Algorithm selection for optimal ecological monitoring design

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Abstract

Comprehensive monitoring of biodiversity to direct conservation action is foundational to addressing the ongoing biodiversity crisis. As integrative monitoring programs increasingly come online in response to multilateral biodiversity agreements, establishing best practices for optimal design is critical. Selecting the appropriate algorithm for identifying sample sites is both necessary for robust inference from biodiversity data and largely neglected from broader monitoring network discussions. Here, we benchmark the performance of four common selection algorithms, outline the characteristics of the suite of algorithms suitable for ecological monitoring design, and offer recommendations for their best use. While all algorithms outperformed simple random samples, performance differences were negligible between algorithms. We recommend instead that practitioners choose algorithms based on feature availability, which varies greatly between algorithms.

Keywords spatially balanced sampling · monitoring network · biodiversity monitoring · generalized random tessellation stratified

0.1 Intro

Monitoring changes in biodiversity through time and across space is fundamental for identifying areas of high conservation value amidst the ongoing sixth mass extinction. Historically, biodiversity data has been dominated by heterogeneous non-probability samples, often collected for snapshots of time using bespoke protocols with low replication (Boyd, Powney, and Pescott 2023). Synthesis of this data for broad-scale assessment of biodiversity suffers from low power, severe data biases (Chapman et al. 2024), and an inability to detect existing trends (Boënnec, Dakos, and Devictor 2024; Johnson et al. 2024; White 2019). With this context, establishment of standardized monitoring protocols across the globe has been a major focus of multilateral biodiversity agreements (Gonzalez and Londoño 2022; Griffith et al. 2024).

Monitoring networks that produce robust data for statistical inference are designed under a pre-established statistical framework (Benedetti, Piersimoni, and Postiglione 2017; Dumelle et al. 2022; Williams and Brown 2019). At its most basic this process involves i) defining a sample frame, ii) identifying potential sampling sites, and iii) applying a site selection algorithm that follows random sampling principles to identify the final sample points. Many algorithms support additional features, including incorporation of site level characteristics, systematic over-samples, and stratification to further tailor the network design. Regardless of the specifics of each algorithm, sets of sampling points recommended in this way should offer a fair representation of the statistical structure of the data used to select them, and therefore adequate information about the status and trends of biodiversity in the region.

Despite significant recent investment in tools for designing and implementing monitoring programs, discussions around choosing the appropriate site selection algorithm have been largely restricted to theoretical differences

Table 1: Available features and implementation for spatial sampling design algorithms.

algorithm	stratification	auxillary variables	legacy sites	master sample	R package
GRTS	yes	no	yes	yes	spsurvey, Sdraw
Cube	yes	yes	no	no	BalancedSampling, sampling
LPM	no	yes	no	no	BalancedSampling
SCPS	no	yes	no	no	BalancedSampling
BAS	yes	no	yes	yes	Sdraw, spbal
HIP	no	no	no	yes	Sdraw, spbal
DAS	no	yes	no	yes	

between algorithms or benchmarking of performance using a limited set metrics rather than practical considerations (Benedetti 2015; Benedetti, Piersimoni, and Postiglione 2017; Kermorvant et al. 2019). This is despite significant differences in computational performance, available features, and ongoing development of better-performing algorithms. Previous evaluations largely focus on spatial balance alone rather than a network's ability to meet the goals of a monitoring project (e.g. Di Biase, Marcheselli, and Pisani (2024)). In biodiversity monitoring this may include for example how completely the full species richness of the region is sampled, how well the network captures landscape heterogeneity, or the ability of a network to detect trends through time. There is therefore a critical need for review of site selection algorithms, the features they provide, and how they perform for ecologically relevant metrics.

Here, we outline the feature and performance considerations for site selection algorithms using the Canadian province of Québec as a case study. We describe a typical process for designing a monitoring network, outline the characteristics of common and more recently developed site selection algorithms for biodiversity monitoring applications, and simulate that process for common algorithms to evaluate performance for multiple management-relevant goals. Based on this simulation study, we offer some specific guidance regarding the selection and use of site selection algorithms for integrative biodiversity monitoring.

0.2 Methods

0.2.1 Algorithm Descriptions

Algorithms vary widely in their approach to balancing samples across space and site characteristics. Below we describe the site selection process for algorithms, their features, and how they might be implemented in the R programming language. We discuss stratification, incorporation of site-level data in the form of auxiliary variables, and inclusion of legacy sites to support iterative network development. We also discuss whether or not the algorithm supports master sampling defined as systematic oversampling to support dynamic sample sizes.

