities of GMM for landrace
242 recognition. Non-normality and uneven variance between groups are sub-
243 optimal for LDA, and whilst LDA results are expected to be reliable (not
244 spurious) they are potentially not as strong as those where optimal
245 conditions are met. The significance of the group separations was further
246 tested by multivariate analysis of variance (MANOVA).

247 ***Experimental charring***

248 Three accessions each of bere and Scandinavian landraces were selected
249 randomly for further morphometric analysis, including charring
250 experiments. Sixty grains (10 per accession) were charred individually,
251 permitting one-to-one comparison pre- and post-charring. Grains were
252 buried in sand, to achieve reducing conditions, and placed in an oven set to
253 230°C for 6 hours ($\pm 1^\circ\text{C}$ accuracy). This charring protocol is designed to
254 produce material representative of well-preserved archaeobotanical
255 material, as discussed elsewhere (Fraser et al. 2013; Charles et al. 2015;
256 Bonhomme et al. 2017).

257 **Results**

258 ***Genotyping indicates three barley clusters***

259 Fifty-four accessions which represent both two- and six-row barleys grown
260 across the UK and Scandinavia during the last hundred years, along with
261 bere barleys from Orkney and the Western Isles, were genotyped with 3072
262 mapped genetic markers (BOPA1&2, Close et al. 2009). For four six-row
263 accessions (three bere and one Scandinavian landrace) SNP data were
264 anomalous, contradicting accession information and, as this casts doubt on

265 the provenance of these accessions, they have been excluded from further
266 analysis (Table S1).

267 SNP data shows three clusters (Fig. 1a and Fig. S1): (i) all two-row accessions
268 including those with a Scottish and non-Scottish British origin, (ii)
269 Scandinavian accessions plus two with a presumed Scandinavian origin and,
270 (iii) a tight cluster of all bere accessions plus the Faroese barley. Within the
271 bere, there is separation between accessions with an Orkney provenance
272 and those with a Western Isles provenance (Fig 1b).

273 ***Grain geometric morphometrics distinguishes barley landraces***

274 A total of 565 grains from all 54 accessions (Table S1) were included in GMM
275 analysis. The GMM data were noisier than the SNP data (for a discussion of
276 intra- and inter-ear variation see SI), though LDA shows these accessions
277 separate into groups with similar membership to those based on SNP data
278 (Fig 2). The overall LOO reclassification rate is low, 61.5%, but the
279 misclassifications are informative in identifying morphologically similar
280 groups of grains (Table 1). Two-row grains tend to group together, with
281 most classified as either non-Scottish British or Scottish British two-row
282 landraces. Scandinavian grains, including those of presumed Scandinavian
283 origin, group together, and most are classified as Scandinavian. The few
284 Faroese grains tend to group with the bere, with most of the bere and
285 Faroese grains classified as bere. Grains from the four six-row accessions
286 with an uncertain origin overlap the six-row groups (Fig. 2a), which is
287 consistent with the genotype data.

288 An LDA based on groupings following the SNP data (for the 50 accessions –
289 525 grains – with reliable results, Table S1) has a high LOO reclassification
290 rate of 81.7% (Fig. 2b and Table S5) and MANOVA indicates that the
291 difference between groups is significant ($Pillai = 1.04625$, $F = 14.5658$, p
292 <0.001). Reclassification can be improved further, to 86.9%, by calculating
293 average shapes for each accession per trial location prior to LDA (Fig. S2 and
294 Table S6).

295 The greatest distinction in grain morphology is for row type (LDA, LOO
296 reclassification = 87.6%; MANOVA, $Pillai = 0.56552$, $F = 35.404$, $p <0.001$),
297 with reclassification slightly better for the Orkney-grown material (92.7%),

298 Fig. 3a) than for the Dundee-grown (83.4%, Fig. 3b). Taking the six-row
299 grains in isolation, the bere plus Faroese group is distinguished from
300 Scandinavian landraces (LDA, LOO reclassification = 85.1%; MANOVA, *Pillai*
301 = 0.53747, $F = 17.081$, $p < 0.001$), and the difference is again more
302 pronounced for the Orkney-grown material (90.9% vs. 80.7%, Fig 3c & 3d).

303 As was the case for SNP data, GMM data indicates differences between bere
304 accessions based on their provenance. The six Orkney bere accessions (65
305 grain) and five Western Isles bere accessions (60 grain) can be distinguished
306 by grain morphology (LDA, LOO reclassification = 81.6%; MANOVA, *Pillai* =
307 0.61352, $F = 8.2548$, $p < 0.001$), and in this case there is little difference
308 between the Orkney-grown and Dundee-grown material (82.1% vs. 83.6%,
309 Fig 3e & 3f).

310 The actual difference in the shape of grains is not easily observed by eye.
311 Through shape amplification, however, it is possible to visualise the average
312 differences in grains for the barley groups (Fig. 4). Shape differences
313 between two-row and six-row central grains appear to be related to the
314 overall roundness and the broadness of the embryo end relative to the apical
315 end (Fig. 4a). Amongst the six-row grains, bere differs from Scandinavian
316 landraces in that Scandinavian grains exhibit a ‘tucking-in’ along the lateral
317 edge near either end of the grain, whereas the bere usually has a continuous
318 gentle curve from the mid-point to the ends (Fig. 4b). Bere of Orkney and
319 Western Isles provenances (Fig. 4c) are both rounded, with Western Isles
320 bere grains broader relative to their overall length.

321 ***Charring has a consistent and modest effect on barley grain shape***

322 In their uncharred state, LDA on the subset of 60 grains selected for
323 experimental charring correctly assigns 95% (57 of 60) as bere or
324 Scandinavian (Table S7). Following charring, LDA reclassifies 80% (48 of 60)
325 correctly (Table S8). The consistency of the charring effect was assessed by
326 comparing the PC1 scores for the subset of 60 uncharred grains with the PC1
327 scores for the same 60 grains in their charred state (Fig. 5). Note that PC1
328 accounts for 62% of the variation, and so serves as a good single-variable
329 summary of grain shape, and that the scores of the charred grains were
330 calculated using the loading matrix of eigenvectors obtained in the PCA of
331 uncharred grain. There is strong correlation between the two PC1 scores

332 ($r_{adj}^2 = 0.76$, $p = <0.001$), indicating that differences in shape before and after
333 charring is similar for all grains. There is some variation between accessions
334 (Fig. S6), suggesting some grains may be effected slightly differently by
335 charring. Nevertheless, taking the results as a whole, the charring effect is
336 largely consistent between grains and is sufficiently modest as to not mask
337 differences in grain shape between the tested landraces (Fig. S7).

338 **Discussion**

339 ***Geometric morphometrics patterns are robust across trial*** 340 ***locations***

341 Geometric Modern Morphometrics (GMM) distinguishes both barley row
342 type and several landrace groups based on grain morphology and,
343 importantly, this has been accomplished for material grown at two trial
344 locations under different growing conditions. The implication is that the
345 primary determinant of grain morphology is genetic, and that effects on
346 grain morphology due to environmental conditions do not mask this. Grain
347 morphology was affected, however, to some extent by trial location, with
348 typically higher LDA reclassification rates for Orkney-grown material.

349 The reason for superior reclassification rates, and therefore more distinctive
350 grain morphologies, for Orkney-grown material is unknown. The possible
351 accidental inclusion of twisted grains (i.e. those from the lateral spikelet
352 position in six-row barley) for the Dundee material (see Materials &
353 Methods) may explain the pattern. Alternatively, differences in growing
354 conditions at the two trial sites may have had an influence. Growing
355 conditions can be predicted to most likely affect grain morphology during
356 the grain formation period (Zadok's stages 71 - 87), which relates to
357 approximately the end of July and start of August for these trials. During this
358 period the Dundee site experienced about one-third less rainfall and was
359 slightly warmer (Table S3), and this might have resulted in differences in
360 grain formation. Finally, it might be hypothesised that landraces are most
361 distinctive when grown in the conditions to which they are adapted, which
362 in this case applies only to the Orkney-grown bere. Orkney bere, however,
363 was less readily distinguished from Western Isles bere on Orkney, casting
364 doubt on this theory. Based on our experiment involving two trial locations,
365 the relationship between growing conditions and grain morphology appears

366 minor, at least compared to the genetic determination of grain morphology,
367 and should be considered neutral until demonstrated otherwise.

368 ***Grain geometric morphometrics distinguishes barley row type***

369 GMM was most effective at distinguishing two-row and six-row barley grains
370 based only on straight grains (i.e. visibly twisted grains from the lateral
371 position in six-row barley were excluded). This finding supports previous
372 work (Ros et al. 2014) in which similar LDA reclassification to row for 300
373 barley grains was 91% correct, but also extends it by demonstrating that the
374 differentiation of two-row and six-row grains does not rely on the presence
375 of twisted grains in the latter. The inclusion in this study of two trial
376 locations strengthens the case for archaeological relevance. The ability of
377 GMM to determine row type for individual grains permits an objective and
378 probabilistic approach to row classification that can be extended to small
379 assemblages or samples, for which the traditional ratio-based approach
380 would be unreliable.

