Adaptive sampling for ecological monitoring using biased data: A stratum-based approach

3 Abstract

Indicators of biodiversity change across large extents of geographic, temporal and taxonomic space are frequent products of various types of ecological monitoring and other data collection efforts. Unfortunately, many such indicators are based on data that are highly unlikely to be representative of the intended statistical populations. Where there is full control over sampling processes, individual spatial units within a geographical population have known inclusion probabilities, but these are unknown in the absence of any statistical design. This could be due to the voluntary nature of surveys and/or because of dataset aggregation. In these cases some degree of sampling bias is inevitable and, depending on error tolerance relative to some real-world goal, we may need to ameliorate it. One option is poststratification to adjust for uneven surveying of strata assumed to be important for unbiased estimation. We propose that a similar strategy can be used for the prioritisation of future data collection: that is, an adaptive sampling process focused on increasing representativeness defined in terms of inclusion probabilities. This is easily achieved by monitoring the proportional allocation of sampled units in strata relative to that expected under simple random sampling. The allocation of new units is thus that which reduces the departure from randomness (or, equivalently, that equalising unit inclusion probabilities), allowing an estimator to approach that level of error expected under random sampling. We describe the theory supporting this, and demonstrate its application using sample locations from the UK National Plant Monitoring Scheme, a citizen science monitoring programme with uneven uptake, and data on the true distribution of the plant Calluna vulgaris. This in silico example demonstrates how the successful application of the method depends on the extent to which proposed strata capture correlations between inclusion probabilities and the response of interest.

 $_{\rm 4}$ $\it Keywords:$ survey error, survey quality, poststratification, weighting, response

⁵ propensity, R-indicators, time-trends

6 Introduction

Ecologists are increasingly concerned with monitoring biodiversity change at
a variety of spatial scales. Whilst this has long been an active area of research
within conservation and related fields (e.g. Spellerberg [57]), in recent years

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its importance has increased, with numerous species' time trends and associ-10 ated multi-species indicators now based on a wide variety of data types [e.g. 11 40, 26, 14]. One consequence of this trend has been the increasing focus on the 12 use of datasets for monitoring that lack any explicit survey design relative to the 13 scientific question of interest. That is, the data used to estimate species' abun-14 dances or occupancies are frequently not a probability sample of the statistical 15 target population. Unfortunately, inference using such nonprobability samples is 16 considerably more difficult than has often been recognised in ecology [10]. The 17 absence of sampling design typically means that model-based adjustments must 18 be made to approach the answer that would have been obtained had sampling 19 actually been probabilistic, and such adjustments can rarely, if ever, be shown 20 to be absolutely reliable [33, 11, 65, 16, 1]. As a result, efforts to characterise 21 biodiversity change from nonprobability samples have often received criticism 22 for not being representative of their inferential target populations (e.g. Gonzalez 23 et al. [20]), leading to a number of high-profile disagreements in the literature 24 [10].25

The technical elements of sampling design underlying these issues have been 26 well-known in the statistical subdiscipline of survey sampling for decades [30, 2. 27 62, 33], yet many of these insights are frequently overlooked or misunderstood by 28 ecologists (although by no means all, e.g. see many chapters within ref. [19]). One 29 stumbling block may be the numerous definitions and types of "bias" available 30 in the literature [19, 43, 49]; the lack of any well-known (to ecologists) unified 31 mathematical definition of sampling bias may also have hindered communication 32 and progress. 33

Within survey sampling focused on descriptive inference (i.e. characterising 34 some directly measurable property of a population from a sample; [24]), statistical 35 error has long been known to be driven in large part by correlations between 36 the probability that any unit is in the sample π , the inclusion probability, 37 and the property of interest y [e.g. 21, 4]. Note that in survey sampling π is 38 also sometimes designated as the "response propensity", because there the key 39 challenge is unknown probabilistic variation in subject responses to designed 40 surveys, rather than the absence of design itself [30]. In ecology, this has also 41 sometimes been discussed under the heading of preferential sampling [e.g. 1]. 42 although that label tends to imply a positive association, whereas the issue 43 applies to correlations of either sign. Probability sampling ensures that this 44 correlation is zero in expectation (i.e. across repeated, normally imaginary, 45 realisations of the sampling mechanism; [33]). A conceptual complication here is 46 that finite probability samples also have non-zero correlations between sample 47 inclusion and the response variable, and that there is variation in the survey 48 sampling literature relative to whether people refer to realised error in a sample 49 as bias (when it may actually be a combination of sampling variance and a 50 biased sampling mechanism), or whether the term sampling bias is reserved for 51 situations where it is known (or strongly expected due to a lack of design) that 52 $E[\rho(\pi, y)] \neq 0$; that is, that the sampling mechanism that produced the data 53 had variable sampling unit inclusion probabilities, which, by definition, were not 54 designed and so cannot be directly accounted for when estimating parameters 55

⁵⁶ like means from the data. This means that the expected value $(E[\cdot])$ of the ⁵⁷ correlation (ρ) between the sample inclusion probabilities π_i and the values of ⁵⁸ the response variable y_i is guaranteed to be non-zero, something that is only ⁵⁹ assured by probability sampling [33].