The first four algorithms are the most widely accepted and therefore included in our performance benchmarking simulations (Generalized Random Tessellation Stratified, Cube Sampling, Spatially Correlated Poisson Sampling, Local Pivotal Method), with three additional algorithms that hold promise but were not included in benchmarking. Algorithm characteristics are also summarized in Table 1.

Generalized Random Tessellation Stratified (GRTS): Generalized Random Tessellation Stratified (GRTS) was developed by the U.S. Environmental Protection Agency for use in the National Environmental Monitoring and Assessment Program (Stevens and Olsen 2004). It uses a hierarchical sampling approach whereby the study extent is hierarchically subdivided by grids until each cell contains only one sample unit. Cells are then ordered on a line by their hierarchical "address", the line is split into a number of equally sized units equal to the sample size and a sample point is randomly selected from each unit (Benedetti, Piersimoni, and Postiglione 2017). Rather than incorporating auxiliary data directly into the site selection process, they can be qualitatively assessed by the user to differentially weight site selection or to define stratification. As this is a more subjective process and not directly comparable to auxiliary inclusion for other algorithms, we did not included GRTS in our auxiliary data simulation scenarios. GRTS is one of two algorithms we discuss that supports legacy site inclusion (Foster et al. 2017). We implemented this algorithm using the `grts` function in the R package `spsurvey`.

Cube Sampling: The cube methods seeks to select a sample that balances across auxiliary variables while maintaining the inclusion probabilities of constituent sites (Chauvet and Tillé 2006; Tillé 2011). It conceptualizes each potential site as a vertex of a hypercube in an N-dimensional space, R^N . The vector of inclusion

probabilities is a vector inside the unit cube, and an affine subspace (hyperplane) defines the set of possible solutions balancing across auxiliary variables. The algorithm therefore seeks to find a point on the linear subspace that satisfies the inclusion probabilities. Inclusion of auxiliary data is fundamental to this approach and it can also handle stratification by selecting samples with an exact sample size within stratum while still maintaining balance for the network of sites as a whole (Chauvet 2009). We implemented this algorithm with the R functions `cube` and `cubestratified` in the R package `BalancedSampling`.

Spatially Correlated Poisson Sampling: Spatially correlated poisson sampling (SCPS) uses a sampler that visits sites one by one, with visit probability initially given by inclusion probability of sites (Grafström 2012). Subsequent sites are visited after calculating a penalization based on distance to previously visited sites. Auxiliary variable information can be incorporated alongside spatial distance to target optimal spread across variables (Zhao and Grafström 2020). Since SCPS is designed to account for differences between site characteristics without stratification we use two different stratification approaches for benchmarking. First, the naive approach which simply treats stratification levels as independent samples, and second, an unequal probability sample which enforces within-strata sample size by setting the total inclusion probability for candidate sites in a strata to the desired sample size for that strata (Benedetti 2015). In benchmarking results below we present the second implementation alongside other algorithms (refereed to simply by SCPS), and discuss the comparison between the two implementations separately. We implemented SCPS using the R function `SCPS` in the R package `BalancedSampling`.

Local Pivotal Method: The local pivotal method (LPM) selects sites based on their euclidean distance in the auxiliary sample space. Sites are selected to maximize the distance between points and therefore coverage of the sample space (Grafström 2012). We implemented LPM using two different algorithms: LPM1, which creates the optimally balanced sample, and LPM2 which selects a sample more efficiently (Benedetti, Piersimoni, and Postiglione 2017). Algorithms performed almost identically, so we report results for only LPM2 here. LPM follows the same philosophy of SCPS in balancing across characteristics without strata, so we also simulated naive and unequal probability stratification scenarios for LPM1 and LPM2. As with SCPS, we include the unequal probability implementation when comparing to other algorithms, and discuss the comparison between naive and unequal implementations separately. These algorithms were implemented using functions `lpm1` and `lpm2` from the R package `Balanced Sampling`.