381 ***Grain geometric morphometrics distinguishes barley landraces***

382 Going beyond the kinds of identifications possible using traditional
383 archaeobotany, the results of this study demonstrate that GMM can
384 characterise the grain morphology of some specific groups of landraces,
385 providing a novel archaeological method for exploring the spread and use of
386 landraces. Neither SNP nor GMM data could distinguish between all landrace
387 groups. The lack of genetic or morphometric difference in two-row grains
388 from Scotland and the rest of Britain may indicate that local differences in
389 landrace naming conventions may not readily translate to biological
390 differences. Indeed, the groups that were genetically and morphologically
391 distinct - Scandinavian landraces, Orkney bere and Western Isles bere - are
392 isolated from each other by sea. Sea barriers reduce the likelihood of
393 outbreeding between landraces and, thus, increase genetic isolation and
394 population divergence (e.g. Hagenblad et al. 2017). It is thus expected that
395 distinctive grain morphology will be most pronounced for island
396 populations. The apparent contradiction of this by the Faroese landraces is
397 discussed in supplementary information

398 Despite the centrality of genetics to grain morphology, it is to be expected
399 that the phenotypic and genotypic uniqueness of landraces will not always

400 manifest as a uniqueness in grain shape. Grain morphology should not,
401 therefore, be considered a proxy for genetic analysis. Rather,
402 archaeobotanical GMM must be considered a tool for detecting landraces
403 that have distinct grain morphology *regardless* of their phenotypic or
404 genotypic character. Nevertheless, while it cannot be expected that the
405 genotypic data will always map onto the morphometric data, it is clear, at
406 least in the case of bere, that genotypically distinct types of the landrace can
407 also be morphologically distinct. Given the limitations of extracting aDNA
408 from charred remains and the necessity of studying the archaeological
409 record in order to establish the rise and fall of bere and other landraces, our
410 morphometric findings are essential for further study of past landrace use
411 and ancestry.

412 ***Bere's past, and the future of archaeological landrace recognition***

413 This novel GMM approach to recognising bere barley provides the means to
414 explore the origins and past usage of this landrace through the
415 archaeological record. The distinctiveness of bere from present-day
416 Scandinavian landraces casts doubt on the Viking introduction theory. This
417 leaves three possibilities: (1) bere derived from landraces of mainland
418 Britain; (2) bere derived from extinct/unavailable landraces from
419 Scandinavia; or (3) bere evolved on the Scottish islands from an earlier
420 introduction. These origins can only be tested by studying the morphology
421 of barley grains in the archaeological record of the Scottish islands, and
422 through comparison with contemporary and archaeological barley from
423 mainland Britain, Scandinavia and other areas.

424 The availability of present-day specimens of bere make it an ideal candidate
425 for exploring the potential of our GMM approach, but the applications of the
426 method are not limited to the study of bere. By studying present-day
427 landraces it is also possible to determine the scope of grain morphologies
428 represented, and identify distinctive forms. The archaeological record,
429 however, is likely to contain landraces for which no parallel survives today
430 – including potential 'lost crops' (Fuller et al. 2012). Analysis of
431 archaeological grains, therefore, must not be restricted to only matching
432 archaeological specimens to modern grain morphologies. An advantage of
433 the GMM approach in this regard is that results are probabilistic, and it is

434 therefore relatively straightforward to identify grains that are a poor match
435 to any of the landraces included in present-day training data.

436 The application of GMM approaches to the archaeobotanical record relies on
437 its suitability for use on charred plant remains, which account for much of
438 the record. The results of our charring experiments corroborate those
439 conducted by others (Bonhomme et al. 2017; Ros et al. 2014), indicating that
440 the effect on grain shape is modest in its magnitude and predictable in terms
441 of the manner of shape change. This consistency provides the opportunity
442 for a 'correction factor' to be developed that infers uncharred shapes from
443 charred grains, and so permitting the direct comparison with present-day
444 barley.

445 Application of GMM approaches to the archaeobotanical record will,
446 however, still pose challenges. Landrace recognition, as opposed to the
447 identification of row type for which the distinction is clearer, will benefit
448 from large sample sizes and the targeting of well-preserved grains that lack
449 gross, charring-induced distortions (Charles et al. 2015). In addition, stable
450 isotope analysis provides information on crop growing conditions and
451 husbandry practices (Bogaard et al. 2013; Wallace et al. 2013; Wallace et al.
452 2015; Bogaard et al. 2016; Styring et al. 2016; Fiorentino et al. 2015) which,
453 if used in tandem with GMM, will provide a detailed picture of ancient crop
454 use.

455 **Conclusion**

456 This study of present-day specimens of bere, one of Europe's oldest
457 surviving barley landraces, and comparison with similar barley landraces
458 has demonstrated the potential of geometric modern morphometric (GMM)
459 analysis of grain to contribute to archaeological research questions through
460 the novel recognition of landraces. Although not all landraces may be
461 detected through GMM analysis, those with distinctive grain morphology can
462 be statistically distinguished from others. The results presented here and
463 elsewhere indicate that sources of uncertainty (e.g. growing conditions,
464 charring, inherent variability) can be overcome, providing the opportunity
465 to use GMM to reach archaeologically invisible landrace-level identifications.

466 The importance of below-species level identification of archaeological plant
467 remains has been highlighted by previous studies of fruit crops. Now
468 archaeobotanical GMM can be extended to cereal crops, the primary source
469 of calories in large parts of the world throughout much of history and
470 prehistory. The recognition of landraces will permit the emergence of locally
471 adapted crop forms to be identified and their spread and exchange between
472 farming communities to be charted, which in turn informs on past
473 economies and cultural identity. For bere, its recognition in the
474 archaeological record will contribute to understanding the origins and
475 history of this important heritage resource, helping in turn to secure its long-
476 term future.

477 **Figure captions**

478 ***Fig. 1***

479 Principal Coordinate Analysis (PCoA1 and PCoA2) of SNP data for the 50
480 barley accessions that were reliably genotyped. Panel A: all 50 non-
481 anomalous accessions. Panel B: non-anomalous bere accessions only.
482 Symbols (and colours) denote barley group: [panel A] circle (red) – six-row
483 bere; filled square (purple) – six-row Scandinavian; open square (purple) –
484 presumed six-row Scandinavian; upward triangle (light blue) – two-row
485 non-Scottish British; downward triangle (dark blue) – two-row Scottish; star
486 (orange) – six-row Faroese; [panel B] circle with + (dark red) – six-row bere
487 of Orkney provenance; circle with × (light red) six-row bere of Western Isles
488 provenance; open circle (black) - six-row bere of unknown provenance.

489 ***Fig. 2***

490 Linear Discriminant Analysis (LD1 and LD2) of GMM data for barley grains.
491 Panel A: 525 grains from the 50 accessions with non-anomalous SNP data,
492 assigned according to accession information with the 20 grains from the four
493 unknown accessions added as new data. Panel B: 525 grains from the 50
494 accessions with non-anomalous SNP data, assigned according to genetic
495 cluster. Confidence ellipses set at level 0.68. Symbols (and colours and
496 ellipse lines) denote barley group: [panel A] circle (red) - six-row bere; filled
497 square (purple) – six-row Scandinavian; open square (purple, dashed ellipse
498 line) – presumed six-row Scandinavian; upward triangle (light blue) - two-
499 row non-Scottish British; downward triangle (dark blue) – two-row Scottish;
500 star (orange) – six-row Faroese; × (black) – six-row unknown origin; [panel
501 B] circle (red) – six-row bere or Faroese; squares (purple) six-row
502 Scandinavian including presumed Scandinavian; diamonds (blue) – two-row
503 British.

504 ***Fig. 3***

505 Separate Linear Discriminant Analyses (LD1) conducted for Orkney-grown
506 and Dundee-grown barley. Percentages refer to the correct L00
507 reclassification rate for each LDA. A: Orkney-grown grains assigned by row
508 type – two-row (105 grains, blue) or six-row (175 grains, pink). B: Dundee-
509 grown grains assigned by row type – two-row (105 grain, blue) or six-row
510 (140 grains, pink). C: Orkney-grown six-row grains assigned by genetic

511 cluster – bere or Faroese (95 grains, red) or Scandinavian including
512 presumed Scandinavian (80 grains, purple). D: Dundee-grown six-row
513 grains assigned by genetic cluster – bere or Faroese (80 grains, red) or
514 Scandinavian including presumed Scandinavian (60 grains, purple). E:
515 Orkney-grown bere grains assigned by provenance – Orkney (35 grains,
516 dark red) or Western Isles (35 grains, light red). F: Orkney-grown bere
517 grains assigned by origin – Orkney (30 grains, dark red) or Western Isles (25
518 grains, light red).

519 **Fig. 4**

520 Amplified ($\times 2$) isometric thin plate splines comparing mean grain shape for
521 different barley groups. Dorsal view of grains with embryo end to left. Fill
522 colours and contour lines indicate similarity with overlaying shape: reddish
523 areas with tight contours indicate large differences, and blueish areas with
524 wide contours indicates similarity. Border colour indicates barley group. A:
525 two-row (210 grains, blue) or six-row (355 grains, pink). B: bere (155 grains,
526 red) and Scandinavian (120 grains, purple). C: Orkney bere (65 grains, dark
527 red) and Western Isles bere (60 grains, light red).

528 **Fig. 5**

529 Principle Component 1 scores for subset of 60 uncharred grains plotted
530 against the Principle Component 1 scores for the same 60 grains in their
531 charred state calculated using the loading matrix of eigenvalues obtained
532 from the PCA of uncharred grains. The linear regression (black) shown was
533 calculated on all grains, $r_{adj}^2 = 0.76$, including the 30 bere grains (red circles)
534 and 30 Scandinavian grains (purple squares).

