Descriptive inference using large, unrepresentative nonprobability samples: An introduction for ecologists

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8 Abstract

9 In the age of big data, it is essential to remember that the size of a dataset is not all that matters. This 10 is particularly true where the goal is to draw inferences about some wider population, in which case it is far more important that the data are *representative* of that population. It is possible to adjust 11 12 unrepresentative samples so that they more closely resemble the population in terms of "auxiliary 13 variables". If the auxiliaries predict sample inclusion and/or the variable of interest well, then the adjusted sample estimates will be closer to the truth. Several survey sampling techniques exist to 14 15 perform such adjustments, but most are not familiar to ecologists. We applied five types of adjustment-subsampling, quasi-randomisation, poststratification, superpopulation modelling, and 16 17 multilevel regression and poststratification—to a simple two-part biodiversity monitoring problem. The first part was to estimate mean occupancy of the plant Calluna vulgaris in Great Britain in two 18 19 time-periods (1987-1999 and 2010-2019); the second was to estimate the difference between the two 20 (i.e. the trend). Calluna vulgaris is an attractive case study because we have good estimates of its true 21 distribution in both time-periods. We estimated the means and trend using large, but (originally) 22 unrepresentative, samples. Compared to the unadjusted estimates, the means and trends estimated 23 using most adjustment methods were more accurate, although their uncertainty intervals generally did 24 not cover the true values. Quasi-randomisation performed especially poorly, and we explain why. 25 Most adjustments were far more successful at bringing the distributions of the auxiliary variables in 26 the samples closer to those in the population than they were at improving the estimates of population 27 means and trends. This implies that the major challenge for adjusting unrepresentative samples in

28 biodiversity monitoring is assembling a suitable set of auxiliary variables (i.e. predictors of sample

29 inclusion and the variable of interest). This challenge will be particularly acute for poorly studied taxa

30 and those whose habitat requirements or sampling biases are not reflected in available data.

31 Introduction

32 As the data revolution gathers pace, it is not surprising to see "big data" being used to monitor

33 biodiversity. Examples include observations submitted to mobile phone apps by amateur naturalists

34 (Johnston et al., 2022) and digitised specimens from museums and herbaria (Nelson & Ellis, 2019).

35 Such data become bigger still when combined in data aggregators such as the Global Biodiversity

36 Information Facility (GBIF; https://www.gbif.org/) or metadatabases such as PREDICTS (Hudson et

al., 2014). Unfortunately, quantity of data does not necessarily imply quality of insight.

38 Monitoring biodiversity is typically a matter of descriptive statistical inference. It is inferential in that

the goal is to infer something about a target population from a sample of that population (Boyd,

40 Powney, et al., 2023). The population might comprise, say, all areal units across some landscape, in

41 which case the sample would be a subset of those units. The inference is descriptive in that the aim is

42 to describe (rather than explain) a variable of interest in the population. A common example is the

43 proportion of patches of land occupied by some species (Bowler et al., 2021; Outhwaite et al., 2020;