Regardless of these terminological issues, Meng [33] demonstrated how a 60 standard formula for statistical error $(\overline{y}_n - \overline{y}_N)$, the difference between the mean 61 of the response variable in the sample and that of the variable in the full pop-62 ulation) can be re-written as the product of three terms. One characterising 63 the aforementioned correlation $\rho(\pi, y)$, given the name "data quality" by Meng, 64 and two others representing the population fraction sampled ("data quantity") 65 and the amount of variation in the response variable in the population ("prob-66 lem difficulty"). (Note, however, that Meng approaches the correlation $\rho(\pi, y)$ 67 from a finite population viewpoint, replacing the latent sampling unit inclusion 68 probabilities π_i with the realised, binary sample inclusion indicators R_i .) The 69 implications of this algebraic identity have been hailed in some areas as a "new 70 paradigm" [3], and in our opinion the formula clarifies many issues that have 71 previously sometimes only been intuitively understood in ecology [11, 7, 10]. 72

The adjustment of nonprobability samples for approaching unbiased inference 73 is one area that has been clarified by Meng's approach: in a subsequent paper, 74 Meng [34] demonstrated how all such techniques (inverse probability weighting 75 and poststratification, imputation or superpopulation modelling, and doubly-76 robust approaches) can be viewed as ways to minimise the correlation $\rho(\pi, y)$. 77 This insight allows us to understand the assumptions of our methods, and 78 therefore to justify our approaches and assess their limitations more clearly [8]. 79 Here we apply these insights to the use of stratification in ecology, particularly 80 its *post hoc* use to adjust unrepresentative sampling, demonstrating its use as an 81 intelligent driver of adaptive sampling for many situations involving data that 82 are biased for the estimation of some "estimand" (i.e. the real-world quantity of 83 interest [32]). 84

A priori stratification is often used in survey design to achieve one or more of 85 the following: good representation of a population relative to target variables of 86 interest; to guarantee certain sample sizes within strata (which may be of intrinsic 87 interest); for the convenience of survey administration, potentially including cost 88 reduction via regional administration; and to increase the statistical efficiency 89 of estimators [30, 62]. For the last point, error can be reduced by randomly 90 sampling within strata of homogeneous units, i.e. those where subpopulation 91 means and variances are expected to be similar [30]. 92

Post hoc stratification, or, as it is more commonly known, "poststratification", can also be used to achieve this latter goal. That is, it can be used to increase the precision of estimators under known sampling schemes [56]. However, it can also be used as a way to remove potential biases arising from the use of nonprobability samples. In this sense it is part of the family of reweighting techniques intended to adjust a sample to better represent some population of interest [56, 65, 11].

The poststratification estimator \overline{y}_{ps} [4], or "basic poststratification identity"

¹⁰¹ [18], used to achieve this can be defined as:

$$\overline{y}_{ps} = \frac{1}{N} \sum_{h=1}^{H} N_h \overline{y}_h \tag{1}$$

where N is the population size (here the total number of spatial units), H is 102 the full set of strata into which the population is divided, N_h is the overall size 103 of stratum h, and \overline{y}_h is the mean within stratum h. The implication of (1) is 104 that within-stratum means substitute for individual unit values, and it is these 105 that are averaged across the entire population once relative stratum sizes in the 106 population have been accounted for (see [11] for a worked ecological example). 107 This formulation implies that all i units within a given poststratum receive the 108 same weight [4, 65], equal to 109

$$w_{i(h)} = \frac{N_h/N}{n_h/n} \tag{2}$$

where n is the total sample size, and n_h is the size of the sample within stratum h. Equation (2) can be understood as upweighting units that are under-represented in the sample relative to the population and *vice versa*. These weights imply an individual unit inclusion probability of $\pi_{i(h)} = n_h/N_h$. And so it can be shown that

$$\bar{y}_{ps} = \bar{y}_{ipw} = \frac{1}{N} \sum_{h=1}^{H} \sum_{i \in n_h} \frac{y_{i(h)}}{\pi_{i(h)}}$$
(3)

[65]. Thus poststratification is a special case of inverse probability weighting 115 (a.k.a. quasirandomization or propensity score weighting) where $\pi_{i(h)}$ is assumed 116 to be constant within strata but to (potentially) vary between strata [65]. In the 117 situation where a set of randomly sampled population units are surveyed with 118 full response (i.e. no "loss" of design-based survey units), then this estimator, 119 whether construed as \overline{y}_{ps} or the inverse probability weighted estimator \overline{y}_{ipw} , 120 is unbiased in expectation [56, 4]. However, as noted above, it is well known 121 that in actual samples error will tend to increase as a function of the correlation 122 between between inclusion probabilities π and the outcome variable y [21, 4]. 123

In the case of uncontrolled (i.e. nonprobability) samples, whether based on a 124 single survey such as a designed citizen science scheme with some nonresponse, 125 or an aggregated sample such as one might retrieve from the Global Biodiversity 126 Information Facility (GBIF) or other meta-database, the lack of statistical design 127 control essentially guarantees that this correlation will be appreciably different 128 from zero [10]. This will not merely be the bad luck of an unrepresentative 129 random sample, but the expectation of a biased sampling mechanism; that is, 130 $E[\rho(\pi, y)] \neq 0$. Here, increases in sample size will not help; in fact, they have 131 been shown to make things worse in realistic scenarios, i.e. when $n \ll N$ and 132 the standard deviation of y, σ_y , does not equal zero, as will generally be the 133 case for most environmental monitoring at small scales [33, 11, 3]. 134

With regards to poststratification, two situations will reduce this undesirable correlation [4]. These rely on the fact that if either of a pair of variables is fixed then they cannot be correlated. These are:

- i. The response of interest y_i is invariable within poststrata (i.e. $\sigma_{y(h)} = 0 \quad \forall h$).
 - ii. The inclusion probabilities π_i are invariable within poststrata (i.e. $\pi_{i(h)} = \pi_i + i \in h$), achieved by simple random sampling (SPS) within strate
 - $\pi_h \quad \forall i \in h$, achieved by simple random sampling (SRS) within strata.