535 **Table captions**

536 **Table 1**

537 Linear Discriminant Analysis LOO reclassification results for GMM data of
538 grains for all accessions assigned by accession information. Group names are
539 abbreviated as follows, Bere-R6: six-row bere; Faro-R6: six-row Faroese;
540 Scand-R6: six-row Scandinavian; ?Scand-R6: presumed six-row
541 Scandinavian; Brit-R2: two-row non-Scottish British; Scot-R2: two-row
542 Scottish.

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787

Fig. 1

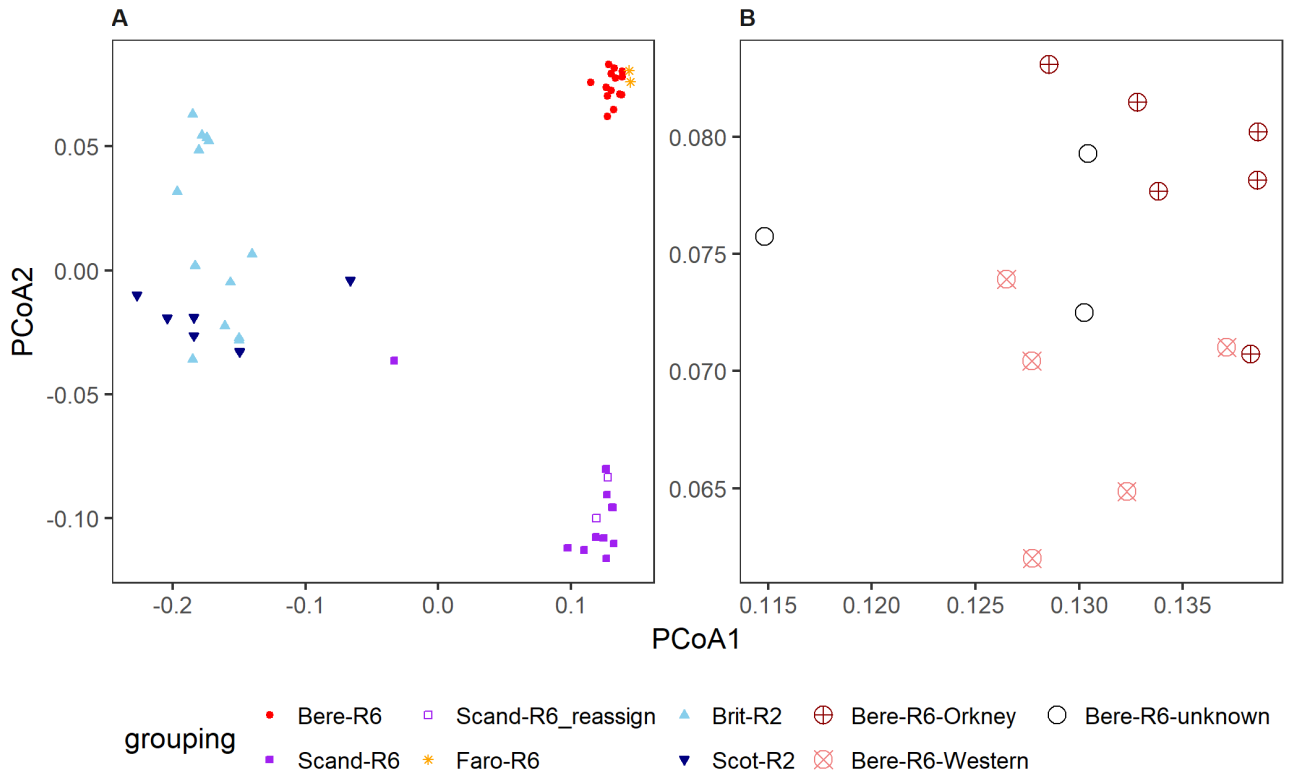


Fig 2

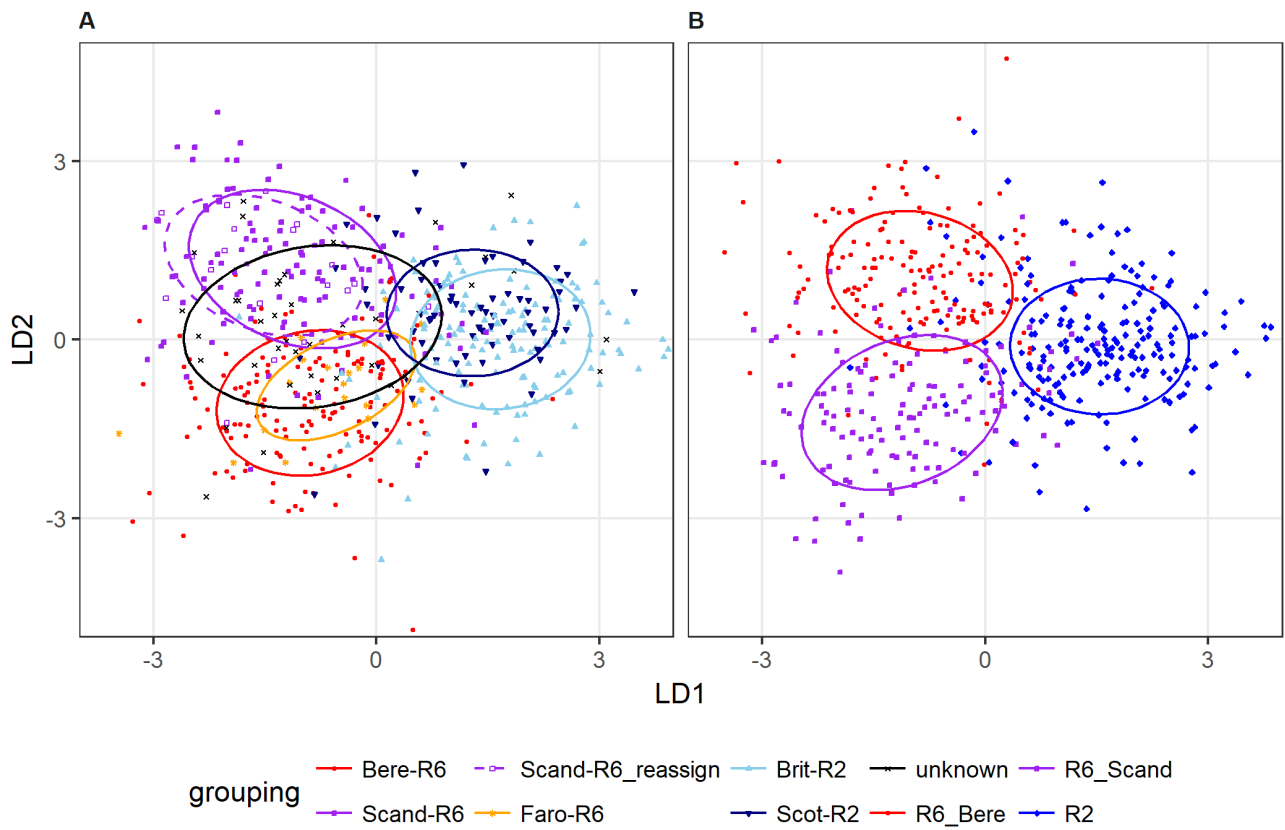


Fig. 3

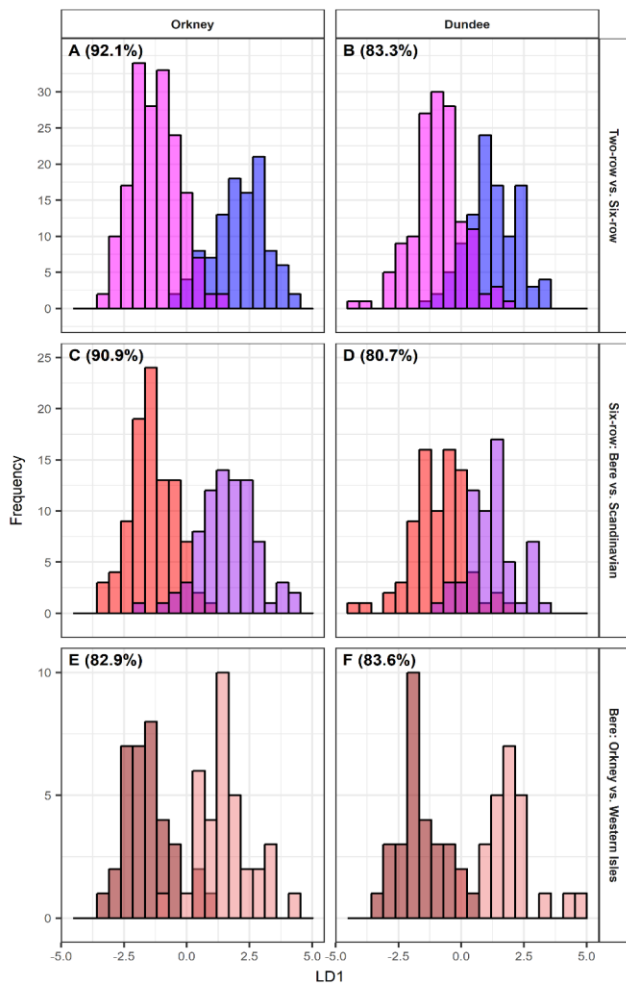


Fig. 4

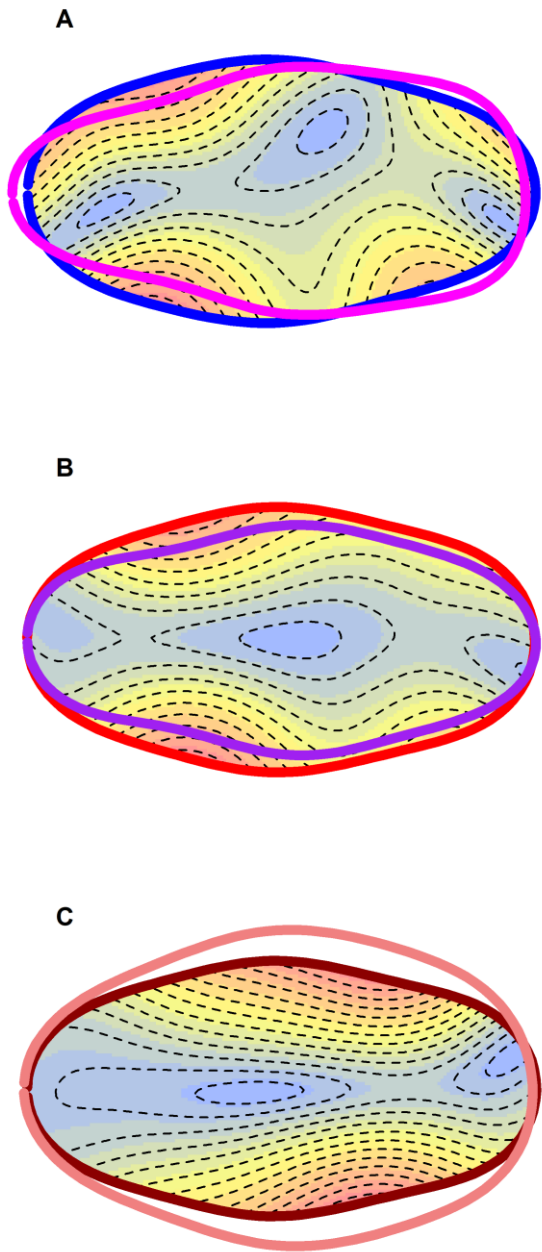


Fig. 5

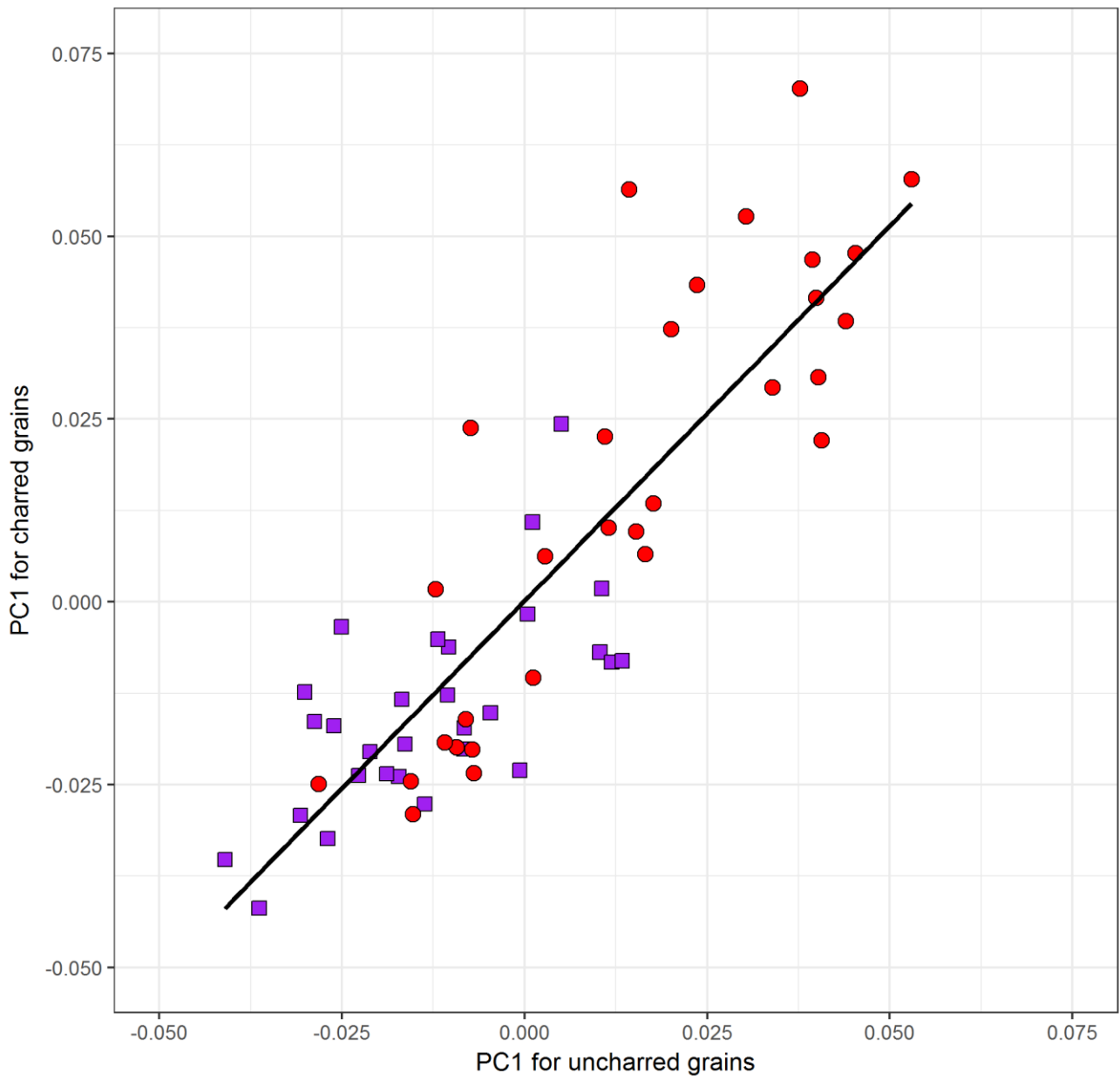


Table 1

	Classified					
Actual	Bere-R6	Faro-R6	Scand-R6	?Scand-R6	Brit-R2	Scot-R2
Bere-R6	124 80%	3 2%	13 8%	2 1%	12 8%	1 1%
Faro-R6	16 80%	0 0%	1 5%	0 0%	1 5%	2 10%
Scand-R6	16 13%	0 0%	85 71%	2 2%	13 11%	4 3%
?Scand-R6	3 15%	0 0%	16 80%	0 0%	0 0%	1 5%
Brit-R2	11 8%	0 0%	3 2%	0 0%	103 74%	23 16%
Scot-R2	4 6%	2 3%	9 13%	0 0%	44 63%	11 16%

Supplementary Information Text

Intra- and inter-ear grain shape variation

For the Orkney-grown barley, grains were selected from individual ears to permit assessment of intra-ear variation in grain shape. The degree of shape variation, represented by PC scores for dimensionality reduction, amongst grains of the same ear can vary markedly, with some ears producing very similarly shaped grains and others very dissimilar (Fig. S5). The degree of grain shape variation does not appear related to the accession origin. This indicates that the GMM dataset is noisy, but not biased.

For six of the Orkney-grown accessions an additional five grains from a second ear were analysed. This permits inter-ear variation to be assessed. Mean PC scores for each ear tend to be similar to that of the other ear of the same accession (Fig S6). LDA of these grains to accession results in 71.7% of grains correctly reclassified to their specific accession with leave-one-out cross-validation, and 100% correctly to their barley group (Fig. S7 and Table S9).

Faroese landraces