44 Powney et al., 2019; Stroh et al., 2023; van Strien & van Grunsven, 2023), but there are many others.

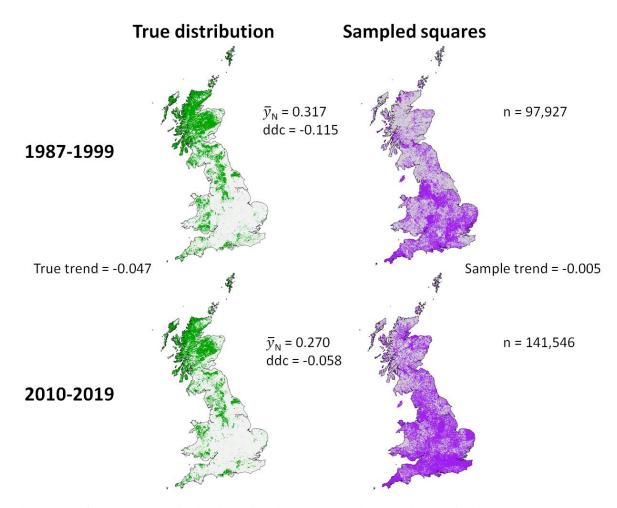
- 45 More important than the size of a sample for descriptive inference is whether it is representative of the
- 46 population (X. L. Meng, 2018). In a representative sample, the distribution of the variable of interest
- 47 is similar to its distribution in the population (Bethlehem et al., 2008). An equivalent definition is that
- 48 there is little to no correlation between inclusion in the sample and the variable of interest—the "data
- 49 defect correlation" (ddc; Meng, 2018). Intuitively, statistics derived from a representative sample,
- 50 such as means and proportions, will be similar to their population equivalents. The challenge is that 51 the variable of interest is unknown in non-sampled population units, so it is typically impossible to
- 51 the variable of interest is unknown in non-sampled population units, so it is typically impossible to 52 coloulete a sample's representativeness exectly.
- 52 calculate a sample's representativeness exactly.
- 53 Rather than measuring sample representativeness in terms of the variable of interest, which is not
- 54 known for all population units, it is possible to approximate it using "auxiliary variables". Auxiliary
- variables are those that are thought to predict the variable of interest or the probability that each
- 56 population unit was sampled. Such variables might be available for every population unit. For
- 57 example, climate variables might explain a species' occupancy, and data on these variables are
- available for every 1 km^2 grid square across the globe (Fick & Hijmans, 2017). If the distributions of
- auxiliary variables in the sample are different to those in the population, then the sample is likely to be
- 60 unrepresentative, at least with respect to those variables (Bethlehem et al., 2008).
- 61 It is possible to adjust an unrepresentative sample by placing more weight on population units that
- 62 were less likely to be sampled. Weighting is simple where the probability that each population unit
- 63 was sampled is known (i.e. in a probability sample). For example, rather than using a sample mean to
- 64 estimate a population mean, the researcher would use a weighted mean with the weights being the
- 65 inverses of the inclusion probabilities (Lohr, 2022). Weighting of this type is known as "design-based
- 66 inference", because the inclusion probabilities are a feature of the sampling design. Unfortunately,
- 67 design-based inference is not applicable for many "big" biodiversity datasets, whose sample inclusion
- 68 probabilities are not known (i.e. they are nonprobability samples), so alternatives are required.
- 69 Most approaches to descriptive inference from nonprobability samples make use of auxiliary
- variables. The details differ, but the general strategy is to weight the sample in such a way that the
- 71 distributions of the auxiliary variables in the sample more closely resemble those in the population
- 72 (Valliant et al., 2018). If the auxiliaries predict the variable of interest and sample inclusion well, then
- this is essentially the same as bringing the distribution of the variable of interest in the sample closer
- to its distribution in the population (i.e. making the sample more representative; see X. Meng, [2022], who demonstrates this mathematically.
- 75 who demonstrates this mathematically).
- 76 Use of sample adjustments in biodiversity monitoring is variable. It is common for monitoring
- schemes to weight samples in such a way that the relative frequencies of habitats or geographic areas
- in the sample are similar to those in the population (Gregory et al., 2005; C.A.M. Van Swaay et al.,
- 79 2002; Chris A.M. Van Swaay et al., 2008; Weiser et al., 2020). But it is also common to see sample
- 80 representativeness ignored, an issue that has led to some high-profile controversies in the biodiversity
- 81 monitoring literature (Boyd, Powney, et al., 2023). We suspect that many of those who do not deal
- 82 with issues of sample representativeness are not familiar with the gravity of the problem or the
- 83 relevant theory and adjustment methods.
- 84 In this paper, we introduce five approaches to descriptive inference using unrepresentative
- 85 nonprobability samples and demonstrate how they relate to each other (conceptually and
- 86 mathematically). We apply each approach to a simple two-part biodiversity monitoring problem. The
- 87 first part is to estimate mean occupancy of the plant *C. vulgaris* across 1 km grid squares in Britain in
- two time-periods; the second is to estimate the difference between the two (i.e. the trend). *Calluna*
- 89 *vulgaris* is an attractive case study because we have good estimates of its true geographic distribution
- 90 in both periods from several sources. The approaches to inference that we demonstrate are
- 91 subsampling, quasi-randomisation (Elliott and Valliant, 2017), poststratification (Little, 1993),

- 92 superpopulation modelling (Valliant, 2009) and Multilevel Regression and Poststratification (MRP;
- 93 Gelman, 2007; Gelman and Little, 1997). Each can be (MRP more loosely than the rest) interpreted as
- an attempt to weight the sample in such a way that it more closely resembles the population, in the
- bope that this results in more accurate descriptive inferences. We demonstrate the effects of each
- approach on the distributions of auxiliary variables in the sample, as well as on the resulting estimates
- 97 of mean occupancy in each period and the time trend between the two. Applying the adjustment
- 98 methods to a real-world example reveals challenges that ecologists are likely to face, and we discuss
- 99 these in detail.

100 Methods

- 101 Estimating the true distribution of *Calluna vulgaris*
- 102 We approximated the true distribution of the dwarf shrub vascular plant *Calluna vulgaris* (Heather) in
- 103 two time periods: 1987–1999 and 2010–2019. For the first period, we used the 1990 UKCEH land
- 104 cover map (Rowland et al., 2020); for the second, we used the 2018 version (Morton et al., 2022).
- 105 From these maps, we identified 1 km grid squares (British National Grid, EPSG:27700) with >0%
- 106 heather or heather grassland cover. To these, we added 1 km squares in which *C. vulgaris* was
- 107 recorded in each time period by the Botanical Society of Britain and Ireland (BSBI); the time periods
- 108 used cover the main periods of recording for two national distribution atlases (Preston, C.D., Pearman,
- 109 D.A. & Dines, 2002; Stroh et al., 2023). Acknowledging that some 1 km squares may have been
- 110 erroneously classed as having some heather or heather grassland coverage by the land cover maps, we
- removed any 1 km squares that fell within 10 km grid squares in which *C. vulgaris* had not been
- recorded by the BSBI in the period 1950–2019. Given that this period includes recording for three
- national distribution atlases (the two cited above plus Perring & Walters, 1962), we assume that the
- 114 union of all 10 km occurrences within this period encompasses all known populations irrespective of
- 115 finer scale changes. Figure 1 maps the resulting estimates of the true 1 km distributions of *C. vulgaris*
- 116 in both time-periods.

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Figure 1. Left column: the distribution of *Calluna vulgaris* in both time-periods. Green squares are occupied and grey squares are not. \bar{y}_N is mean occupancy or, equivalently, the proportion of squares

121 occupied. The ddc's are the correlations between sample inclusion (1 if the square is in the sample

122 and 0 otherwise) and occupancy. Right column: the nonprobability 1 km samples for each time-

123 period. Purple squares were sampled and grey squares were not. n is the number of squares sampled.