Balanced Acceptance Sampling: Balanced Acceptance Sampling (BAS) selects points based on a random-start Halton sequence, which gives a quasi-random number sequence (B. L. Robertson et al. 2013). The multi-dimensional study space, which could be for example a two-dimensional space defining latitude and longitude, is scaled and enclosed by a unit box of the same dimensions as the study space. Points are then assigned an element of the Halton sequence based on their location in the multi-dimensional box and selected for the final sample set based on the ordering of the sequence. This algorithm does not allow for the inclusion of auxiliary data beyond the ad hoc modification of inclusion probabilities based on site characteristics however it does support the inclusion of legacy sites.

Halton Iterative Partitioning: Halton Iterative Partitioning (HIP) builds on the concepts of BAS, but rather than selecting points from the space of the multi-dimensional box it iteratively partitions the box and selects points from the nested boxes based of the halton sequence ordering (B. Robertson et al. 2018). It has been recently expanded from it's original implementation to facilitate master sampling (B. Robertson, Dam-Bates, and Gansell 2022). It does not incorporate stratification or the inclusion of auxiliary variables.

Dynamic Assignment Sampling: Dynamic Assignment Sampling (DAS) was designed to facilitate the inclusion of auxiliary variables and master sampling in a single algorithm (B. Robertson, Price, and Reale 2024). It draws a balanced sample from the auxiliary sample space sequentially as units are iteratively assigned to a candidate set. A candidate set is then chosen as the core set of seed sites before a sufficient number of sites are assigned to reach the desired sample size. DAS has not yet been implemented in open source software at the time of writing.

0.2.2 Design Process

Here we give a general outline for the steps in the simulated network design, with details of data and simulation methods to follow.

Candidate Points: We identified a set of candidate points using a hexagonal sampling algorithm implemented by the R function `st_sample` from the R package `sf`. This algorithm establishes a grid of evenly spaced sample points across the sampling extent while accounting for irregularity in sample extent boundaries. The initial grid had 10000 candidate points evenly spaced across the province of Quebec, with a euclidean distance

between points of ~13 km. We excluded points on water or ice as identified by the landcover data described below. The final candidate set had 9992 potential sites. For simulations stratified by ecoregion, we excluded ecoregions with an insignificant area in Québec, defined by 10 or fewer candidate points in the ecoregion.

Auxiliary Variables: For each potential sample site in the candidate set we assembled a suite of auxiliary variables describing the site characteristics from existing open source environmental data. Data included landcover, climatic variables, and site topography. To account for covariation in variables, we performed whitening on the matrix of auxiliary variables using the function `whiten` from the R package `whitening`. Whitening transforms the sample matrix to a matrix of orthogonal, and therefore independent, variables with unit variance and zero covariance (Kessy, Lewin, and Strimmer 2018).

Identifying Sample Points: For each algorithm of interest we simulated a suite of design scenarios by sampling from the set of candidate points under different conditions. We included a simple random sample as a baseline for performance and evaluated the following algorithms: Generalized Random Tessellation Stratified (GRTS), Cube sampling, Spatial Correlated Poisson Sampling (SCPS), and two implementations of the Local Pivotal Method (LPM1, LPM2). For each algorithm we sampled 100 replicates for each sample size sample size ranging from 10 to 545 on an approximate log scale (10, 15, 22, 33, 49, 74, 110, 164, 245, 365, 545). This process was executed for each algorithm for four different sampling scenarios: unstratified (equal probability) and stratified by ecoregion, with and without auxiliary environmental data. For stratified samples, the complete monitoring network sample size was allocated across ecoregion strata proportional to the ecoregion's area in the study extent.

Evaluation of Algorithm Performance: Algorithm performance was evaluated based on three complementary metrics representing different goals for monitoring programs. Spatial balance, or the variance in site inclusion probabilities across space; species coverage, or how comprehensively the network samples existing species on the landscape; and environmental coverage, or how balanced sampling is across combinations of environmental variables. Species and environmental coverage were averaged across simulation replicates and spatial balance was measured as the variance across all simulation metrics. See the Algorithm Evaluation Metrics section below for details on how metrics were calculated.

0.2.3 Data

Landcover data for candidate point exclusion and auxiliary variables was obtained from the ESA WorldCover dataset for 2020 (Zanaga et al. 2021). Additional auxiliary variables included slope and elevation from the Earthenv topography data (Amatulli et al. 2018), and all 19 CHELSA-BIOCLIM+ variables (Brun et al. 2022). Ecoregions for stratification simulations were taken from the WWF defined ecoregions (Olson et al. 2001). We used IUCN range maps for mammals to evaluate biodiversity coverage of the simulated network and included all mammals whose range intersects with Québec.