Although the genetic and grain morphometric similarity of Faroese landraces and bere appear to contradict this, a possible explanation is that the Faroese landraces in this study were derived from introductions of bere to the Faroes. This could have happened during visits by Faroese fishermen to the Northern Isles during the 19th and early 20th Centuries (Djurhuus, personal communication) and, if this had not been documented, such material might then have been included in collections of Faroese landraces made in the 1920s. More generally, informal imports of bere may have often been important in renewing Faroese seed stocks following poor harvests and this might have prevented the appearance of genetically and morphologically distinct local landraces.

Supplementary Information Figure and Table Captions

Fig. S1. Neighbour joining tree based on SNP data for the 50 accessions with non-anomalous SNP data. Colours and icons denote group membership based on accession information: red with circle – six-row bere, orange with star – six-row Faroese, purple with solid square – six-row Scandinavian, purple with open square – presumed six-row Scandinavian, dark blue with downward triangle – two-row Scottish, light blue with upward triangle – six-row non-Scottish British.

Fig. S2. Linear Discriminant Analysis (LD1 and LD2) of GMM data for 525 barley grains (from the 50 accessions with non-anomalous SNP data) after calculation of mean shape per accession per trial location. Confidence ellipses set at level 0.68. Symbols (and colours) denote barley group: circles (red) – six-row bere or Faroese; squares (purple) six-row Scandinavian including presumed Scandinavian; diamonds (blue) – two-row British.

Fig. S3. Box-and-whisker plots for Principle Component Analysis scores (PC1 to PC5) for each analysed ear of Orkney-grown barley. Dundee-grown accessions excluded because the relationship between grains and ears is unknown. Colours denote barley group: red – six-row bere, orange – six-row Faroese, purple – six-row Scandinavian, white – presumed six-row Scandinavian, dark blue – two-row Scottish, light blue – two-row

non-Scottish British, grey - unknown. Suffixed 'e' number denotes ear designation; second ear also denoted by dashed line on boxes.