124 We assume that *C. vulgaris* was recorded in all sampled grid squares that it occupied in the relevant

time-period. The true trend is the difference between population means, and the sample trend is the

126 difference between sample means (i.e. mean occupancy across purple squares).

127 Sample data on *Calluna vulgaris* occupancy

- 128 The 1 km samples for both time periods ("Sampled squares in Fig. 1) encompass any vascular plant
- data assigned to a single day, either at the 1 km scale or finer, collected by the BSBI for the national
- 130 distribution atlases of Preston et al. (2002) and Stroh et al. (2023).
- 131 Auxiliary data
- 132 We used five auxiliary variables for which data are available for all 1 km grid squares in Great Britain
- 133 (Table 1). Most of the auxiliary variables indicate the accessibility or attractiveness of grid squares,
- 134 which tend to be associated with site selection in citizen science datasets (Geldmann et al., 2016).
- 135 Elevation is a potential predictor of *C. vulgaris* occupancy.
- 136 Originally, we included three additional predictors of *C. vulgaris* occupancy—the first and third
- 137 principal components of climate space in Britain and soil pH—but later omitted them. We had
- 138 previously found the climate variables to be important predictors of 1 km habitat suitability for *C*.
- 139 vulgaris using species distribution models (Boyd, Harvey, et al., 2023). Including these predictors did
- 140 not improve the estimates of mean occupancy, a point that we expand on in the discussion. Reducing

- 141 the set of auxiliary variables simplifies matters for some of the adjustment methods that we present
- 142 below.
- 143 For simplicity, we assume that the auxiliary variables are constant between time-periods. This
- 144 assumption is obviously violated for some variables (e.g. road length and postcode density). However,
- this should not matter if, in reality, the variables in period one are correlated with those in period two,
- because any given grid square will generally have a higher or lower value than the others regardless of
- 147 the period. We think that this situation is plausible: for example, there is a higher density of postcodes
- 148 in London in period two than in period one, but in either period, it has a higher density than
- elsewhere. Another reason to use one set of auxiliary data for both time-periods is to make our
- 150 findings more applicable to situations in which temporally resolved data are not available (e.g. in data
- 151 poor countries or periods in the distant past).
- 152 Table 1. Auxiliary variables used for sample adjustment.

Variable	Reason for inclusion	Details	Reference(s)
Postcode density	Indicates population	Total number of	ONS (2021)
	density in vicinity	postcodes in the focal	
		grid square and its 299	
		nearest neighbours	
Road length	Indicates accessibility	The total length of all	Data from
		"Roads" and "Link	https://www.openstree
		roads" ("Highways"	tmap.org/ under an
		class of the	open database license
		OpenStreetMap	
		ontology) in the focal	
		grid square and its 299	
Duonoution in	Indiantas notantial	nearest neighbours	UNEP-WCMC &
Proportion in protected area	Indicates potential attractiveness to surveyor	Proportion of the focal grid square with some	IUCN (2020)
protected area	attractiveness to surveyor	level of "protection".	10CN (2020)
		Includes everything	
		from SSSIs to e.g.	
		local nature reserves	
Proportion open	Indicates accessibility	Proportion of land	All open access land
access land	5	legally designated as	datasets in GB are
		open access within 1	available via an Open
		km grid square	Government License.
			For England, we used
			the CRoW act 2000
			layer. For Wales, we
			combined the
			registered common
			land, other statutory
			access land, open
			country and public
			forest datasets. All of
			the Scottish
			countryside is open
Average elevation	Predictor of <i>C. vulgaris</i>	Average elevation of 1	access.
Average elevation	occupancy	km grid square	Intermap (2009)
	occupancy	calculated from 50 m	
		digital terrain model	

154 Estimating the per-period population mean

- 155 The first step in our biodiversity monitoring problem is to estimate mean occupancy of *C. vulgaris* in
- 156 each time-period. Although not usually written this way, it is helpful for what comes later to re-

157 express the population mean as a weighted sum

$$\bar{y}_N = \frac{1}{N} \sum_{i=1}^N y_i = \sum_{i=1}^N \frac{y_i}{N} = \sum_{i=1}^N \frac{y_i w_i}{\sum_N w_i},$$
 (1)

158

where y is occupancy (1 = occupied and 0 = unoccupied), N is the population size, i indexes 1 km grid squares and $w_i = 1/N$ (N is the same in both time-periods). The denominator in the rightmost

- 161 expression might seem unnecessary, because it equals one. We have retained it to illustrate the
- 162 similarity between this expression and the sample-based estimators below, which have a similar form
- 163 but whose sampling weights *w* do not necessarily sum to one. For notational simplicity, we do not
- 164 index the time-period, and the reader should remember that \bar{y}_N is time-period specific. In practice, y
- 165 is not known for all *i* in the population, so sample-based estimators of \bar{y}_N are needed.

166 The design-based estimator

- 167 The design-based estimator of the population mean, which is applicable only where a probability
- sample of some sort is available (Lohr, 2022), has a similar form to 1)

$$\overline{y}_{db} = \sum_{i=1}^{n} \frac{y_i \, w_i}{\sum_n w_i}.$$

- 169 The differences are that the sums are over the sample size n rather than N and that the weights w_i are
- not necessarily constant. Rather, the weight for unit *i*, w_i , is equal to the reciprocal of the probability that it was included in the sample = $1/p_i$.
- 172 Sample inclusion probabilities are, by definition, not known for nonprobability samples, so alternative
- 173 estimators are required. We present five such estimators below, three of which–quasi-randomisation,
- 174 poststratification and superpopulation modelling-are explicit attempts to come up with a set of
- 175 weights w_i that produce a reasonable estimate of \bar{y}_N under 2). The other two, subsampling and MRP,
- are conceptually similar.