0.2.4 Algorithm Evaluation Metrics

We evaluated algorithm performance using three metrics that represent key goals of biodiversity monitoring networks: spatial balance, species coverage, and environmental coverage. Spatial balance was assessed following Benedetti (2015) and Stevens and Olsen (2004), as the variance in total inclusion probability of points contained in each Voronoi polygon. Environmental coverage was measured by calculating the Jensen-Shannon divergence (JSD) for the environmental values represented by a sample network using the function `JSD` in the R package `philentropy` (Drost 2018). Jensen-Shannon distance was calculated for each environmental variable, with the JSD for a potential sampling design calculated as the square root of the mean distance of all environmental variables. JSD therefore measures how completely the sample distribution covers the environmental space of the sample landscape. We assessed species coverage using the IUCN range maps to compile species checklists for each sample point and the sample extent as a whole. Coverage was quantified as the percent of species in the landscape not sampled by a given sample monitoring network.

0.3 Results

Algorithms generally showed very similar performance across metrics, despite having visually different samples (Fig. 1), and showed saturating performance with increasing sample size, particularly for species and environmental coverage (Fig. 2). Across all metrics and simulation scenarios algorithms performed better than the simple random sample. For species and environmental coverage performance differences were negligible, though LPM, and SCPS consistently performed better for all metrics. Cube sampling alone showed marked difference after adding stratification. Surprisingly, including environmental variables did not change

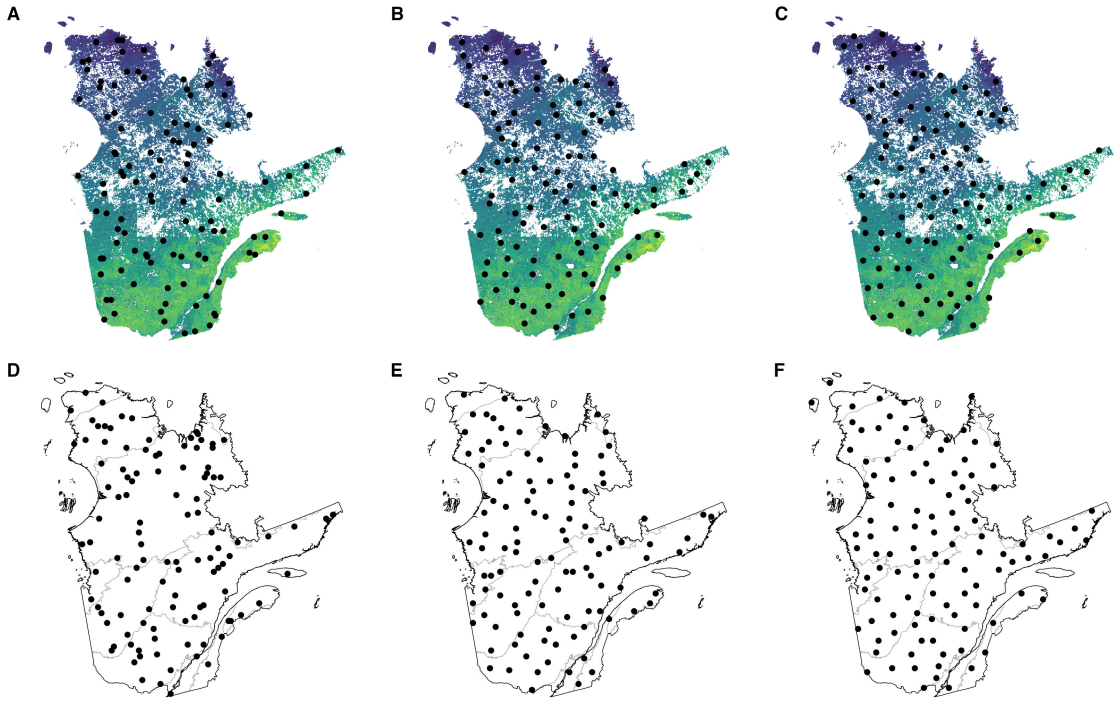

Figure 1: Example designs for unstratified (A-C) and stratified (D-F) monitoring network designs for Cube (column 1), LPM (column 2), and SCPS (column 3) algorithms, all with a sample size of 110. Unstratified designs are show with NDVI, stratifeid designs are shown with ecoregion boundaries.

algorithm performance significantly for the majority of algorithms, with the exception of cube sampling (Fig. 3).