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In the first of these situations, the poststratification estimator (1) will be 142 more efficient (lower variance) than the arithmetic mean, and will reduce error 143 wherever a random sampling design has yielded an unbalanced sample by chance 144 [25]. In the second of these situations, the poststratification estimator reduces 145 the bias, but not the variance [28, 27]. This is linked to the assertion of Gelman 146 and Carlin [18] that poststratification is most important when correcting for 147 differential nonresponse *between* poststrata. Assuming that inclusion probabilities 148 are uniform within poststrata, but correlated with y within the overall population, 149 then adjusting for poststratum membership renders $\rho(\pi, y)$ equal to zero [65, 34]: 150 that is, π and y are independent conditional on some X, where here X is the 151 vector of unit poststratum memberships [56]. 152

Whilst poststratification and its variants [e.g. see 17] can be useful tools for 153 adjusting existing samples [11], where monitoring is ongoing and survey organisers 154 have some power to alter data collection, combining adaptive sampling with 155 poststratification may be a more efficient way to reduce error compared to 156 relying on poststratification of unrepresentative samples alone [54, 52]. Larger 157 samples may be also desired for other reasons irrespective of the potential 158 for using the poststratification estimator on a sample in hand (increases in 159 power for example). The situations in which poststratification is likely to assist 160 the sampler given above suggest a simple approach to adaptive sampling for 161 researchers seeking to characterise a population parameter such as a mean. As 162 noted above, such descriptive targets are increasingly important for ecological 163 monitoring and conservation, especially where nonprobability samples are used 164 [10]. Straightforward approaches to adaptive sampling, with few assumptions, 165 are therefore likely to be of wide utility [22]. 166

Here we propose an approach to the problem based on assessments of post-167 stratum sampling coverage. We show how this can be implemented easily with 168 standard binomial formulae within an adaptive framework using data collected 169 between 2015–2023 for the UK National Plant Monitoring Scheme, a designed 170 citizen science programme with uneven site uptake [45]. Our approach has a 171 direct link to the literature on the monitoring of survey quality via assessments of 172 potential nonresponse bias [63, 38], and we use one such indicator (the R-indicator 173 of Schouten, Shlomo and colleagues [50]) of variation in response propensities (or, 174 as we have styled them here, inclusion probabilities) across strata to explore the 175 potential improvements in survey representativeness (a measure of survey quality 176 [51]) achievable using our approach. Finally, we investigate the performance 177 of the approach through simulation and when confronted with a real dataset. 178 Specifically, we examine how well stratum-based adaptive sampling performs 179 in estimating the true 1 km^2 occupancy of the subshrub Calluna vulgaris (L.) 180 Hull in Great Britain. We use both simulated locations and actual sampled sites 181 from the NPMS to explore the potential strengths and weaknesses of the method 182

¹⁸³ relative to its key assumptions.

184 Methods

¹⁸⁵ A stratum-based adaptive survey strategy

The approach proceeds as follows: for the population of interest (e.g. some 186 geographic area over which the mean of some attribute of a population of 187 units is desired), select a set of strata H considered to have some differential 188 relationship with sample inclusion and/or the response variable(s) of interest. 189 Each stratum need not be a single spatially contiguous unit, but each population 190 unit should be assignable to a single stratum (geographical units may often 191 require assigning to the stratum with the largest overlapping area). Many such 192 strata will likely already exist, although the approach is not limited to existing 193 strata, as any set of geographically indexed variables could be discretised and 194 crossed to create strata [e.g. see 11]. For example, in the UK "land classes" 195 have previously been erected based on covariation in numerous geographical 196 and environmental variables [12] and then amalgamated into broader zones [61]; 197 for Europe, biogeographic zones based on patterns of terrestrial and marine 198 biodiversity exist [15]. Note that the strata do not have to be absolutely believed 199 to have an invariable one-to-one relationship between stratum unit membership 200 and inclusion probability, only that there is some nontrivial relationship, such 201 that adjusting for its contribution to the correlation $\rho(\pi, y)$ will be better than 202 assuming that the sample is equivalent to one selected at random [34]. 203

For the existing sample for which future adaptive selections are required, 204 compare the current distribution of units across strata to that expected for the 205 same sample size under simple random sampling; this is known as proportional 206 allocation in the survey sampling literature [62]. That is, a given set of strata 207 H partitioning N will be sampled in proportion to n/N, such that, for stratum 208 $h, n_h = (n/N) \cdot N_h$; if achieved, all response propensities would be equal, both 209 within and between strata. The stratum for which the next unit should be 210 collected will then be the one with the current largest negative departure from 211 212 random expectation, quantified using z-statistics.

213 Monitoring representativeness

The link between inclusion probabilities and indicators of representativeness noted above was formalised by Schouten and colleagues [51]. They provide the following operational definition of "representative" in the survey sampling context:

$$\bar{\pi}_h = \frac{1}{N_h} \sum_{i=1}^{N_h} \pi_{i(h)} = \pi \quad \forall h.$$
(4)

Equation (4) is a weaker version of statement (ii) given in the Introduction, as it does not state that all unit inclusion probabilities within a stratum are identical, only that the means across strata are equal. Based on this, the Schouten *et al.* R-indicator is $R(\pi) = 1 - 2s_{\pi_h}$, where s_{π_h} is the weighted standard deviation of the mean inclusion probabilities across strata [51]. $R(\pi) = 1$ denotes maximum representativeness when the variance in inclusion probabilities across strata is zero.