Fig. S4. Principal Component Analysis (PC1 and PC2) of all grains to show inter- and intra-ear variation between the accessions for which two ears were analysed. Grey symbols indicate grains from accessions with only one ear analysed, and included for reference. Other colours denote grains from the same accession (see legend below figure). Solid shapes indicate the ear from which each grain was derived: circle – ear 1, diamond – ear 2. Lines indicate the difference between each grain and the mean PC scores for that ear, which is indicated by a hollow square. Accession details abbreviated: BET1 = Bere_T1_Western_Isles_SASA (six-row Bere); BORK = Bere_OM1_Orkney_SASA (six-row Bere); BSUI = Bere_SU2_Western_Isles_SASA (six-row Bere); BJOR = Bjerneby_Norway_NGB (six-row Scandinavian); MJOS = Mjos_1918_Norway_NGB (six-row Scandinavian); UFOR = Uforaedlet Jamtland_Sweden_NGB (six-row Scandinavian).

Fig. S5. Linear Discriminant Analysis (LD1 and LD2) of grains from accessions for which two ears were analysed, classified to their accession. Colours denote barley group: reds – bere, purples – Scandinavian. Symbols distinguish accessions. Ellipses are confidence ellipses set at 0.68. Accession details abbreviated: Scand = Scandinavian, R6 = six-row, BET1 = Bere_T1_Western_Isles_SASA (six-row Bere); BORK = Bere_OM1_Orkney_SASA (six-row Bere); BSUI = Bere_SU2_Western_Isles_SASA (six-row Bere); BJOR = Bjerneby_Norway_NGB (six-row Scandinavian); MJOS = Mjos_1918_Norway_NGB (six-row Scandinavian); UFOR = Uforaedlet Jamtland_Sweden_NGB (six-row Scandinavian).

Fig. S6. Principle Component 1 scores for subset of 60 uncharred grains plotted against the Principle Component 1 scores for the same 60 grains in their charred state assigned to the Principle Components Analysis calculated for the uncharred grain. Linear regressions were calculated for each sample of bere (circles) – Bere_T1_Western_Isles (red, $r = 0.84$), Bere_OM1_Orkney_SASA (green, $r = 0.39$), Bere_SU2_Western_Isles_SASA (light blue, $r = 0.61$) – Scandinavian (squares) – Bjerneby_Norway_NGB (yellow, $r = 0.65$), Mjos_1918_Norway_NGB (dark blue, $r = 0.43$), Uforaedlet Jamtland_Sweden_NGB (pink, 0.76) - landraces.

Fig. S7. Isometric thin plate splines (no amplification) comparing mean grain shape before and after charring. Dorsal view of grains with embryo end to left. Fill colours and contour lines indicate similarity with overlaying shape: reddish areas with tight contours indicate large differences, and blueish areas with wide contours indicates similarity. Border colour indicates barley group and charring state. A: 60 bere grains either uncharred (red) or charred (black). B: 60 Scandinavian grains either uncharred (purple) or charred (black).

Table S1. Details of barley accessions included in the study, and their group membership.

Table S2. Linear Discriminant Analysis leave-one-out reclassification results of grains for all accessions assigned by genetic cluster (see Table S1 and Fig 1a). Group names abbreviated: R6_bere - six-row bere or six-row Faroese; R6_Scand - six-row Scandinavian or presumed six-row Scandinavian; R2 – British (including Scottish) two-row.

Table S3. LDA leave-one-out reclassification results of grains for all accessions assigned by genetic cluster (see Table S1 and Fig 1a) after calculation of mean shape per accession per trial location. Group names abbreviated: R6_bere - six-row bere or six-row Faroese; R6_Scand - six-row Scandinavian or presumed six-row Scandinavian; R2 – British (including Scottish) two-row.

Table S4. Inputs applied to the Orkney and Dundee barley trials in 2016.

Table S5. Meteorological data for the two trial sites during 2016. NA denotes not available.

Table S6. LDA leave-one-out reclassification results of grains from accessions for which two ears were analysed classified to their accession. Accession names abbreviated: BET1 = Bere_T1_Western_Isles_SASA (six-row Bere); BORK = Bere_OM1_Orkney_SASA (six-row Bere); BSUI =

Bere_SU2_Western_Isles_SASA (six-row Bere); BJOR = Bjorneby_Norway_NGB (six-row Scandinavian); MJOS = Mjos_1918_Norway_NGB (six-row Scandinavian); UFOR = Uforaedlet Jamtland_Sweden_NGB (six-row Scandinavian).

Table S7. Linear Discriminant Analysis leave-one-out reclassification results of subset of 60 grains in uncharred state assigned by genetic cluster type of landrace.

Table S8. Linear Discriminant Analysis leave-one-out reclassification results of subset of 60 grains in charred state assigned by genetic cluster type of landrace.