We found that the naive implementation of LPM and SCPS, where strata were each treated as independent samples, gave significantly worse performance than the unequal probability approach to stratification (Fig. 4). Rather than reaching a saturation point, spatial balance for the naive implementations increased with increasing samples, indicating worse balance with larger sample size. This also manifested in species and environmental coverage, where naive implementations saturated at worse performance than the unequal probability implementations.

0.4 Discussion

Appropriately selecting sample locations is critical for generating robust inference from biodiversity monitoring data. Despite a variety of existing algorithms for designing a sampling network, and on going development of available features, discussions around the most appropriate algorithm for ecological sampling has been limited.

We found the performance differences between most of the best-performing algorithms to be negligible; this was particularly true for species and environmental coverage, and robust across study design. This may simply reflect the fact that ecological processes tend to be correlated to one another in addition to being spatially auto-correlated (Legendre 1993). Whereas auto-correlation can be a source of bias by masking actual trends in biodiversity (Diniz-Filho, Bini, and Hawkins 2003), it can be a net positive for the design of biodiversity monitoring networks by artificially driving algorithms to suggest designs with similar performances. In some sense, these results suggest that site selection algorithms can fall victim to the Rashomon effect (Paes et al. 2023): potentially different designs may be equally effective at biodiversity monitoring. The performance of biodiversity monitoring may be limited more by the environmental and biogeographic characteristics of the region to monitor than by the choice of algorithm (we moderate this statement for specific cases further on).

Coherently to the previous discussion about equivalency of different selection methods, we found that even when spatial balance indicated relatively poor performance (different runs of the algorithm suggested markedly