177 Estimators for nonprobability samples

- 178 The following estimators are used in survey sampling to estimate population means from
- nonprobability samples. More detail on each can be found in Valliant et al. (2018), Lumley (2010)
- 180 and Lohr (2022).

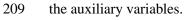
181 Naïve sample mean

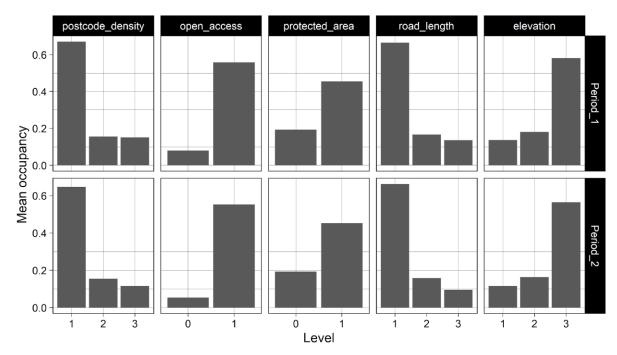
- 182 Where sample inclusion probabilities are unavailable, a simple option is to assume that $w_i = 1/n$ for
- all *i*. In this case, 2) is the (naïve) sample mean. As the weights are constant, the sample mean does
- 184 not adjust for differences in y between the sampled and non-sampled population units. It is
- 185 nevertheless widely used in biodiversity monitoring.

186 Quasi-randomisation

- 187 An alternative approach is to imagine that the nonprobability sample was selected probabilistically
- and to estimate the implied inclusion probabilities. Any binary model and auxiliary data can be used.
- 189 Once inclusion probabilities p_i have been estimated, the weights $w_i = 1/p_i$ (as in the design-based
- 190 estimator). In our example, we used random forests and the auxiliary data in Table 1 to estimate
- 191 pseudo-inclusion probabilities. More complex appraoches are possible and have been used to map
- 192 species distributions (Johnston et al., 2020).

- 193 Poststratification
- 194 Another approach to estimating sampling weights is poststratification. Poststratification requires
- 195 categorical auxiliary data, so continuous variables must be discretized prior to analysis (Valliant,
- 196 2020). The auxiliary variables are crossed (think contingency tables) to create poststrata. Each
- 197 poststratum *j* has a sample size n_j and population size N_j . The sampling weight w_i for population unit
- 198 *i* in poststratum *j* is given by N_j/n_j .
- 199 In our example, we split most auxiliary variables into three categories using their terciles (i.e. cut
- 200 points at the 33rd and 67th percentiles). This did not make sense for the variables denoting the
- 201 proportion of each grid square that is open access land and protected area, because most squares took
- the value one or zero. We split these variables into two categories, 0 and >0, i.e. whether or not there
- is some open or protected land in the grid square. Discretization initially gave $3 \times 3 \times 3 \times 2 \times 204$ 204 2 = 108 poststrata, from which we subtracted one poststratum that contained no population units,
- 205 leaving 107.
- 206 It is sensible to discretize the auxiliary variables in such a way that the variable of interest varies
- among categories. Otherwise, the adjustment from poststratifying will be minor (or unnecessary!).
- Fig. 2 shows that mean occupancy of *C. vulgaris* in the samples differs appreciably among levels of





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Figure 2. Mean occupancy of *Calluna vulgaris* for each level of the auxiliary variables (Table 1) in each time-period. The auxiliary variables were originally on a continuous scale, but we discretized them to enable poststratification. See the main text for details.

- 214 Superpopulation modelling
- 215 Superpopulation modelling is conceptually different to the adjustment methods described above. The
- 216 premise is that there exists some model that describes the variable of interest in the population. If this
- 217 model can be recovered from the sampled outcome variable y and the auxiliary data, it can be used to
- 218 predict the variable of interest in non-sampled units. Given a prediction for each non-sampled *i*, it is
- then simple to estimate the population mean.
- 220 A general (i.e. multiple) linear regression model of *y* has the form

$$E_M(y_i) = \boldsymbol{x}_i^T \,\boldsymbol{\beta},\tag{3}$$

221 where the subscript M indicates that the expectation (mean) is with respect to the model, x_i is a vector

- 222 of predictors for unit *i*, the superscript T indicates that the vector x_i has been transposed (to a row
- 223 vector) and β is a column vector of parameters. There is some matrix notation in 3) and what follows, 224 but the logic should be apparent to those who do not understand the precise detail. A prediction of y
- 225 for unit *i* is

$$\hat{y}_i = x_i^T \,\hat{\beta}.\tag{4}$$

The accent on β indicates that it is an estimate. Given a sample s, one estimator of β is $\hat{\beta} = A_s^{-1} X_s^T y_s$, 226

where $A_s = X_s^T X_s$, X_s is an n x p matrix of covariates and y_s is an n vector of y's (Valliant, 2020). If 227 \overline{s} is the set of non-sampled population units, the superpopulation model prediction of the population 228 229 mean is

$$\bar{y}_{sp} = \frac{\sum_{i \in s} y + \sum_{i \in \bar{s}} \hat{y}}{N}.$$
 5)