225 Adaptive sampling algorithm

This proceeds as follows (also see the R code in Supplementary Material 1): **Step 1**: Assign all population units N_i to a unique corresponding stratum h_i .

Step 2: Calculate each stratum's current z-statistic, z_h , by comparing the current empirical count $(\bar{x}_h = N_h \cdot (n_h/N_h) = n_h$, the current sample size) and binomial count standard deviation $(s_h = \sqrt{N_h \cdot n_h/N_h \cdot (1 - n_h/N_h)})$ to the expected count $(\hat{\mu}_h)$ based on proportional allocation (i.e. $n/N \cdot N_h$). Then, $z_h = (\bar{x}_h - \hat{\mu}_h)/s_h$, the difference between the empirical and expected counts in standard deviation units.

Step 3: Across the H strata, select that h with the smallest z_h as the stratum most in need of additional sampling to reach the simple random sample benchmark. Call this the focal stratum h_f .

Step 4: Given the addition of a new site to stratum h_f , calculate the new values of \overline{x}_h and s_h directly from the standard binomial formulae. The new target stratum site count expected under simple random sampling is also updated as $\hat{\mu} = (n+a)/N \cdot N_h$. In the following examples a = 1, but it could be any positive integer as there is no requirement to evaluate the switch after the addition of every single new sampling unit.

Step 5: After updating the current focal stratum h_f with the newly added site(s), recalculate the z-statistics for all strata, including h_f . Compare the updated $z_{h(f)}$ with the minimum z_h across all strata. If $z_{h(f)}$ is no longer the smallest, switch the focus to the stratum with the new smallest $z_{h(f)}$ denoted h_{f^*} . Begin sampling h_{f^*} if required, otherwise continue with h_f .

Step 6: Repeat Steps 2 to 5 K times until the desired new sample size allowed by current resourcing, n + aK, is reached, or until all strata are at their expected simple random sampling counts $(n + aK)/N \cdot N_h$.

We can monitor the progress of this algorithm by following the empirical stratum sampling proportions (n_h/N_h) , and by calculating the corresponding R-indicator at each step.

²⁵⁵ Investigating performance

256 Stratum sampled proportions and the *R*-indicator

The UK National Plant Monitoring Scheme (NPMS) asks volunteers to record 257 plant abundances in small plots located in particular habitats [64]. Plots are 258 located within 1 km² squares (hereafter "sites") of the relevant country grid (the 259 scheme currently covers Great Britain, Northern Ireland, the Isle of Man and the 260 Channel Islands). The available sites within the scheme (see https://www.npms. 261 org.uk/square-near-me-public) are originally a weighted-random selection, 262 stratified by 100×100 km cells of the larger relevant grid; see [45] for more 263 detail. Due to variable population density and other factors across the region, 264

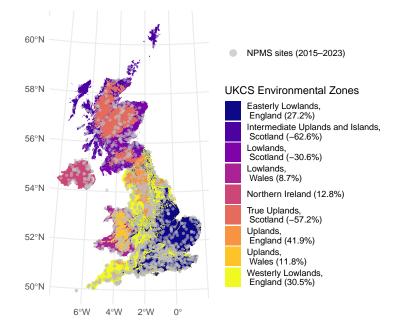


Figure 1: UK Countyside Survey (UKCS) Environmental Zones plus Northern Ireland. The numbers following the UKCS zone names give the difference between the empirical National Plant Monitoring Scheme (NPMS) square count and that expected under simple random sampling (SRS), expressed as a percentage difference (+/-) relative to the expected count. Percentages closer to zero therefore approach SRS counts. Grey circles are surveyed NPMS sites, 2015–2023.

uptake of these sites is uneven, and some areas have far fewer survey returns 265 than others [45]. A primary aim of the NPMS is the production of nationally 266 representative indicators of habitat quality [41], and so, ideally, coverage of the 267 area would be relatively even. We know that inclusion probability (i.e. site 268 uptake) is related to such factors as human population density and correlated 269 environmental variables such as altitude and land cover type, and that these 270 variables are also correlated with the local abundances and occupancies of plant 271 indicator species and their habitats [45]. North-west to south-east gradients of 272 all these variables are well-known for Britain and Ireland [48, 58, 44, 23, 47]. We 273 therefore assume that representation of broad environmental strata, in tandem 274 with poststratification of results, is likely to be a positive step towards reducing 275 potential bias in monitoring scheme outputs. One widely-used set of strata 276 for Great Britain is the UK Countryside Survey (UKCS) Environmental Zones 277 [61], based on a larger set of "land classes" created originally for the *a priori* 278 stratification of national ecological and biogeographical surveys [12]. To these 279 we add Northern Ireland as an additional stratum to better cover our area (Fig. 280 1). Surveyed NPMS sites [39] are overlaid on these zones in Figure 1 to show 281 their current overall (2015–2023) coverage. 282