Fig. S1

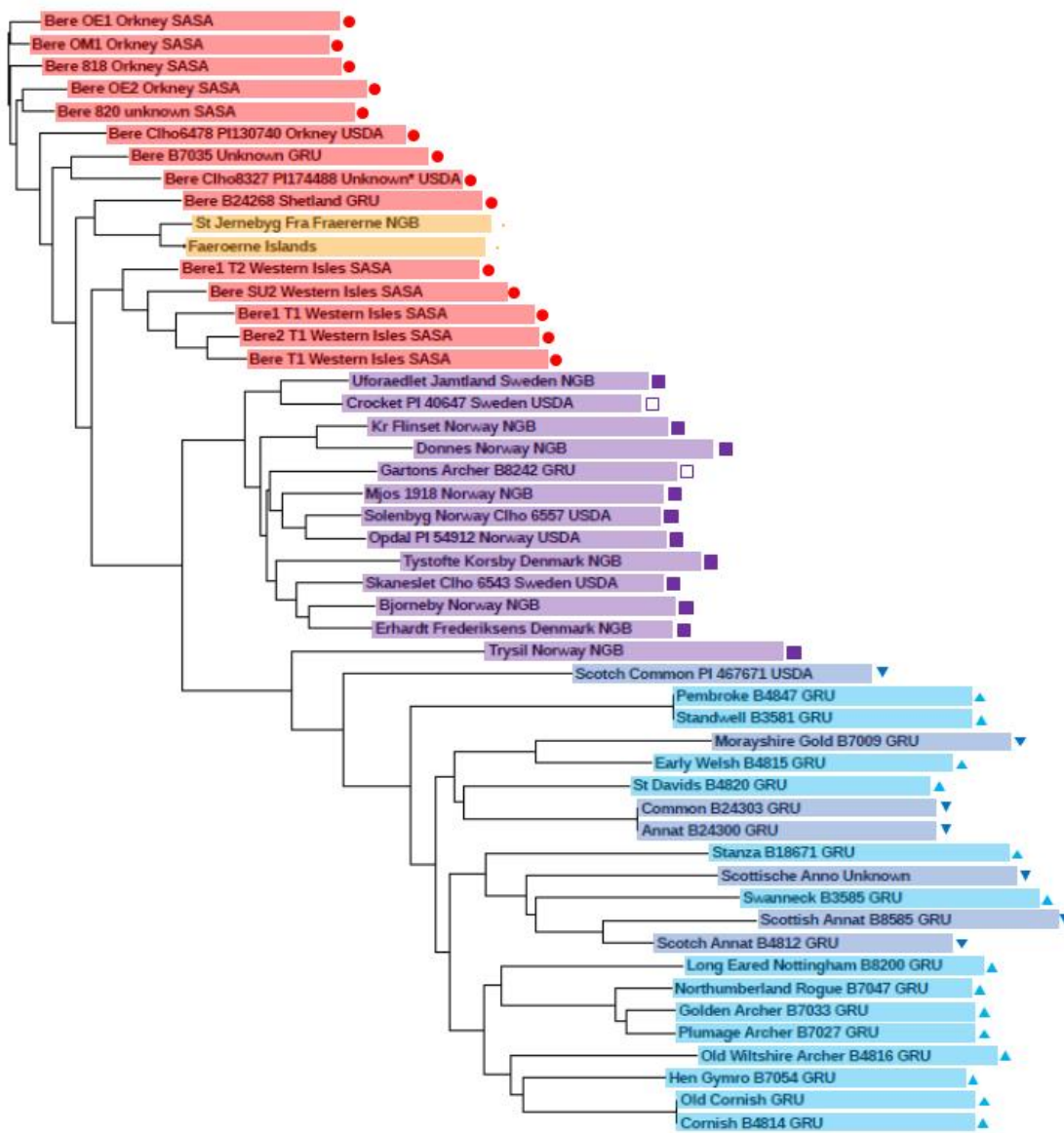


Fig. S2

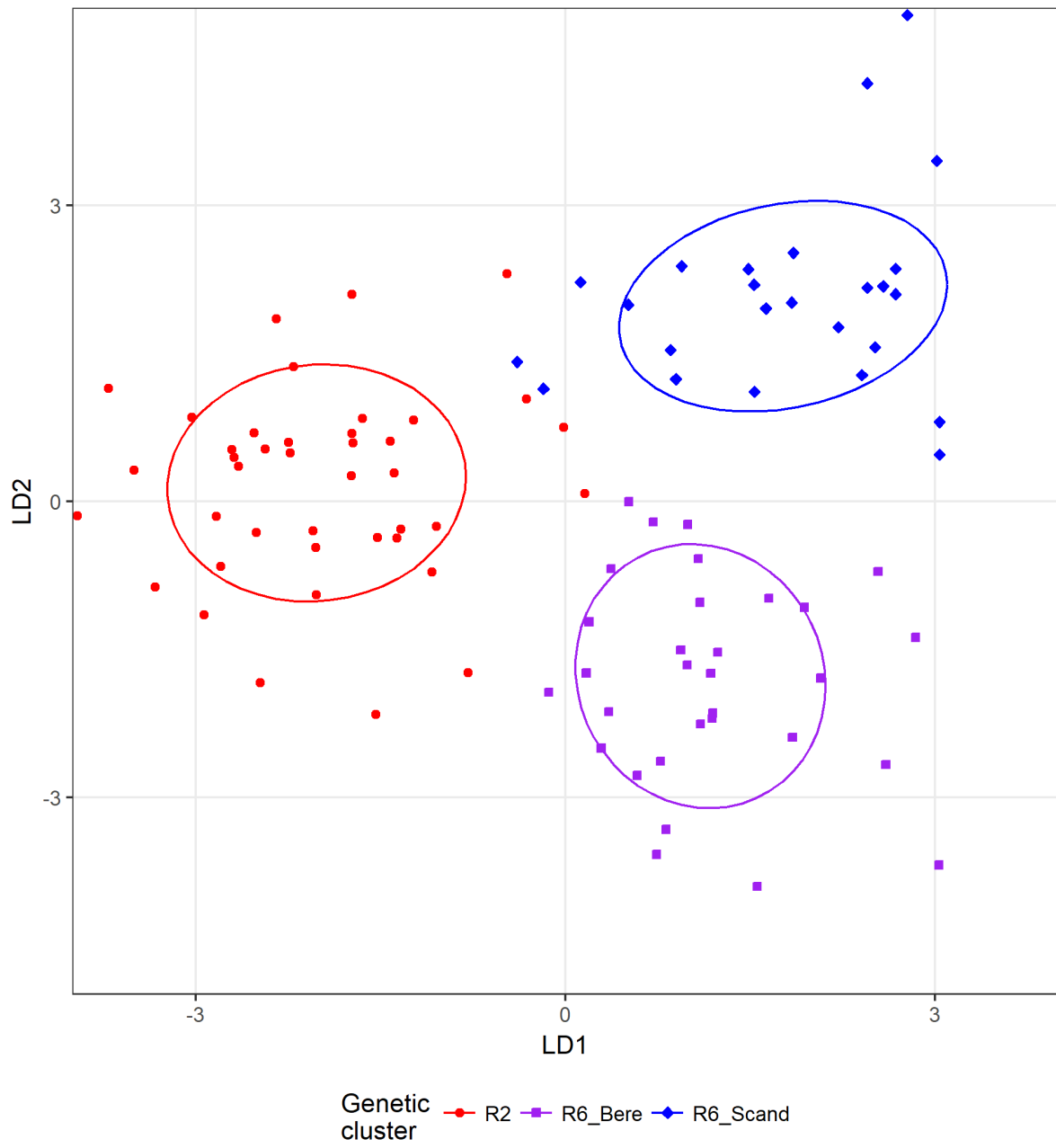


Fig. S3

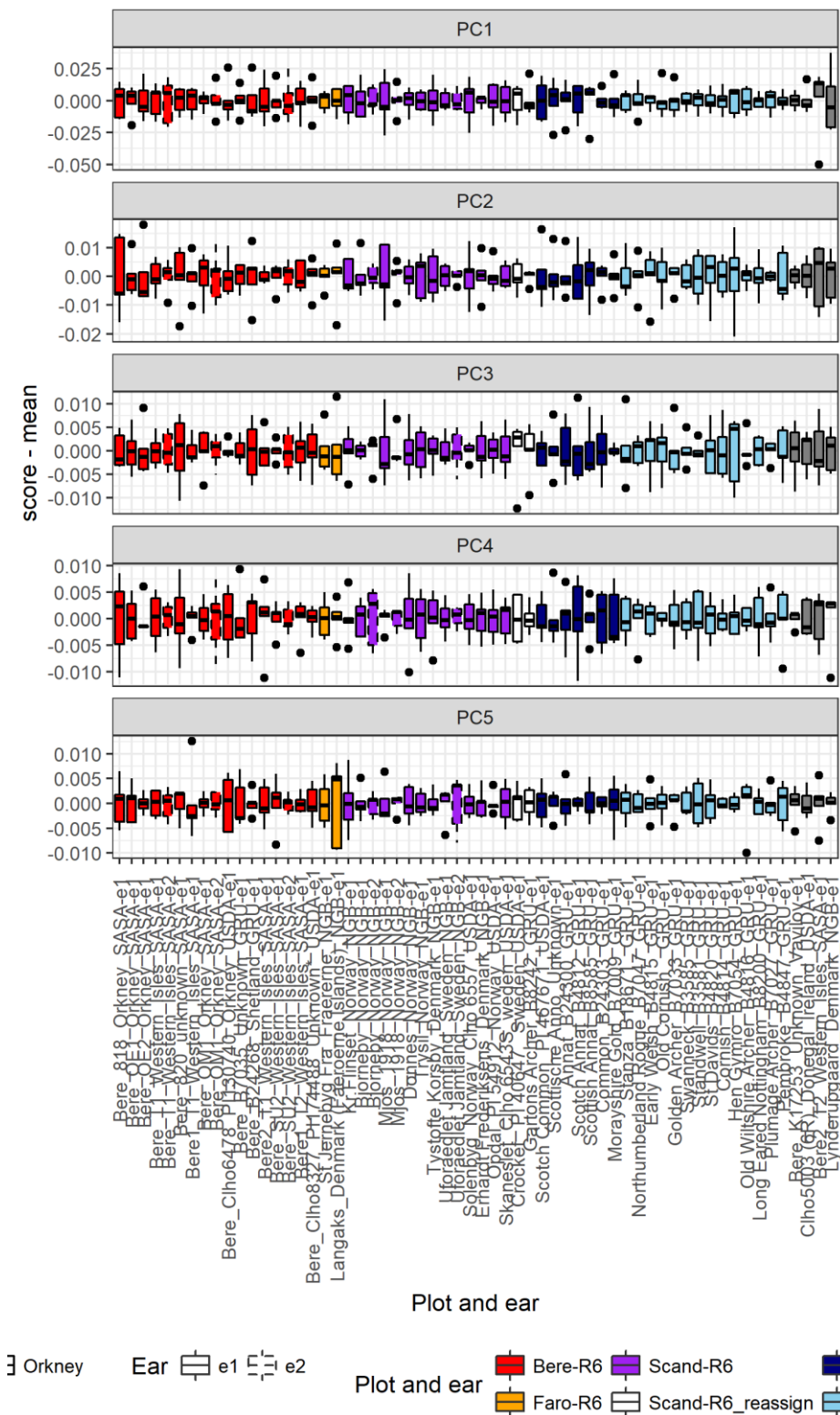


Fig. S4