That is, it is the sum of the known outcome values in the sample and those predicted by the model for 230

- the remainder of the population divided by the population total. A feature of \bar{y}_{sp} is that it can be 231
- expressed in the same form as the design-based estimator in 2), with $w_i = 1 + t_{\bar{s}}^{x} A_{s}^{-1} x_i$ and $t_{\bar{s}}^{x}$ being 232
- 233 the vector of population totals of the auxiliary variables in non-sampled population units (Elliott and
- 234 Valliant, 2017). (Code to verify this numerically is available at
- 235 https://github.com/robboyd/selectionBiasEffects/tree/master/R.) Like the other adjustment models,
- 236 then, the superpopulation estimator is an approach to estimating the sampling weights w_i .
- 237 Linear regression might seem like an unusual choice of model for a binary outcome (occupancy), but
- 238 we felt that it was the best option here. One reason is that the implied model is actually linear for an
- 239 estimator of the form 2) (Valliant, 2020). Most important, however, is that the use of a linear model
- 240 enables the estimation of sampling weights (Valliant et al., 2018; supplementary material 1). This is
- 241 helpful, because those weights can be used to show the effects of superpopulation modelling on the
- 242 distributions of the auxiliary variables in the sample (see "Evaluating the effects of the adjustments"
- 243 below). Alternative models can be used where weights are not required (e.g. Wu and Sitter, 2001). In
- 244 our example superpopulation model, we used the auxiliary variables in Table 1 as predictors.
- 245 Subsampling
- 246 Perhaps more familiar to ecologists than the above approaches is subsampling (Beck et al., 2014;
- 247 Steen et al., 2020). The idea is to create a representative "miniature" of the population out of the
- 248 sample (Meng, 2022) and to calculate the quantity of interest (mean occupancy) from this subsample.
- 249 Subsampling trades sample size for representativeness.
- 250 Our approach was to draw weighted random samples of size 500 with replacement from the original
- samples [note that these weights are different to sampling weights in 2)]. The decision to set n = 500251
- 252 was somewhat arbitrary, but changing the subsample size makes little difference to the point estimates
- 253 of the population means (although they become more precise with increasing subsample size;
- 254 supplementary material 1). We assigned each grid square i in poststratum j (using the same strata as
- 255 described above under Poststratification) a weight of n_i/N_i . The result was subsamples whose
- members were more likely to be from strata comprising a larger fraction of the population. The 256
- 257 subsample mean is the estimator of the population mean.
- 258 Rather than using a single subsample, we repeated the process 1000 times and used the mean of the
- 259 estimated means (i.e. bootstrapping). This was necessary, because the estimated means were sensitive
- 260 to the random component of the subsampling.

261 Multilevel regression and poststratification (MRP)

- 262 MRP is an extension of poststratification and a variation of superpopulation modelling (Gelman,
- 263 2007; Gelman & Little, 1997; Valliant et al., 2018). A hierarchical model is used to estimate mean
- 264 occupancy in each poststratum. The advantage of using a hierarchical model is that cells with few or
- 265 no data borrow information from cells with more data (i.e. partial pooling or shrinkage is exploited).
- 266 The population mean is the weighted mean of the stratum means, where the weights are equal to the
- 267 proportion of the population in each stratum.
- 268 Our hierarchical model is a simple one. It is a binomial GLM with a logit link function, a fixed
- 269 intercept and a random intercept for each auxiliary variable (see https://mc-
- 270 <u>stan.org/rstanarm/articles/mrp.html</u> for a similar formulation). A more complex model might include
- 271 interactions among the auxiliaries (e.g. Ghitza and Gelman, 2013), but we found these take several
- times longer to run. Long run times may be undesirable for production-type statistical workflows in
- biodiversity monitoring, where models might need to be fitted for thousands of species in tens of
- time-periods. Even without interactions, and on a computer cluster, the models took around ten hours
- to run per time-period. We fitted the model in a Bayesian framework using 5 Markov Chain Monte
 Carlo (MCMC) chains, each with 1000 iterations. This was sufficient to achieve convergence on all
- 277 parameters in both time-periods.

278 Confidence intervals

- 279 We present 95% confidence/credible intervals for all estimates of mean occupancy (credible intervals
- for MRP, which was implemented in a Bayesian framework). The *survey* package (Lumley, 2010),
- which we used to calculate the sample means, the superpopulation model estimates and the
- 282 poststratified estimates, calculates the confidence intervals automatically. It accounts for the sampling
- 283 weights where relevant. We used percentile confidence intervals from the bootstrapped subsamples.
- 284 Estimating the trend in mean occupancy
- Having estimated mean occupancy in each time-period, the next step was to estimate the difference between the two = $\bar{y}_2 - \bar{y}_1$ (i.e. the trend). The standard errors of the trends are
- 287 $\sqrt{var(\underline{y}_2) + var(\underline{y}_1)}$ (Gelman, 2007), where the variances are sampling *not sample* variances (i.e.
- the square of the standard error rather than a measure of variability in the samples). We used the
- standard errors returned by the *survey* package, which accounts for the sampling weights. We present
- 290 95% confidence intervals for the trends from most estimators ($\pm 1.96 \times$ the standard errors). MRP is
- 291 one exception, because the 95% credible interval can be calculated directly from the posterior
- distribution of $\bar{y}_2 \bar{y}_1$. Similarly, we extracted percentile 95% confidence intervals for the
- subsampling estimator from the bootstrapped distribution of trends.

