A GENERAL FRAMEWORK FOR PREDICTING THE OPTIMAL COMPUTING CONFIGURATIONS FOR CLIMATE-DRIVEN ECOLOGICAL FORECASTING MODELS

by

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ABSTRACT
A GENERAL FRAMEWORK FOR PREDICTING OPTIMAL COMPUTING CONFIGURATIONS FOR CLIMATE-DRIVEN ECOLOGICAL FORECASTING MODELS
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Rapidly growing databases are swiftly transforming the field of biodiversity modeling into a big-data science, characterized by high volume, heterogeneous datasets with high uncertainty. As climate warming and land use change accelerate, it is imperative that scientists leverage all available data to generate robust, high resolution, and accurate predictions of biodiversity changes, in order to protect vital ecosystem services and minimize loss. In recent years, cloud computing's flexibility and scalability has caused it to emerge in many fields as the standard for analyzing massive datasets. However, cloud computing has been underutilized in biodiversity studies and climate-driven ecological forecasting specifically. While the cloud's novel operating model allows users to provision and release virtual instances from a utility provider on demand, ecological researchers currently have little guidance about the most efficient configuration to use. Researchers face tradeoffs between model accuracy, computing cost, and model execution time, and the choice of configuration has scientific and financial ramifications.

In this thesis, I present a general conceptual framework for approaching these tradeoffs and introduce a model for determining the optimal data-hardware configuration for a species distribution modeling (SDM) workflow. I develop and test three hypotheses relating model accuracy and cost to algorithm inputs and computer hardware and collect an empirical dataset of over 25,000 experimental trials of four leading SDMs (generalized additive models, GAM; boosted regression trees, GBM-BRT; multivariate adaptive regression splines, MARS; random forests, RF), using Bayesian regression trees and to model the drivers of SDM accuracy and execution time. The computing performance models (CPMs) demonstrated explained more than half of the variance in the dataset in all cases and can improve future allocation of time and money, as well as inform model developers on future priorities. The CPMs are also a key component in identifying the data-hardware configurations that maximize accuracy and jointly minimize SDM execution time and cost.

In general, the SDMs examined were most accurate when fit with a large number of training examples and many covariates and accuracy was largely unaffected by hardware configuration. The optimal hardware for GAM, GBM-BRT, and MARS were low memory with few CPUs. RF, an ensemble technique, can more easily leverage parallel infrastructure, resulting in an optimal hardware configuration of four to seven CPU cores. Many widely used SDMs are structurally unable to take advantage of the increased computing power offered by cloud computing. As datasets continue to grow, new algorithms and software packages must be developed to explicitly take advantage of the modern high performance computing techniques. The CPMs developed here are extensible to other forms of biodiversity and ecological modeling studies. Efficiency studies such as the one presented here are valuable in facilitating uptake of new technologies by providing rigorous evidence of their utility.

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1. Introduction

Human-induced global environmental change, including climate warming, land clearance, and the spread of invasive species, threatens to severely alter biodiversity patterns worldwide in the coming century (Lowe et al., 2011; Root et al., 2005; Thuiller, 2007; Thuiller et al., 2008), potentially causing the extinction of over one-sixth of all species (Urban 2015). Species ranges, particularly those of vascular plants, are strongly controlled by climatic factors (Salisbury, 1926; Woodward, 1987), and global changes in climatic gradients are expected to have a substantial impact on future patterns of biodiversity (Lowe et al., 2011). Statistical methods that quantify a species' biophysical response to environmental factors, known as *species distribution models* (SDMs), can be used to forecast future species distributions and biotic assemblages under different greenhouse gas emission scenarios (Clark et al., 2014; Guisan & Thuiller, 2005; Guisan & Zimmerman, 2000; Guisan et al., 2013; Maguire et al., 2015; Thuiller et al., 2008). A rapidly growing volume of ecological data is available for modeling species-specific responses to the climate system, both at present and in the geologic past (Fig. 1). Environmental monitoring efforts, such as the Long Term Ecological Research program (LTER, Hobbie et al., 2003) and the National Ecological Observatory Network (NEON, Schimel et al., 2009); databases of the fossil record, including the Neotoma Paleoecology Database (Neotoma; http://neotomadb.org) and the Paleobiology Database (PBDB, http://paleobiodb.org); and modern species occurrence databases, such as the Global Biodiversity Information Facility (GBIF, http://www.gbif.org), all organize, store, and distribute large amounts of information to researchers in pursuit of understanding and forecasting biological responses to perturbations in the earth system (Brewer et al., 2012; Michener & Jones, 2012; Howe et al., 2008; Uhen et al., 2013). While growing collections of modern and paleo biodiversity data can improve predictive ecological modeling studies, data volume and heterogeneity challenge successful uptake and

implementation (Hampton et al., 2013). Cloud computing may offer a technological solution to some of the problems posed by the increasing 'bigness' of ecological data (Hampton et al., 2013; Michener & Jones, 2012), by allowing users to easily access configurable and convenient virtual resources (Mell & Grance, 2012). However, little guidance exists for researchers about tradeoffs between model accuracy, performance and cost. The present study develops a method for identifying the optimal computing configuration on which to run SDMs, describing a flexible and skillful framework that can be used to inform computing provisioning strategies and suggest future priorities for SDM developers.