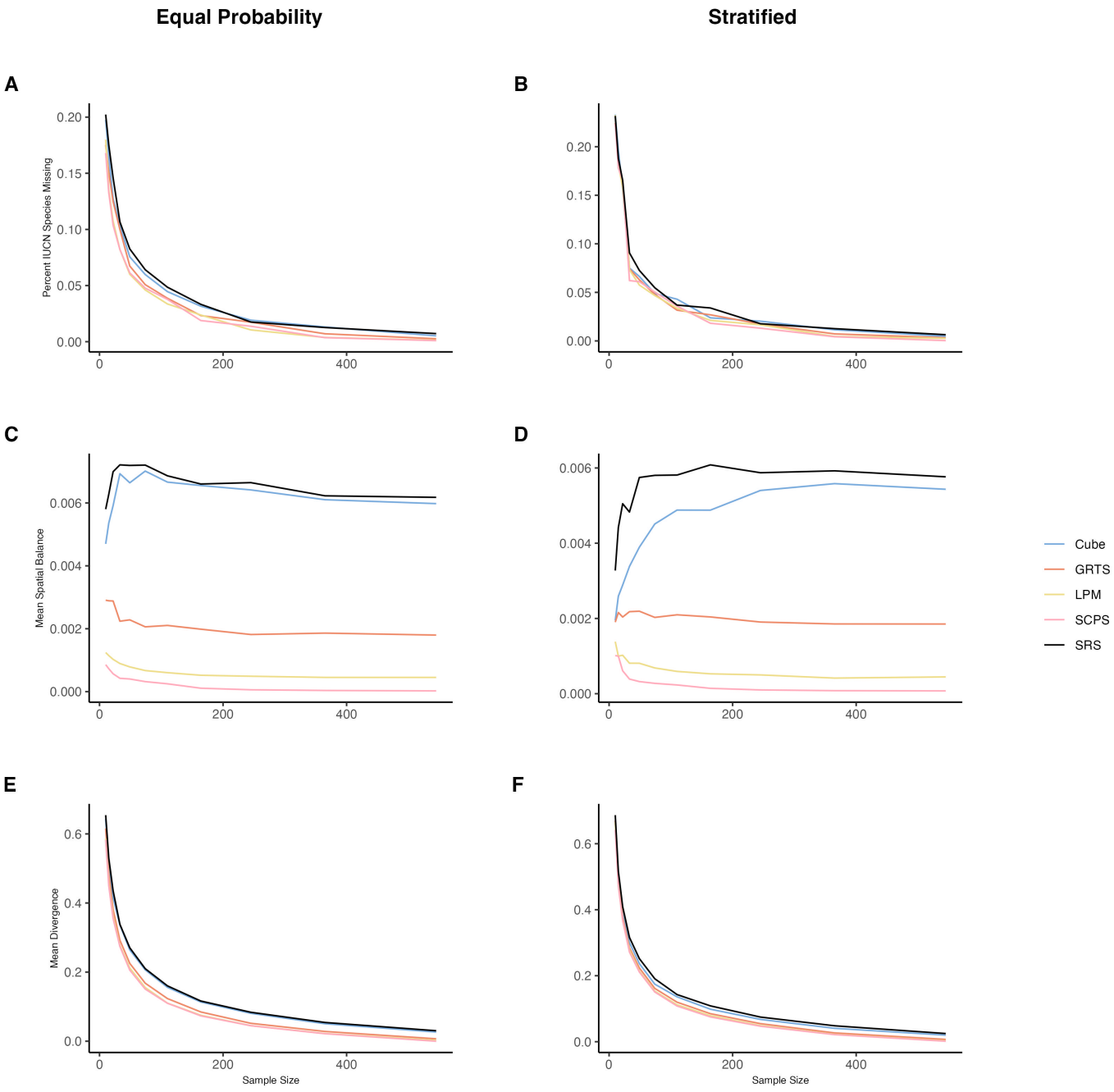

Figure 2: Three evaluation metrics for each of the algorithms for all of Quebec and stratified by ecoregion. Y axis is scaled between zero and one, with lower values indicating better performance for all metrics.