294 Evaluating the effects of the adjustments

- 295 We used relative frequency plots (c.f. Makela et al., 2014) to assess whether the adjustments brought
- the distributions of the auxiliary variables in the samples closer to their distributions in the population.
- 297 The first step was to split each auxiliary variable into fifty bins of equal width spanning its range. The
- relative frequency of grid squares (the *i*'s) in each bin k is $N_{i,k}/N$, where $N_{i,k}$ is the number of grid
- squares in each bin k in the population and N is the population size (we use k to index the bins to
- 300 distinguish them from the strata described earlier). Similarly, the relative frequency of sampled grid
- 301 squares in each k is $n_{i,k}/n$, where $n_{i,k}$ is the number of sampled grid squares in bin k and n is the

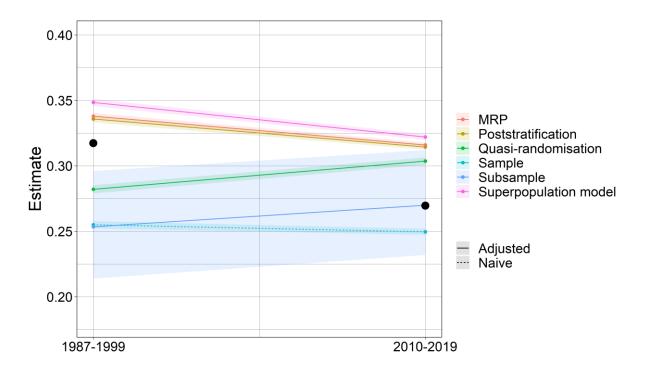
total sample size. In the adjusted samples, the equivalent relative frequency is $\frac{\sum_{i \in k} w_i}{\sum_N w_i}$ (slightly

- 303 different for subsampling; see below). We compared the original and adjusted samples' deviations
- 304 from the population using the Mean Absolute Error (MAE) of the relative frequencies across all k. If
- the MAE from the adjusted sample is smaller than the original sample, then the adjustment brought
- 306 the distribution of the auxiliary variable closer to its population distribution.

- 307 We were not able to construct adjusted relative frequency distributions from MRP so omit it from this
- 308 portion of the analysis. The problem is that, whilst it has been shown how to derive unit-level
- 309 sampling weights where the multilevel model is linear (Gelman, 2007), no formula has yet been
- derived for the case of the binomial GLM (Valliant et al., 2018). There is no obvious way to derive
- 311 weights from the subsampling estimator either. However, for this estimator, the adjusted relative
- frequencies of the auxiliaries are simply their distributions in the subsamples so are simple to obtain.
- 313 Assessing whether the estimates of mean occupancy in each period and the trend were improved by
- each adjustment method was simpler. We measured the difference between the point estimates of
- mean occupancy and the truth using the absolute error = $|\bar{y}_N \bar{y}_{est}|$, where \bar{y}_{est} is the estimate. For
- the trends, whose signs are of interest, we simply used the differences between the estimates and the
- truth. We also assessed whether the confidence/credible intervals produced by each method covered
- the true means and trend.

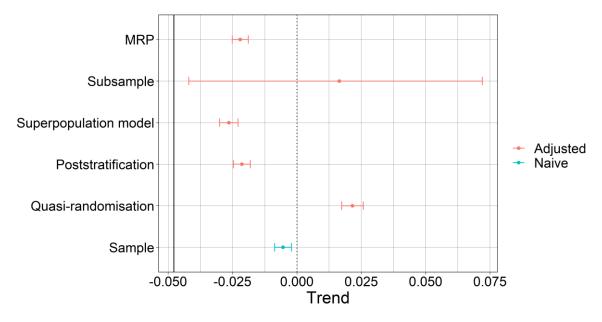
319 Results

- 320 Per-period sample representativeness and estimated mean occupancy
- 321 The samples are large but somewhat unrepresentative (Fig. 1). Forty-three percent of grid squares
- were sampled in period one, and the ddc is -0.115; in period two, 62% of grid squares were sampled,
- and the ddc is -0.058. A consequence of these ddc's is that the naive sample means underestimate the
- 324 population means, especially in period one where the magnitude of the ddc is greater (Fig. 3).
- 325 The adjustment methods did not always result in improved point estimates of mean occupancy
- relative to the naive sample means (Fig. 3). In period one, the adjusted estimates were generally better
- in terms of absolute errors, with the exception of the subsample estimate, which was worse. In period
- two, on the other hand, the estimate from the subsample was the only one to get closer than the naive
- sample mean (again, in terms of absolute error). The absolute errors are provided in supplementary
- 330 material 3.
- 331 In terms of confidence/credible interval coverage, the estimators were generally very poor. With the
- exception of the subsample means, none covered the population mean in either period. The fact that
- the confidence intervals from the subsamples did cover the population means is not surprising: the
- subsamples are small (n = 500), so the confidence intervals are wide. Of course, increasing the size
- of the subsamples reduces the width of the confidence intervals, as we show in supplementary
- material 1.