With over 700 million modern and historical occurrence records in GBIF and 3.5 million fossil observation records in Neotoma (Fig. 1), traditional statistical methods for analyzing, modeling, and forecasting ecological distributions often cannot be applied without compromising analysis scope. Many SDM methods, though popular in the literature and highly skillful, are not designed to leverage parallel processing or distributed computing, and cannot be scaled to huge datasets. Other scientific fields, including bioinformatics (Schatz et al., 2010), genomics (Stein, 2010), climate analytics (Schnase et al., 2015), as well as private industry (Mosco, 2014), have adopted these and other computing techniques to cope with large datasets. As the volume of ecological data increases and the need for accurate, high-resolution projections of biotic distributions and extinction risk become more pressing, solving data volume challenges by reducing project scope (e.g., Bolker et al., 2009) is no longer a valid option. *Cloud computing* provides a platform for large-scale ecological analysis (Hampton et al., 2013; Michener & Jones, 2012), by providing "ubiquitous, convenient, and on-demand network access to a shared pool of configurable computing resources that can be rapidly provisioned and released with minimal management effort" (Mell & Grance, 2012). The rapid commercialization of cloud computing

and the widespread availability of public cloud services through providers like Amazon Web Services (AWS) and Google's Cloud Compute Engine (GCE) have put a seemingly unlimited supply of computing resources at scientists' disposal.

Moreover, the cloud's novel business model of charging for the use of virtual machines (VMs) rather than the purchase of physical hardware provides a highly flexible platform for scientific computing. This operating model lets consumers scale their resources depending on computational demand (Hassan, 2011). Users are therefore not locked in to a single hardware configuration and can add or remove hardware components as the problem changes (Armbrust et al., 2009). The costs of migrating to cloud environments can be difficult to estimate (but see Sun & Li, 2013), but the time gains can be significant (Yang et al., 2011a).

Given the cloud's flexible computing options, biodiversity modelers are faced with tradeoffs on at least three distinct axes: computing cost, model run time, and model accuracy. Moreover, in some situations, biodiversity modelers may seek to reduce variability and uncertainty in these three dimensions.

I hypothesize that, for any SDM modeling experiment, there exists an optimal data-hardware configuration that maximizes SDM accuracy while jointly minimizing the runtime and cost. In this thesis, I develop a framework for predicting this optimal configuration for four widely popular SDMs. I build a large empirical dataset (n=26,730) by observing the cost, runtime, and accuracy of SDMs run under different parameterizations and on different cloud computing configurations. Subsequently, I fit a Bayesian computing performance model (CPM) to predict the execution time and accuracy of modeling scenarios, understand the factors that contribute to the runtime and accuracy of these models, and identify the optimal hardware for the

task. I conclude by discussing priorities for future computing development in biodiversity modeling.

2. Background and Previous Work

2.1 Big Data in Ecology

In ecology, big data is emerging from the on-going building of massive biological datasets, including genomic sequences, long-term ecological monitoring (remote sensing, NEON, LTER), phylogenetic histories, trait databases, and biodiversity occurrence data. This emergence has required the development of robust quantitative methods in the biological sciences and has promoted advances in techniques for data management, analysis, and accessibility (Howe et al., 2008). Worldwide data volume doubled nine times between 2006 and 2011, and successive doubling has continued into this decade (Chen et al., 2014). This rate of data volume increase is faster than the annual doubling of computing power predicted by Moore's Law (Villars et al. 2011). Challenges include the inability to move large datasets across networks, increased metadata requirements for storage and data discovery, and the need to support novel data uses (Schnase et al., 2014).

Ecological occurrence data consist of spatiotemporally-explicit records of presence, absence, or abundance of individuals of a species or higher taxonomic grouping. These data form the backbone of many contemporary biodiversity analyses and environmental change forecasts. Increasingly, these data are being stored in large, dedicated, community-curated databases like Neotoma, GBIF, and PBDB (Uhen et al. 2013; Brewer et al. 2012; Williams et al., in press). Since the early 1990s, the Internet, an increased willingness to share primary data among scientists, and substantial investments by governmental and non-governmental organizations has precipitated rapid influxes of digital occurrence records (Soberón & Peterson, 2004). While there

are known problems with the quality and consistency of data records in large occurrence databases (Soberón et al., 2002), they provide a low-friction way of consuming large amounts of data that would otherwise be prohibitively time consuming to obtain from the literature or new fieldwork (Beck et al., 2014; Grimm et al., 2013). Entire new fields, e.g. 'biodiversity informatics' (Soberón & Peterson, 2004), 'ecoinformatics' (Michener & Jones, 2012), and 'paleoecoinformatics' (Brewer et al., 2012), have been delineated to address the growing challenges and opportunities presented by the management, exploration, analysis and interpretation of observations of biotic patterns now housed in biodiversity databases (Soberón & Peterson, 2004).