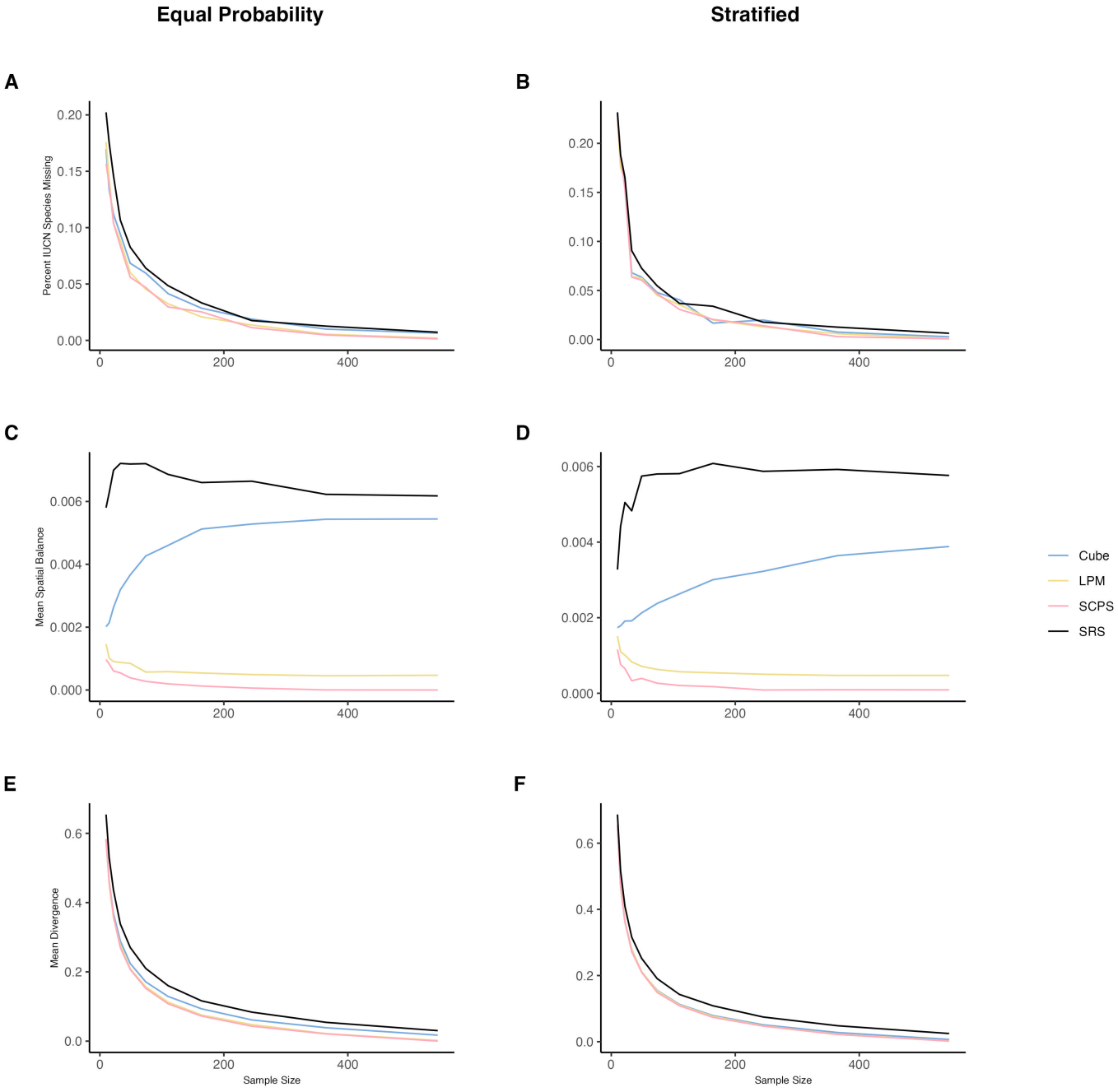

Figure 3: Three evaluation metrics for each of the algorithms for all of Quebec and stratified by ecoregion, including only algorithms that can take environmental data as auxiliary variables. The Y axis is scaled between zero and one, with lower values indicating better performance for all metrics.