283 Reducing bias in a response variable of interest

Investigating the likely benefits of our strategy for a response variable of 284 interest, such as a species' occupancy or average abundance, is more challeng-285 ing, as it requires access to a species' true underlying state to evaluate (or a 286 good estimate of this via a probability-based survey). Whilst pure simulation 287 approaches could be used, we consider that these would be less illuminating than 288 investigations more closely aligned to real-world datasets, because the theoretical 289 principles underlying the approach are already well characterised. We use an 290 approximation of the true 1 km^2 distribution (for 2000–2019) of the heathland 291 subshrub Calluna vulgaris (L.) Hull ("Heather"), originally created for Boyd 292 et al. [11]. This "true" distribution is based on the 2018 UKCEH Land Cover 293 Map [37] (where "Heather" and "Heather grassland" are land covers derived from 294 satellite images and other information) and occurrence data from the distribution 295 mapping project *Plant Atlas 2020* [58]. See [11] for more information on the 296 construction of the *Calluna* map. 297

Adaptive sampling based on simulated locations. First, we demonstrate the 298 performance of the method when the key assumption regarding random sampling 299 within strata is met. Here we only use empirical data from the NPMS [39] 300 dataset to initialise stratum sample sizes for the adaptive algorithm. (Specifically 301 we use data from 2019 for these investigations.) The initial samples themselves 302 are new random selections within strata; the adaptive addition of sites uses 303 our suggested algorithm. We refer to this approach as "Stratum SRS [Simple 304 Random Sampling] + adaptive". The iterative estimates of the mean occupancy 305 of Calluna for this scenario use the poststratification estimator from the R306 package "survey" [31]. 307

Adaptive sampling based on empirical locations. Second, we investigate the 308 performance of the method using the actual sampled sites from 2019 in the 309 NPMS [39] dataset. This approach provides insight into how the method might 310 perform when the key assumption of random sampling within strata is unlikely to 311 be fully met. We refer to this approach as "NPMS + adaptive". Again, iterative 312 estimates of *Calluna* occupancy use the poststratification estimator from the 313 R "survey" package [31]. We also include a scenario where our proposed strata 314 are ignored, and new sites added to the existing NPMS 2019 sample are chosen 315 randomly from the total site population of Great Britain. We call this approach 316 "NPMS + SRS". Calluna occupancy estimates from this procedure are the simple 317 mean rather than the poststratified mean. For all three scenarios new sites added 318 to the sample are labelled as unavailable for future iterations of the algorithm. 319

320 **Results**

Table 1 gives the current distribution of NPMS 1 km² sites by UKCS Environmental Zone stratum. These are given in order of their discrepancy from proportional allocation (i.e. simple random sampling) of the 2015–2023 sample of 1,204 sites that could be assigned to strata, from under- to over-sampled [39].

Table 1: The current distribution of NPMS sites by UKCS Environmental Zone strata, ordered from under- to over-sampled relative to simple random sampling (SRS). Exp. count is the expected number of squares under SRS. Pct sampled is the current percentage of the stratum area sampled; Count discrepancy is the difference between the actual square count and the expected count expressed as a percentage difference (+/-) relative to the expected count.

Stratum no.	Stratum	No. sites	Exp. count	$\begin{array}{c} \text{Stratum} \\ \text{area} \\ (\text{km}^2) \end{array}$	Pct sampled (%)	Coun discrep ancy (% o expected)
5	Intermediate Uplands and Islands, Scotland	53	142.2	29866	0.18	-62.7
6	True Uplands, Scotland	65	152.5	32034	0.20	-57.4
4	Lowlands, Scotland	76	109.9	23084	0.33	-30.
7	Northern Ireland	73	67.4	14156	0.52	8.
8	Lowlands, Wales	60	53.8	11309	0.53	11.
9	Uplands, Wales	55	48.9	10272	0.54	12.
1	Easterly Lowlands, England	395	311.6	65441	0.60	26.3
2	Westerly Lowlands, England	321	246.7	51815	0.62	30.
3	Uplands, England	106	74.9	15739	0.67	41.

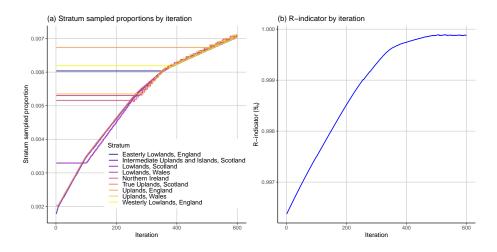


Figure 2: Evolution of UKCS Environmental Zone stratum mean sampled proportions and their R-indicator by iteration.

325 Figure 2 demonstrates the progress of the stratum-based adaptive sampling algorithm in terms of stratum sampled proportions and R-indicator. The example 326 here uses 600 iterations (i.e. the final target sample size was n+600 = 1804). This 327 amount of adaptive sampling may be unrealistic in most real world situations 328 where there is existing nonresponse, but we use this number to demonstrate 329 the point at which all strata become proportionally allocated, and to show the 330 evolution of the R-indicator towards its maximum possible value of 1 (Fig. 2). 331 As per Table 1, Figure 2a shows how, initially, only the Intermediate Uplands 332 and Islands and True Uplands of Scotland are underallocated. These have the 333 lowest stratum proportions sampled initially: up to around the 100th iteration it 334 is only these sites that are being selected for new sampling locations. The other 335 strata "flatline" up to this point, indicating that they are over-sampled relative 336 to the number of samples they would expect if the total sample had actually 337 been proportionally allocated. The most over-sampled stratum is the Uplands 338 of England, as this does not see its sample size increased until around the 500th 339 iteration. This is also the point at which the R-indicator (Fig. 2b) approaches 340 its maximum value of 1 and itself flatlines; this indicates that all strata are now 341 being sampled relative to the proportions expected under proportional allocation. 342 Table 2 gives abridged output of the adaptive sampling algorithm underlying 343