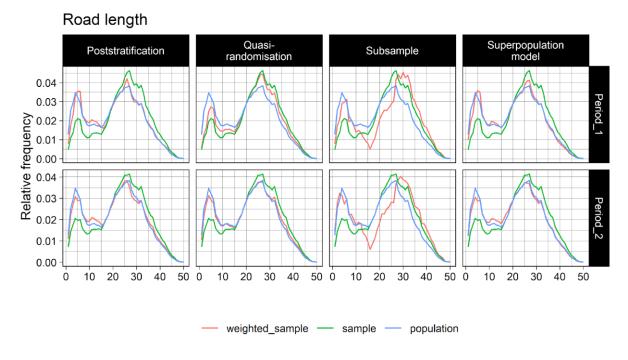




- Figure 3. Naive (i.e. unadjusted) and adjusted sample-based estimates of mean occupancy in each
- time-period. The shaded regions are 95% confidence/credible intervals (see the main text for
- information on how these have been constructed for each method). The large black circles are the true
- 341 population means in each time-period.
- 342 Estimated trend in mean occupancy
- 343 Three of the five adjusted point estimates of the trend in mean occupancy are closer than the
- 344 difference in naive sample means to the true population trends. The other two, the trends from quasi-
- randomisation and subsampling, are poor. Their point estimates even have the wrong sign. No
- 346 estimator's credible/confidence interval covers the true trend. The fact that the naïve sample trend
- 347 underestimates the true trend is a consequence of the time varying representativeness (Bowler et al.,
- 348 2022; Oliver L. Pescott et al., 2019).



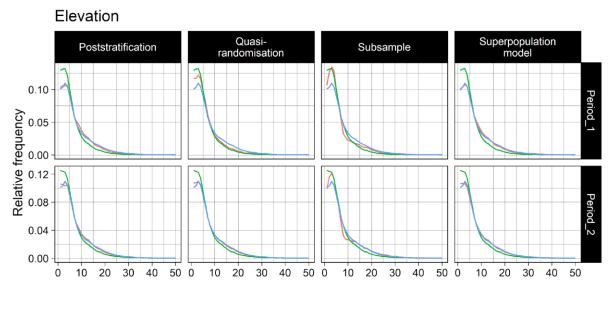
- 350 Figure 4. Trends in mean occupancy between periods one and two produced by the estimator from
- ach adjustment method, in addition to the naive sample estimate. Error bars delimit 95%
- 352 confidence/credible intervals. The solid vertical black line denotes the true population trend (-0.047).
- 353 Distributions of auxiliary variables
- 354 As measured using Mean Absolute Errors (MAEs), the adjustment methods were generally very good
- at bringing the distributions of the auxiliaries in the samples closer to those in the population. Figs 5
- and 6 show the sample and population distributions of two auxiliary variables, road length and
- 357 elevation, but the MAEs for these and the others can be found in supplementary material 3.
- 358 Superpopulation modelling and poststratification performed particularly well. Quasi-randomisation
- 359 offered only a minor improvement in period one. Subsampling was the only approach that did not
- 360 bring the distributions of the auxiliaries in the sample closer to those in the population.



361

362 Figure 5. Sample, population and weighted sample distributions of the auxiliary variable road length

363 (Table 1) in periods one and two.



— weighted_sample — sample — population

364

Figure 6. Sample, population and weighted sample distributions of the auxiliary variable elevation (Table 1) in periods one and two.

367 Discussion

368 Our experience is that analysts using large, nonprobability samples to monitor biodiversity tend not to 369 account for issues of representativeness. Even where such issues are dealt with, there has been little 370 acknowledgement of the broader panoply of relevant survey sampling methods available to the 371 analyst, no exploration of how these are conceptually (or mathematically) linked and no comparison of their performance in realistic (i.e. relatively data poor) biodiversity monitoring situations. Evidence 372 373 that a method can work in some discipline, or in simulation studies, is not proof that it will work in all 374 situations. We have demonstrated how such adjustments might be applied using a realistic example of 375 distribution change in a vascular plant over a period of 32 years. This example is realistic in that we 376 do not have access to perfect predictors of occupancy or of sample inclusion. However, it is still likely to be closer to a best-case scenario than otherwise, due to the intense survey effort expended on 377 378 vascular plants over the British landscape in the recent past (Stroh et al., 2023) and the fact that 379 auxiliary data are relatively accessible in this area.

Our key finding is that the ability to bring the distributions of auxiliary variables in the sample closer to those in the population does not automatically mean that an adjustment will produce a more accurate estimate of a population quantity. For example, poststratification and superpopulation modelling were highly successful at redistributing the auxiliary variables in the samples (Figs 5 and 6). However, this did not translate into large improvements in the estimates of mean occupancy in each time-period or the trend (Figs 3 and 4). It must be the case that the auxiliary variables were not sufficient to describe the key differences between sample and population.

So, what makes a good auxiliary variable? Caughey et al. (2020) listed three criteria: 1) it should predict the response; 2) it should predict sample inclusion; and 3) its distribution in the population should be known. Four of the five auxiliary variables in our example were chosen on the basis that they predict sample inclusion, whereas only one was thought to be a reasonable predictor of the response (occupancy). Whilst it might seem like we prioritised the second criterion over the first, note that we originally included additional predictors of the response. These included soil pH, a known

393 predictor of *C. vulgaris* occupancy (Stroh et al., 2023), and the first and second principal components

of climate space in Britain, which we previously found to be important predictors of *C. vulgaris*habitat suitability (Boyd, Harvey, et al., 2023). Including these variables did not improve the estimates
of mean occupancy or the trend, as we show in supplementary material 2. We suspect that these

- variables were redundant, because they are highly correlated with those in Table 1, so it is of little
- 398 consequence which of these auxiliaries we included.