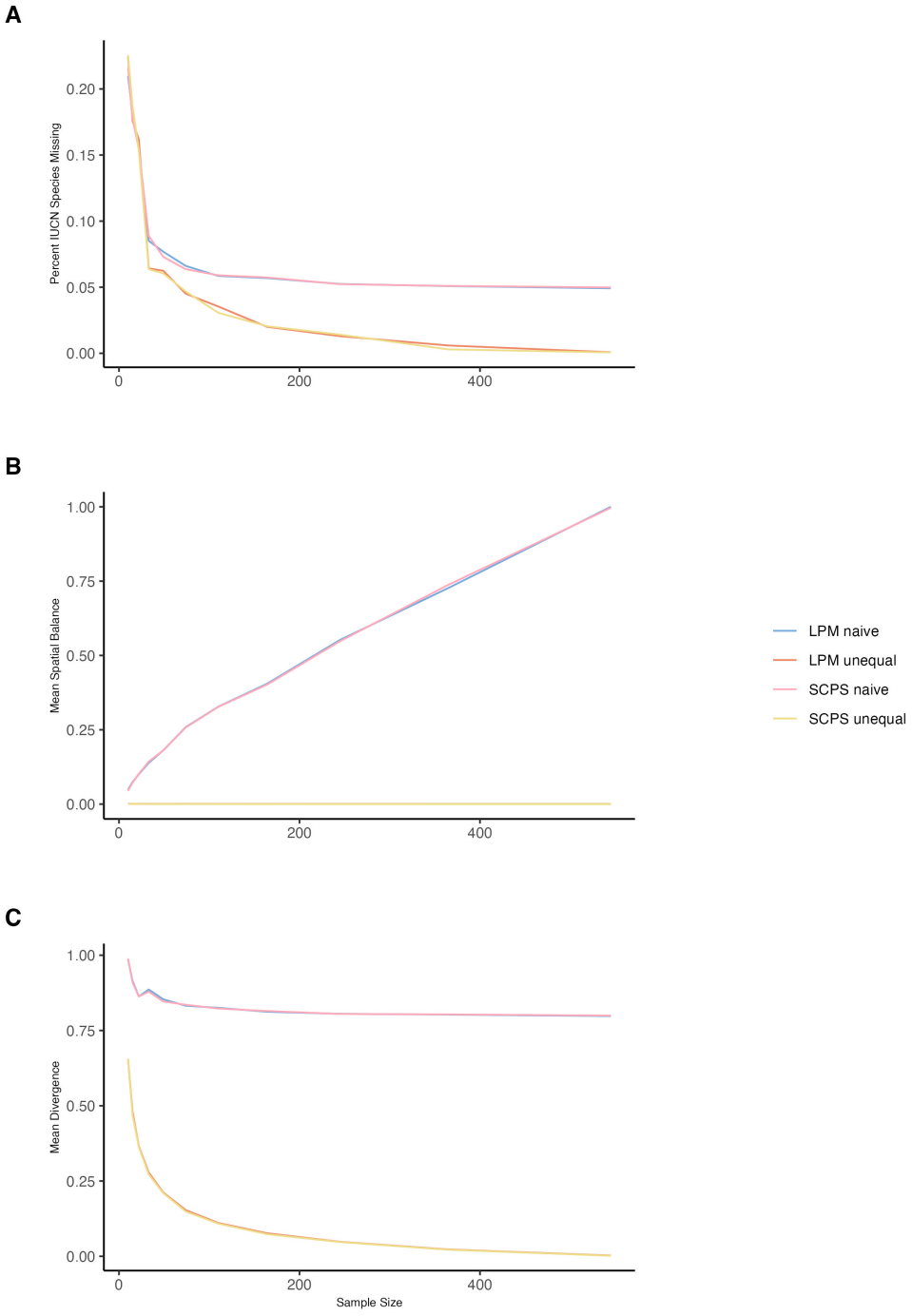

Figure 4: Three evaluation metrics for naive (stratum treated completely independently) and unequal probability (enforcing strata sample size by modifying inclusion probabilities) implementations of LPM and SCPS algorithms. Unequal implementations are the same show in benchmarking in Fig 2 and Fig 3.

different locations to survey), ecological performance metrics were mostly determined by sample size. Notably, the saturation of performance for ecological performance metrics was similar across algorithms. This, again, reinforces the idea that the "best" designs generated by each algorithm may be equivalent, and that the difficulty in monitoring a region is determined by ecological processes. Although the monitoring networks got progressively better with more samples, we observed a clear saturation, suggesting that past this saturation point adding additional sites does not result in more informative monitoring.

There are two important algorithm-specific recommendations we can formulate based on our results. First, the naive implementation of stratification for SCPS and LPM performed far worse than other algorithms in all metrics. In particular, spatial balance metrics increased (poorer performance) when sample size increased, meaning that more investment in monitoring would yield worse outcomes. For applications where stratification concepts are important, users should enforce differing sample sizes by unequal probability sampling for these algorithms rather than treating strata independently. Second, the performance of cube sampling is increased when auxiliary data are used; this makes this algorithm unsuitable when there are no readily available information about non-ecological data at the candidate locations. Although this is a limitation, the wealth of publicly available high-resolution geospatial data means that this limitation is unlikely to ever affect the viability of cube sampling as a site selection algorithm. Beyond those specific use cases, algorithm selection is largely dependent on the features needed by the user and implementation availability (Table 1), even more so since no algorithm was able to generate a monitoring network that saturated with fewer sampled locations.

We benchmarked algorithms for a single case study landscape, defined by its large extent and strong latitudinal gradient in species richness, composition, and environmental features. The performance of some algorithms may respond to changes in the landscape of interest. For example, highly heterogeneous landscapes may be more comprehensively sampled by algorithms that take into account site-level information; this is particularly likely since fine-scale heterogeneity can over-rule the effect of auto-correlation (Tardanico and Hovestadt 2023), which can reveal additional differences between algorithms. Similarly, ecosystems in which species distributions are not tightly tracking the environmental gradient may lead to some algorithms achieving better performance; we specifically expect that in these cases, algorithms with good spatial balance may be more apt at capturing ecological variables. In all cases, because the computational requirements of these algorithms remain fairly low, it is not unrealistic to proceed with a location-specific benchmark in a systematic way.

The option to produce a master sample is a key distinguish feature of algorithms with particular relevance to ecological sampling (B. Robertson, Price, and Reale 2024) . Master sampling creates a systematic oversample that allows you to increase or decrease the sample size dynamically while maintaining the probabilistic sampling frame (Dam-Bates, Gansell, and Robertson 2018). This approach facilitates modifications to the complete set of sampling locations due to common logistical constraints such as site inaccessibility, changing landownership, or budgetary constraints. Of the algorithms we benchmarked only GRTS can create a master sample, however it is increasingly recognized as a critical feature for robust implementation of monitoring designs. This is reflected in recent algorithm development with BAS, HIP, and DAS all supporting master sampling (Table 1).

In adopting a practical approach to benchmarking, we suggest that the different algorithms are able to achieve similar best performances. In more concrete terms, this allows users to give more importance to the capabilities of each algorithm when selecting a subset to benchmark against a specific region of interest. All the algorithms we benchmarked were able to outperform simple random sampling, suggesting their use in the monitoring design process will result in more robust biodiversity monitoring networks than naive or expert-informed sampling alternatives. Although all but one of these algorithms had available implementations, they used very different interfaces and programming conventions. The development of a unified interface for sampling is a natural next step in ensuring sampling algorithm uptake for future monitoring design.

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