Figure 2. The top of the table shows how, initially, stratum number 5, the "Intermediate Uplands and Islands" zone of Scotland is targeted in isolation (as expected from its position at the top of Table 1). The bottom of Table 2 shows how, once all strata are undersampled relative to the addition of new sites, the target stratum switches with every iteration of the algorithm. The total population size of UK 1 km² sites assigned to UKCS Environmental Zone strata is 257,502; 1804/257502 = 0.0070, hence the stratum sampled proportions

Iteration	Stratum no.	z-value	Mean prop.	Site count	$^{\mathrm{SD}}$
1	5	-1.2e+01	1.8e-03	54	7.3
2	5	-1.2e+01	1.8e-03	55	7.4
3	5	-1.2e+01	1.8e-03	56	7.5
4	5	-1.2e+01	1.9e-03	57	7.5
5	5	-1.1e+01	1.9e-03	58	7.6
6	5	-1.1e+01	1.9e-03	59	7.7
595	3	1.1e-01	7.1e-03	111	10.5
596	1	1.0e-01	7.0e-03	460	21.4
597	5	9.9e-02	7.0e-03	214	14.6
598	4	9.1e-02	7.0e-03	164	12.8
599	2	8.7e-02	7.0e-03	368	19.1
600	7	8.5e-02	7.1e-03	102	10.1

Table 2: Abridged adaptive sampling output for the first and last six added sites across 600 iterations. Stratum no. = stratum number of focal stratum (see Table 1 for stratum name); Mean prop. = sampled proportion for target stratum; SD = binomial st. dev. for site count within stratum.

achieved for the final six iterations at the bottom of Table 2 ("Mean prop." column).

Figure 3 shows the results of applying our algorithm to the case of estimating 353 our "true" 1 km² occupancy of *Calluna vulgaris* (0.27). The unadjusted sample 354 mean occupancy of the existing 2019 NPMS data for *Calluna* is 0.33. Taken 355 together, the four elements of Figure 3 reveal both the potential strengths and 356 weaknesses of the proposed method in improving on the unadjusted sample 357 mean through the adaptive sampling algorithm. Figure 3a demonstrates how 358 three different data/model scenarios can lead to better estimates of the true 359 mean with increasing sample size. Given that both simple random sampling and 360 stratified random sampling are standard methods in survey sampling, this is not 361 surprising; it is the differences between the strategies investigated that provide 362 useful insights into the likely performance of our approach when applied to 363 real-world datasets. Figure 3a also shows that the initial poststratified estimate 364 (iteration 1) of Calluna occupancy using the 2019 NPMS locations ("NPMS + 365 adaptive"; see also Table 3) leads to the most biased estimate. In addition, the 366 "NPMS + adaptive" estimates are worse than those estimated using the sample 367 mean with new sites added through simple random sampling ("NPMS + SRS"). 368 However, the "NPMS + adaptive" poststratified estimates approach the true 369 value more quickly than "NPMS + SRS", presumably due to the important 370 variation in *Calluna* occupancy across the strata used (Fig. 3d). 371

The third scenario, "Stratum SRS + adaptive", indicates the reason for the initially poor poststratified estimates under "NPMS + adaptive": the 2019 NPMS locations are biased towards the presence of *C. vulgaris* within all strata. Evidence for this can be seen within Figure 3c; for example, the estimated occupancy within the Uplands of England is very strongly overestimated before it is incorporated into the adaptive sampling algorithm. Other strata show

Iteration	Mean	SE	Method	Estimator
1	0.33	0.024	NPMS + SRS	Unadjusted
600	0.28	0.014	NPMS + SRS	Unadjusted
1	0.41	0.021	NPMS + adaptive	Poststratified
600	0.31	0.012	NPMS + adaptive	Poststratified
1	0.25	0.021	Stratum SRS $+$ adaptive	Poststratified
600	0.27	0.011	Stratum SRS $+$ adaptive	Poststratified

Table 3: Initial and final mean occupancies (with standard errors) of *Calluna vulgaris* for different adaptive sampling methods and starting data.

weaker patterns, but the pattern of initial overestimation is clear (Fig. 3d 378 provides the "true" values for comparison). This means that some stratum 379 occupancy estimates require the addition of many new sampling locations before 380 their estimates increase in accuracy: before this point the poststratification 381 estimator simply weights the biased stratum estimates according to their areas, 382 resulting in important residual bias in the overall estimate. The "Stratum 383 SRS + adaptive" scenario shows that rejecting the existing locations within 384 the 2019 NPMS dataset and selecting new random sets of sites within strata 385 results in more accurate poststratified estimates that rapidly improve (Fig. 3a, 386 "Stratum SRS + adaptive"). This highlights that if the assumptions of the 387 poststratification model are approximately correct (i.e. sampling is random 388 conditional on the strata), then our approach can perform well: the estimates 389 also show slightly decreased standard errors over the iterative series relative 390 to the simple random sampling site-addition approach (Table 3). Finally, the 391 R-indicators shown in Figure 3c demonstrate how these metrics are only as 392 useful as the accuracy of the underlying assumptions [53]: the R-indicator for the 393 "NPMS + adaptive" scenario shows the expected pattern of decreasing variation 394 in the mean sample inclusion probability across strata (note that "Stratum SRS 395 + adaptive" is not shown as it is identical to "NPMS + adaptive"), whereas the 396 simple random sampling additions to the original NPMS sample do not aim to 397 harmonise stratum sampling proportions on this basis. 398