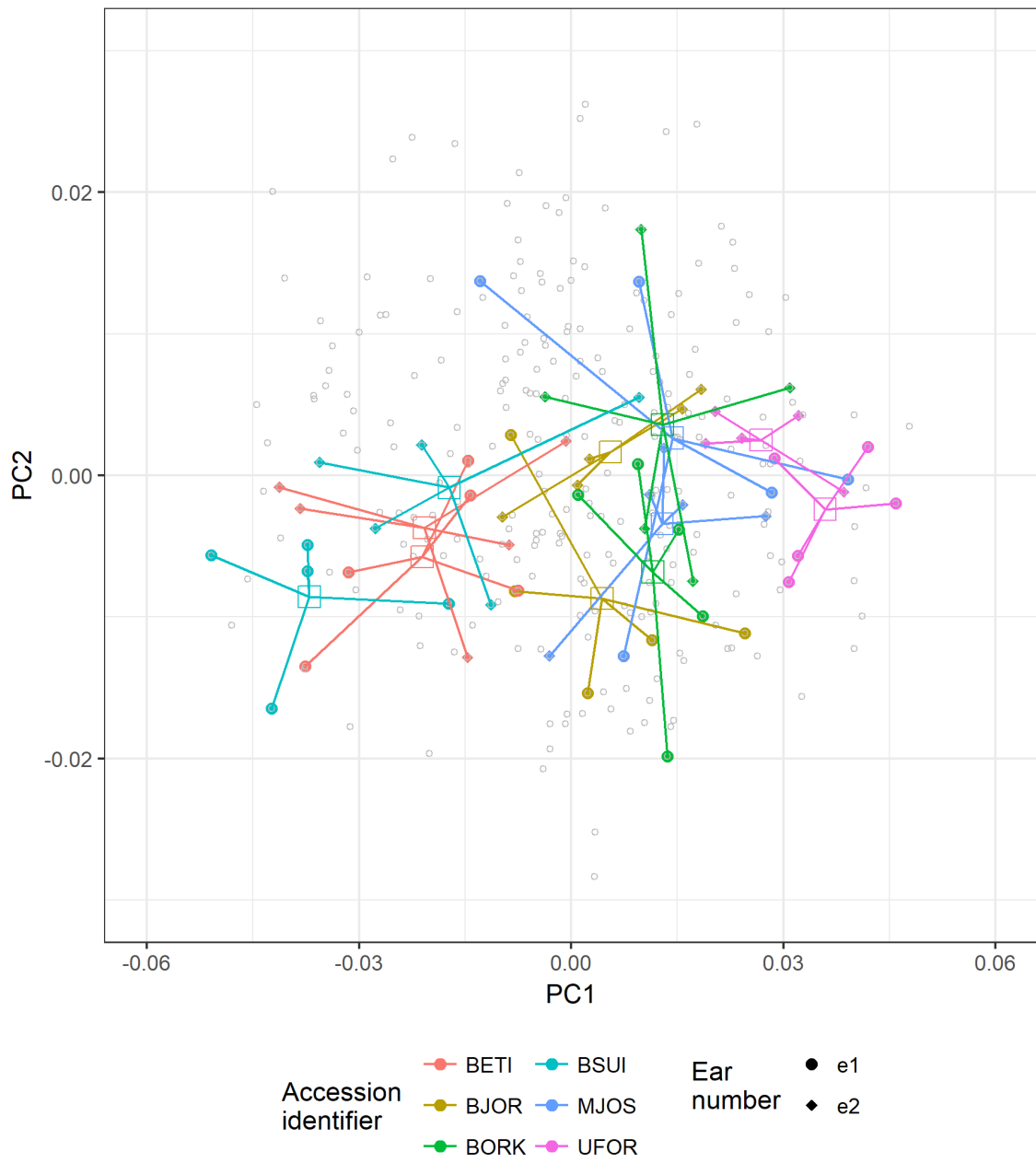


Fig. S5

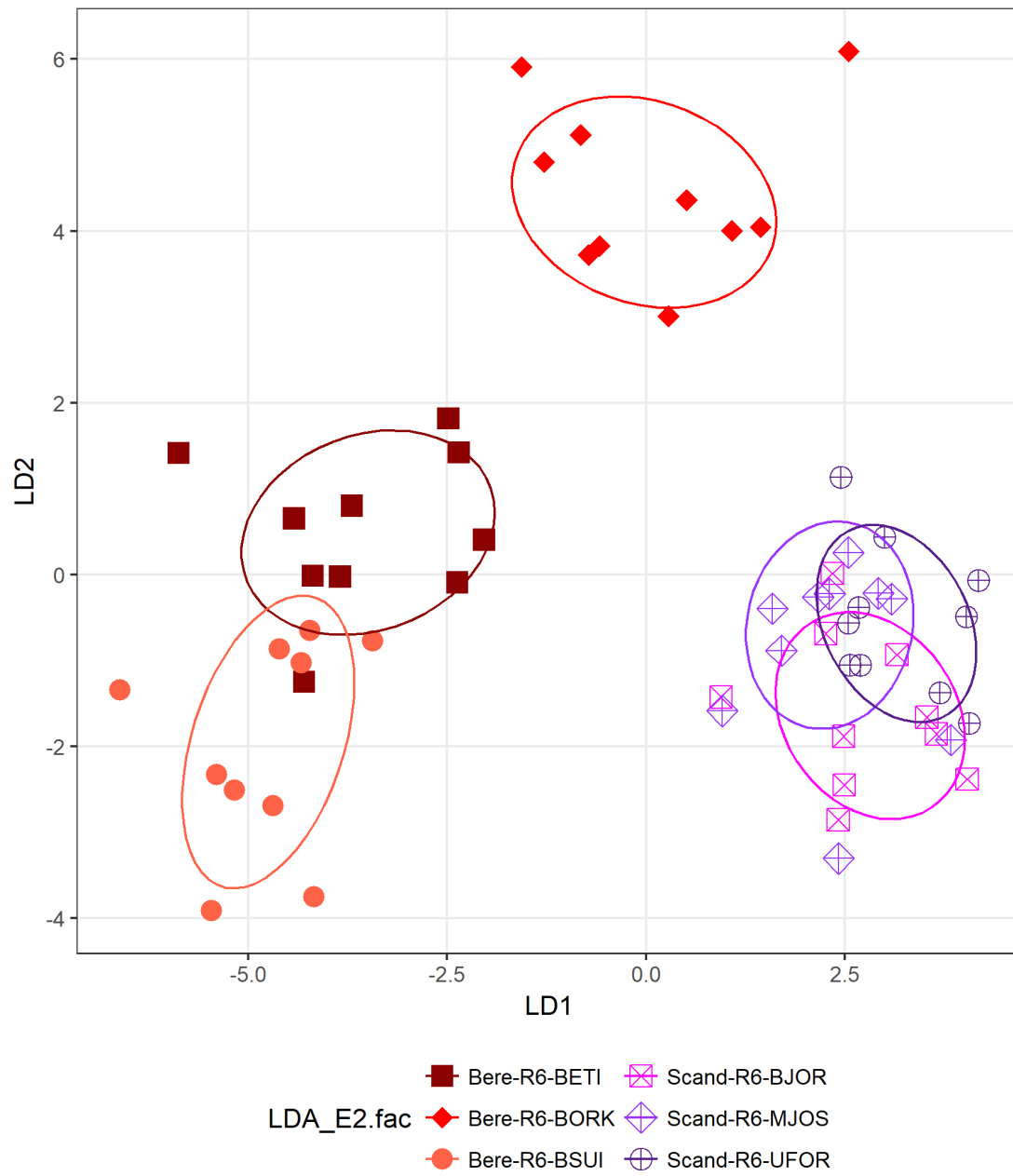


Fig. S6

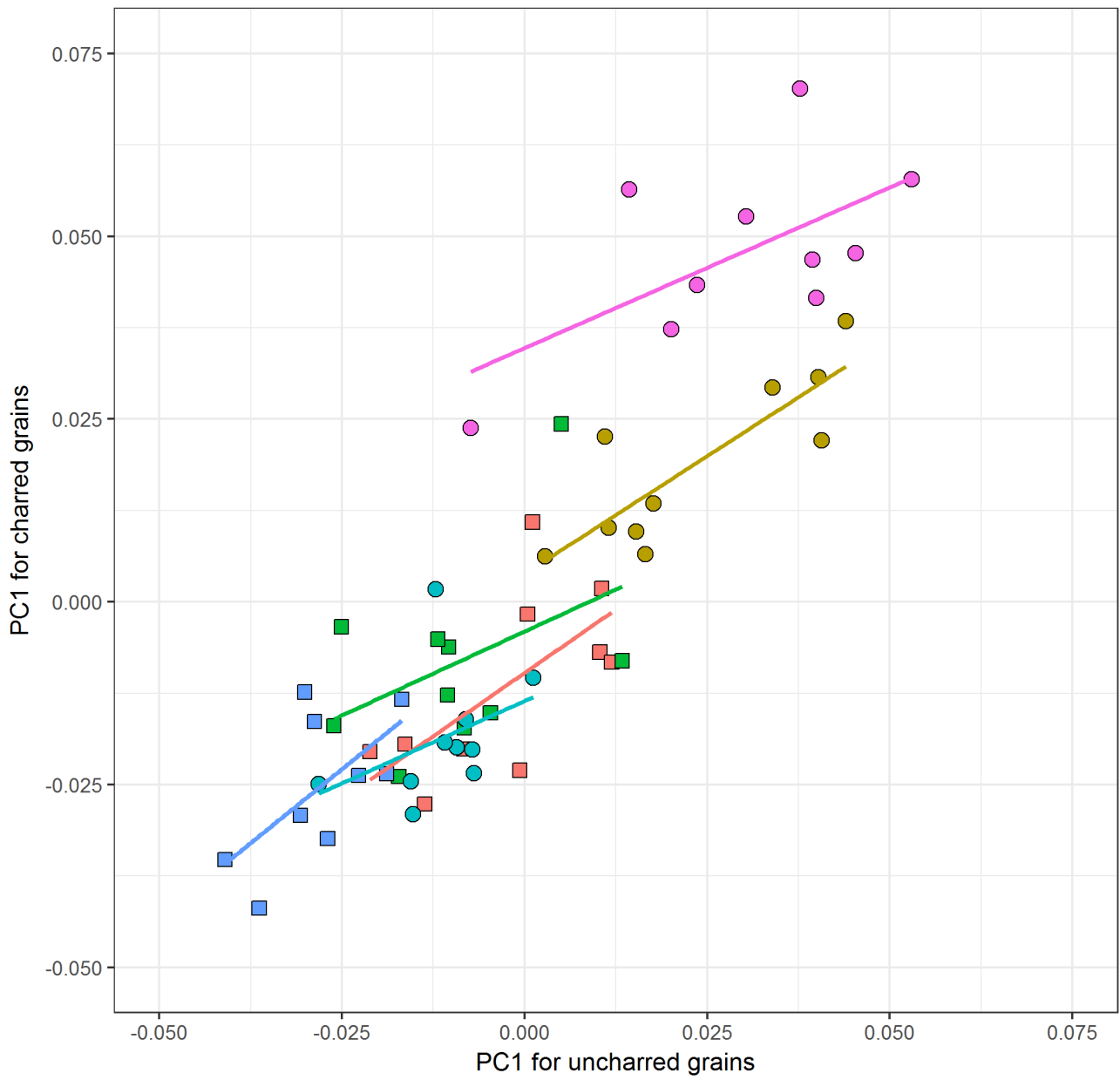
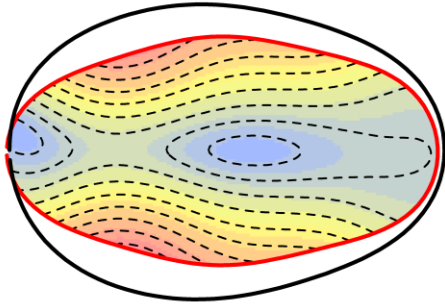