399 Identifying auxiliary variables that satisfy Caughey and colleagues' (2020) criteria is likely to be the 400 most challenging part of adjusting samples in biodiversity monitoring. In many situations, predictors of the variable of interest and sample inclusion are unknown. Where they are known, data might not 401 402 be available at the required scale (i.e. their distribution in the population is not known). To illustrate 403 this point, consider the hoverfly Criorhina asilica, whose larvae require decaying timber from 404 particular tree species (Stubbs & Falk, 2002). Without data on the locations of those decaying trees, it 405 would likely be impossible to adjust for what is presumably a major determinant of its distribution. 406 For taxa whose habitat requirements are well understood and reflected in available data (e.g. birds), selecting auxiliary variables should be simpler. Nevertheless, in practice, the analyst does not know 407 408 the truth, so there will always be some guesswork (if this were not the case, statistical modelling 409 would not be required). Transparency regarding availability and choice of auxiliary variables should be an important component of reporting for all biodiversity monitoring. 410

- 411 Whilst we are confident that the appropriateness of the auxiliary variables was the limiting factor in
- 412 our example, it is possible that improvements to the estimators themselves could have improved
- 413 matters. Potential improvements to MRP are most obvious. For example, interactions between the
- 414 auxiliary variables could be included in the multilevel model (Ghitza & Gelman, 2013), and multiple
- 415 time-periods could be modelled at once (Gelman et al., 2018). The question is whether fine-tuning
- 416 models, which might make them more expensive to run (including interactions in MRP certainly
- 417 does), is worth marginal gains in accuracy. As Mercer et al., (2018), writing in the context of
- 418 adjusting survey samples, put it, "[t]he right variables make a big difference for accuracy. Complex
- 419 statistical methods, not so much."
- 420 Some have questioned whether it is worth weighting nonprobability samples at all. In opinion polling,
- for example, there are many examples where weighting or other adjustments did little or nothing to
 improve the accuracy of inference from nonprobability samples, or even made matters worse (Bailey,
- 423 2023). In terms of the accuracy of the sample-based estimates, our results suggest that the situation in
 424 biodiversity monitoring is similar. Importantly, however, we have also showed that most adjustment
- 425 methods do what they are supposed to: they turn an unrepresentative sample into a representative one,
- 426 albeit strictly with respect to the chosen auxiliaries. First principles dictate that, if the auxiliaries are
- 427 appropriate, this would translate into a more representative sample in terms of the variable of interest
- 428 and improve the accuracy of inference. We see taxon experts as having a crucial role in identifying
- 429 appropriate auxiliaries (e.g. Boyd, Harvey, et al., 2023; Smart et al., 2019).
- It is worth commenting on how we measured the accuracy of the estimated trends. We compared the magnitudes of the estimated and true trends and assessed whether the estimates' confidence/credible intervals covered the true value. Others defined accuracy as the power to "detect" a trend, whereby a method is considered successful if it gets the sign of the trend correct and its uncertainty interval does not span zero (e.g. Valdez et al., 2023). In this power setting, four of the estimators that we considered were able to detect the true trend, including the difference between the naive sample means.
- 436 We prefer to use the magnitude of the trend as a measure of accuracy for biodiversity monitoring,
- 437 because many applications in this area are descriptive-inferential, not decision-theoretic (Greenland,
- 438 2022; Hurlbert et al., 2019; Oliver L. Pescott et al., 2019). That is to say, the final objective of
- 439 exercises in biodiversity trend estimation is frequently a descriptive indicator, not a binary
- 440 accept/reject conclusion of change or no change (e.g. Dennis et al., 2019; Powney et al., 2019). The
- 441 link between Neyman-Pearsonian power and such exercises is often unclear (Amrhein et al., 2019):

- they are essentially descriptive exercises and as such should be evaluated in terms of the closeness of
- the sample-based estimate to the truth, not merely in terms of rejecting (typically unrealistic) null
- 444 hypotheses. The ability to report and consider uncertainty in the trend estimation is essential in
- 445 making judgements about the risk of bias in biodiversity data (Boyd et al., 2022).
- Also worth remembering is that we have only applied the adjustments to one species and using a
 relatively "good" dataset. It is plausible that the adjustments would improve estimates from a smaller
- 448 or less representative dataset to a greater extent. They will certainly work better for species whose
- 449 auxiliary variables are easier to identify and reflected in available data.
- 450 Repeating our analysis with other taxa and datasets would provide a better understanding of in what
- 451 circumstances we can expect adjustments to perform well. The difficulty will be finding species
- 452 whose true occupancy (or other variable of interest) is known. One option is to use simulations, but it
- is extremely important that they are not designed in such a way that the auxiliary variables explain
- sample inclusion and the variable of interest completely. In this case, the methods will all work very
- 455 well, but that is not a true reflection of reality.
- 456 Our concluding message is that statistical adjustments might improve descriptive statistical inference
- in ecology, but only when combined with expert knowledge and appropriate data. Where there is
- doubt about the suitability of available auxiliary variables, a safer strategy is to assess the risk of bias
- 459 qualitatively (Boyd et al., 2022; Meineke & Daru, 2021). If there is deemed to be a risk, it should be
- reflected in the way that findings are reported (Boyd, Powney, et al., 2023; O L Pescott et al., 2022).
 This might include using more conservative language and acknowledging that traditional uncertainty
- 462 intervals are not guaranteed (or even likely) to cover the truth (X.-L. Meng, 2022).

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