399 Discussion

Nonprobability samples of different types are now routinely used within 400 ecology and conservation for various monitoring aims, often with minimal critical 401 assessment [8, 10]. Not infrequently such projects relate to the desire to produce 402 large-scale indicators of biodiversity change, with representativeness of large 403 geographical areas implied as a consequence. Whilst estimates based on such 404 data can potentially be partially adjusted for sampling bias using a family of 405 reweighting techniques including poststratification [11, 34], targeting new effort 406 in order to reduce such biases is likely to be a useful complementary strategy 407 [52, 54]. We suggest that the use of strata, hypothesized to capture important 408 relationships between inclusion probabilities and the response variable(s) of 409

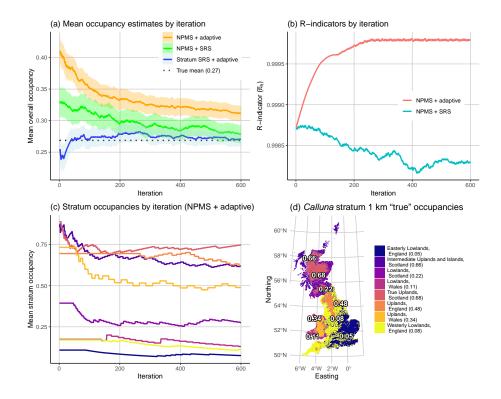


Figure 3: Adaptive sampling of *Calluna vulgaris* occupancy within the National Plant Monitoring Scheme, 2019. (a) Overall Great Britain occupancy estimates for different adaptive sampling scenarios, with binomial proportion standard error ribbons, compared to the true mean (0.27). The unadjusted sample mean of the initial 2019 NPMS data is 0.33; (b) Rindicators for stratum unit inclusion probabilities, NPMS + adaptive and + SRS scenarios; (c) Stratum occupancies for the NPMS + adaptive method by iteration, colour-coding follows (d); (d) Estimated "true" mean occupancies of *Calluna* by UKCS Environmental Zone stratum (these are displayed at, or near, stratum centroids on the map).

interest, is a useful and simple theoretical starting point for adaptive sampling
for projects with descriptive goals (i.e. where the aim is to estimate some directly
measurable property of a population from a sample; [24]).

If the strata are well-chosen relative to their potential to reduce correlations 413 representing sampling bias, our adaptive approach aimed at a random sample 414 stratified using proportional allocation can improve matters. An example would 415 be where a common plant has near 100% occupancy at some broad scale (e.g. a 416 10 x 10 km grid), but its average local cover (e.g. at the square-metre scale) 417 varies with an environmental gradient. If sampling co-varies along the same 418 gradient (e.g. due to population density, as in the UK National Plant Monitoring 419 Scheme: [45]) then estimates of average abundance are likely to exhibit important 420 bias. However, if some set of strata partition the environment into areas where 421 sampling is close to random with respect to regional variation in the species? 422 abundance, then this bias will be significantly reduced: the national correlation 423 is removed by estimating means within smaller areas and then combining these 424 in relation to their expected national proportions to better represent the total 425 population [11]. Whilst it is true that in such a case the poststratification 426 estimator will theoretically reduce bias anyway [4, 18, 13, 53], the combination 427 of adaptive sampling and reweighting has been shown to be superior to relying 428 on reweighting alone, both in theory and in empirical investigations in the survey 429 sampling literature [52, 53]. Adding new sites to the sample in this way can 430 reduce variance, as well as keeping bias low [66]. Regardless of this, monitoring 431 programs will often have a focus on increasing uptake for other reasons (e.g. 432 engagement, increasing power; [22]), and so targeted approaches to selecting 433 new sites are likely to be required irrespective of existing analytical options for 434 potential bias reduction of the sample in hand [11]. In theory, such approaches 435 could also be applied to sampling in other dimensions, e.g. to prioritise the 436 digitisation of literature or museum records to improve spatial and/or temporal 437 representativeness in historic time periods. 438

Researcher domain knowledge is crucial to the successful application of the 439 strategy explored here and elsewhere [53]. Reweighting nonprobability samples 440 via any analytical technique requires a substantive understanding of plausible 441 relationships between variables driving the sampling process and those driving 442 the response [11, 13, 35]. If strata are in fact random with respect to both y and 443 π , that is they have no relationship with the correlation between sample inclusion 444 and variable of interest, then new locations based on them should not contribute 445 to estimator bias, although variance may be increased. It is also possible that 446 selected strata increase bias. As our *Calluna* example demonstrates, this may 447 be due to the poststratification step amplifying poor within-stratum estimates 448 (i.e. those with substantial remaining biases). Theoretically the adaptive sampling 449 step itself should not increase bias if it is a probability-based selection. In reality, 450 constraints on the sampling of new locations within strata could increase or 451 maintain bias for the same reasons that the sample in-hand was initially biased. 452 for example due to land access issues. 453