Fig. S7

A



B

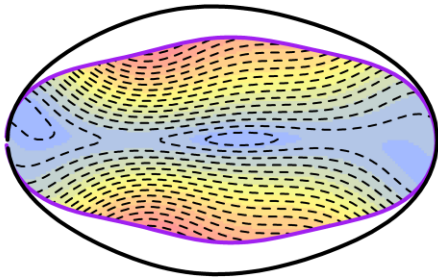


Table S1

Accession name	Accession origin and row type	Accession gene cluster	Orkney grains from ear 1	Orkney grains from ear 2	Dundee grains
Bere_818_Orkney_SASA	Bere-R6	R6-Bere	5	0	5
Bere_820_unknown_SASA	Bere-R6	R6-Bere	5	0	5
Bere_B24268_Shethland_GRU	Bere-R6	R6-Bere	5	0	5
Bere_B7035_Unknown_GRU	Bere-R6	R6-Bere	5	0	5
Bere_Clho6478_PI130740_Orkney_USDA	Bere-R6	R6-Bere	5	0	5
Bere_Clho8327_PI174488_Unknown*_USDA	Bere-R6	R6-Bere	5	0	5
Bere_OE1_Orkney_SASA	Bere-R6	R6-Bere	5	0	5
Bere_OE2_Orkney_SASA	Bere-R6	R6-Bere	5	0	5
Bere_OM1_Orkney_SASA	Bere-R6	R6-Bere	5	5	5
Bere_SU2_Western_Isles_SASA	Bere-R6	R6-Bere	5	5	5
Bere_T1_Western_Isles_SASA	Bere-R6	R6-Bere	5	5	5
Bere1_T1_Western_Isles_SASA	Bere-R6	R6-Bere	5	0	5
Bere1_T2_Western_Isles_SASA	Bere-R6	R6-Bere	5	0	5
Bere2_T1_Western_Isles_SASA	Bere-R6	R6-Bere	5	0	5
Bere_K17253_Unknown_Vavilov	Bere-R6	Omitted	5	0	5
Bere2_T2_Western_Isles_SASA	Bere-R6	Omitted	5	0	5
Clho5003 (6R)_Donegal_Ireland_USDA	Bere-R6	Omitted	5	0	5
Langaks_Denmark (Faeroerne Islands)_NGB	Faro-R6	R6-Bere	5	0	5
St Jernebyg Fra_Fraererne_NGB	Faro-R6	R6-Bere	5	0	5
Cornish_B4814_GRU	Brit-R2	R2	5	0	5
Early Welsh_B4815_GRU	Brit-R2	R2	5	0	5
Golden Archer_B7033_GRU	Brit-R2	R2	5	0	5
Hen Gymro_B7054_GRU	Brit-R2	R2	5	0	5
Long Eared Nottingham_B8200_GRU	Brit-R2	R2	5	0	5

Northumberland Rogue_B7047_GRU	Brit-R2	R2	5	0	5
Old Cornish_GRU	Brit-R2	R2	5	0	5
Old Wiltshire Archer_B4816_GRU	Brit-R2	R2	5	0	5
Pembroke_B4847_GRU	Brit-R2	R2	5	0	5
Plumage Archer_B7027_GRU	Brit-R2	R2	5	0	5
St Davids_B4820_GRU	Brit-R2	R2	5	0	5
Standwell_B3581_GRU	Brit-R2	R2	5	0	5
Stanza_B18671_GRU	Brit-R2	R2	5	0	5
Swanneck_B3585_GRU	Brit-R2	R2	5	0	5
Bjorneby_Norway_NGB	Scand-R6	R6-Scand	5	5	5
Donnes_Norway_NGB	Scand-R6	R6-Scand	5	0	5
Erhardt Frederiksens_Denmark_ NGB	Scand-R6	R6-Scand	5	0	5
Kr Flinset_Norway_NGB	Scand-R6	R6-Scand	5	0	5
Mjos_1918_Norway_NG B	Scand-R6	R6-Scand	5	5	5
Opdal_PI 54912_Norway_USDA	Scand-R6	R6-Scand	5	0	5
Skaneslet_Clho 6543S_Sweden_USDA	Scand-R6	R6-Scand	5	0	5
Solenbyg_Norway_Clho 6557_USDA	Scand-R6	R6-Scand	5	0	5
Trysil_Norway_NGB	Scand-R6	R6-Scand	5	0	0
Tystofte Korsby_Denmark_NGB	Scand-R6	R6-Scand	5	0	5
Uforaedlet Jamtland_Sweden_NGB	Scand-R6	R6-Scand	5	5	5
Crocket_PI 40647 _Sweden_USDA	Brit-R6	R6-?Scand	5	0	5
Gartons Archer_B8242_GRU	Brit-R6	R6-?Scand	5	0	5
Lynderupgaard_Denmar k_NGB	Scand-R6	Omitted	5	0	5
Annat_B24300_GRU	Scot-R2	R2	5	0	5
Common_B24303_GRU	Scot-R2	R2	5	0	5
Morayshire Gold_B7009_GRU	Scot-R2	R2	5	0	5
Scotch Annat_B4812_GRU	Scot-R2	R2	5	0	5
Scotch Common_PI 467671_USDA	Scot-R2	R2	5	0	5
Scottische Anno_Unknown	Scot-R2	R2	5	0	5
Scottish Annat_B8585_GRU	Scot-R2	R2	5	0	5

Table S2

Trial/Input	Type	Date of application	Rate of application
i. Orkney			
Fertiliser	Compound nitrogen (N), phosphorus (P) and potassium (K) fertiliser (14% N: 14% P: 21%K)	21-Apr	50 kg ha ⁻¹ each of N and P (as P ₂ O ₅) and 75 kg ha ⁻¹ of K (as K ₂ O)
Herbicides	Ally Max (143 g kg ⁻¹ metsulfuron-methyl and 143 g kg ⁻¹ tribenuron-methyl)	29-May	21 g ha ⁻¹
	Optica (600 g l ⁻¹ mecoprop-p)		1.0 l ha ⁻¹
	Axial (100 g l ⁻¹ pinoxaden)		0.3 l ha ⁻¹
ii. Dundee			
Fertiliser	Compound nitrogen (N), phosphorus (P), potassium (K) and sulphur (S) fertiliser (24% N: 4% P: 14% K: 7% S)	29-Mar	43 kg ha ⁻¹ of N; 7 kg ha ⁻¹ of P (as P ₂ O ₅); 25 kg ha ⁻¹ of K (as K ₂ O); 13 kg ha ⁻¹ of S (as SO ₃)
		11-May	Half the above rate
Pre-emergence herbicide	Stomp Aqua (455 g l ⁻¹ pendimethalin)	19-Mar	2.9 l ha ⁻¹
Herbicides	Charge (600 g l ⁻¹ mecoprop-p)	06-May	1.0 l ha ⁻¹
	Traton SX (111 g kg ⁻¹ metsulfuron-methyl and 222 g kg ⁻¹ tribenuron-methyl)		45 g ha ⁻¹
Fungicides	Siltra Xpro (60 g l ⁻¹ (6.2% w/w) bixafen and 200 g l ⁻¹ (20.2% w/w) prothioconazole)	24-May	0.4 l ha ⁻¹
	Joules (500 g l ⁻¹ (40.2% w/w) chlorothalonil)		1.0 l ha ⁻¹
	Vegas (50 g l ⁻¹ cyflufenamid)		0.25 l ha ⁻¹
	Siltra Xpro (as above)	20-Jun	0.4 l ha ⁻¹
	Joules (as above)		1.0 l ha ⁻¹

Table S3

Month	Orkney mean temperature (°C)	Orkney total rainfall (mm)	Dundee mean temperature (°C)	Dundee total rainfall (mm)
January	4.7	152	3.8	192
February	4.2	92	3.4	56
March	6.4	68	5.6	22
April	6.5	48	6.5	65
May	9.6	33	11.6	15
June	11.7	32	13	99
July	13.8	101	14.9	82
August	13.8	85	15.3	43
September	13.6	103	14.9	38
October	10.5	40	9.7	23
November	6.8	40	NA	NA
December	7.8	118	NA	NA

Table S5

	Classified		
Actual	R6_Bere	R6_Scand	R2
R6_Bere	144 (82%)	13 (7%)	18 (10%)
R6_Scand	20 (14%)	101 (72%)	19 (14%)
R2	17 (8%)	9 (4%)	184 (88%)

Table S6

	Classified		
Actual	R6_Bere	R6_Scand	R2
R6_Bere	35 (83%)	4 (10%)	3 (7%)
R6_Scand	1 (3%)	29 (91%)	2 (6%)
R2	2 (8%)	1 (4%)	22 (88%)

Table S7

	Classified	
Actual	Bere	Scandinavian
Bere	29	1
Scandinavian	2	28

Table S8

	Classified	
Actual	Bere	Scandinavian
Bere	22	8
Scandinavian	4	26

Table S9

	Classified					
Actual	BETI	BORK	BSUI	BJOR	MJOS	UFOR
BETI	8	1	1	0	0	0
BORK	0	10	0	0	0	0
BSUI	8	0	8	0	0	0
BJOR	0	0	0	5	4	1
MJOS	0	0	0	4	4	2
UFOR	0	0	0	0	2	8