A similar situation might occur if an adaptive sampling strategy was applied to a finite pool of interested surveyors, and the strategy ended up merely shifting

attention from one area to another, introducing a bias that might change over 456 time if left unadjusted. Whilst poststratification could continue to reduce such 457 biases if the underlying strata were effective, survey organisers would presumably 458 want to monitor such situations given that they may represent no net gain in 459 accuracy. There would be little point in attempting to manipulate data collection 460 if it merely led to a new sample configuration with biases of a similar size unless 461 other inferential aims were in play: the desire to cover some environmental 462 gradient to better estimate predictive or causal regression coefficients for use in 463 species distribution modelling or similar across broader time-slices, for example 464 [36]). A related issue is that our algorithm only considers the addition of new 465 sampling units, not their removal. In theory, removing existing sites could also 466 reduce bias: for example, in our *Calluna* example, even if we did not have access 467 to the "true" distribution, a coarser map of habitat types might clearly indicate 468 oversampling of heathland and other relevant habitats within strata. Whether 469 or not reducing survey effort in this way is a sensible option will of course be 470 survey specific. 471

Other practical issues also need considering. Spatial bias in citizen science 472 surveys is not unexpected given the vounteer effort underpinning them [46], and 473 so it may not be realistic to recruit surveyors for locations selected according to 474 theories of statistical optimisation. Some schemes may be able to avoid this issue 475 through the combination of volunteer and professional effort; for example, the 476 UK Pollinator Monitoring Scheme currently relies on both [60]. In other cases 477 low uptake in some areas can be very challenging, and substantial effort may be 478 required to understand the reasons for nonresponse. An example is the "Upland 479 Rovers" scheme of the UK Breeding Bird Survey, where substantial effort has 480 gone into trialling different approaches to increasing surveyor uptake of upland 481 squares [5]. 482

Even if practical implementation is difficult, our approach can have value as a 483 conceptual tool for the investigation of existing biases via simulation exercises in 484 a similar way to the *Calluna* example given here. Discretised species distribution 485 models, or simply habitat or land cover maps, could still provide insight into likely 486 biases affecting the sampling of a species' abundance or occupancy, and this type 487 of information could be used to better construct adjustment poststrata and/or 488 adjust uncertainty intervals for estimates [11, 42]. If large biases are suspected to 489 remain, even after the exploration of adaptive sampling or poststratification, then 490 other bias reducton strategies should be explored, the simplest being to adjust 491 the estimate to a population that one has more confidence of being sampled 492 representatively. That is, do not make inferential claims that are significantly 493 larger than the evidence [8]. An example would be claiming that a time series of 494 a butterfly's local abundance was actually indicative of that across the whole of 495 a country in the face of strong evidence for geographic bias and temporal shifts 496 in such over time [cf. 6]. 497

Adaptive sampling in environmental monitoring is not new [e.g. 55], however, a majority of previous investigations in this area have primarily aimed at taking "advantage of population characteristics to obtain more precise estimates of population abundance or density, for a given size or cost, than is possible with

conventional designs" [59]. Indeed, work in this area of ecology has tended to 502 focus on the reduction of variance conditional on controlled design, and seems 503 rarely to have asked the question from the point of view of adding units to 504 reduce estimator bias relative to a baseline of unrepresentative sampling for 505 descriptive inference [22]. Whilst there is considerable mathematical overlap 506 between these existing approaches to adaptive sampling [59] and that considered 507 here, those approaches have tended to use the response values of interest to guide 508 the selection of new sampling locations [59], whereas here we follow the recently 509 developed survey sampling approach of focusing on how to equilibriate inclusion 510 probabilities across units to reduce correlations between these and the response 511 variable(s) of interest [53]. Such approaches fall within the second category of 512 Wagner's typology of nonresponse bias indicators [63], as they require data on 513 survey response and sampling frame information at the population level (here 514 stratum membership), but not on the survey outcome variables themselves. 515

516 Conclusion

We have laid out the relationship between poststratum-based adjustment 517 strategies and inverse probability weighting in the context of reducing bias 518 (or, equivalently, improving representation) for descriptive inference. Following 519 Meng [33] and others [4, 65], we have characterised this bias as a non-zero 520 correlation between inclusion probabilities and the variable(s) of interest and 521 clarified the assumptions required to justify this approach. A recent review 522 of adaptive sampling in ecology [22] suggested that the complexity of some 523 techniques in the literature likely constituted an important barrier to uptake, 524 and our simple approach may help to overcome this problem. The approach 525 proposed here relies on assumptions that are typically impossible to verify 526 without separate survey efforts, but this is no different to the assumptions 527 required to reweight existing samples to improve representativeness [3, 2, 11]528 and the ongoing development of R-indicators and related tools points to numerous 529 opportunities for ecologists in these areas [e.g. 52, 38, 53]. We have focused on a 530 single categorical driver of sampling bias to target adaptive sampling, but, in 531 principle, one could cross-tabulate many categorical variables and/or discretise 532 continuous ones for crossing [62]. It may be that modelling inclusion probabilities 533 using multivariable approaches, and using "partial" R-indicators based on these, 534 will allow finer-grained exploration and control of adaptive sampling strategies 535 relative to inclusion probability variance in the future [54]. 536

We reiterate that our approach is not a panacea. In general, if sample inclusion 537 probabilities and the response variable are still correlated after poststratification 538 (i.e. $|\rho(\pi_{i(h)}, y_{i(h)})| >> 0$), then calculated statistics may still contain important 539 bias relative to any given research question. However, this applies to all such 540 strategies based on weighting adjustments, and certainly applies to ignoring 541 the problem altogether (i.e. assuming that the sampling mechanism is already 542 equivalent to a probability sample without critical inspection). Best practice 543 is likely to involve sensitivity analyses [29, 42], and both quantitative [9] and 544 qualitative assessments of the potential for bias relative to key research goals 545 [8, 43].546

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549 Supplementary Material 1

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