Although *'big data'* often is used loosely, there are two prominent frameworks for identifying big data. One characterizes big data as "data sets so large and complex that they become awkward to work with using standard statistical software" (Snijders et al., 2012). This ambiguous delineation is often echoed in the advertising and marketing literature that accompanies products, such as Apache Hadoop, a popular distributed computing framework, which describes Big Data as "datasets which could not be captured, managed, and processed by general computers within an acceptable scope" (Chen et al., 2014).

Under this framework, a dataset's bigness depends on both the duration of analysis and the entity attempting to analyze it. Manyika et al. (2015) suggest that the volume of data required to be 'big' can change over time, and may grow as technology advances. Today, big data usually refers to datasets between terabytes and petabytes (2^{40} to 2^{50} bytes), but varies among problem domains (Chen et al., 2014), the size of datasets common to that domain, and the software tools commonly used in that domain (Manyika et al., 2015). The rapid growth of databases and concurrent development of increasingly complex data models to store spatiotemporal

biodiversity occurrence records and their metadata (Grimm et al., 2013) suggests that traditional methods of data handling are insufficient for modern ecological analyses. Further developments, such as application programming interfaces (APIs) and language-specific bindings (e.g., R packages or python modules), facilitate accessing, filtering and working with large occurrence datasets (Goring et al., 2015; Hernández & Sgarbi, 2016; Chamberlain et al., 2016). Thus, new, custom-built tools are required to store, analyze, visualize, and use multiple large ecological occurrence datasets.

A second framework by which to assess Big Data is the 'Four V's Framework,' a popular and flexible framework that was first introduced by IBM in the early 2000's and used by large technological companies to characterize their data. Here a dataset is described by its volume, variety, veracity, and velocity, under which "volume refers to the size of the data; velocity indicates that big data are sensitive to time, variety means big data comprise various types of data with complicated relationships, and veracity indicates the trustworthiness of the data" (Yang & Huang, 2013).

Biodiversity data clearly meets at least three of these criteria. With respect to volume, since the late 1990s, the rapid growth and scale of biodiversity information has become challenging to manage (Fig. 1). Today, Neotoma holds over 14,000 datasets containing more than 3.5 million individual occurrence records and associated spatial, temporal, and taxonomic attributes, corresponding to an average growth rate of 358 occurrences per day for the past 27 years. All Neotoma records were originally gathered during fieldwork (e.g. sediment cores, paleontological or archaeological digs, or other efforts) -- techniques that require large expenditures of time and effort (Glew et al., 2002). GBIF houses well over 700 million digital records of field observations, living and fossil specimens, and reports from the scientific

literature. Since its launch in the early 2000s, GBIF's holdings have grown nearly 300%, from about 180 million records in 2001 to over 700 million records in 2016. GBIF includes both contemporary and historical observations, though 98.9% of its holdings are from 1900 onwards[1].

Biodiversity data also have a high variety, complicated by many interrelationships. For example, Neotoma's holdings feature 23 dataset categories (Figure 2a). Categories are separated for different taxonomic groups (e.g. plants, vertebrates, diatoms, ostracodes), fossil sizes (microfossils vs. macrofossils), geochronological datasets used to estimate time, and physical and geochemical measurements such as X-ray fluorescence (XRF) and loss-on-ignition (LOI). Each dataset type has somewhat different metadata requirements and is managed by different sets of Data Stewards and virtual Constituent Databases within Neotoma (Williams et al., in prep.) GBIF delineates nine record classes, including human observations, living and fossil specimens, literature review, and machine measurements (Figure 2b). Though the records coexist in GBIF, they are distinct, derived using different protocols by different communities of researchers. Moreover, the data are both spatial and temporal. All of Neotoma's records and 87.6% of GBIF's records are georeferenced[2]. Digital representations of spatial phenomena must grapple with unique challenges, including discrete representations of continuous physical processes, correlations between parameters in space and time, and differences in scale, that make storage and management difficult (Yang et al., 2011a). Finally, occurrence data represents the work of many dispersed individual researchers and research teams – the 'long tail' of ecological data (Hampton et al. 2014; Heidorn, 2008). While controlled vocabularies and defined data structures help to efficiently assemble large numbers of records, nearly every record was collected, analyzed, and published by a different scientist. While some scientists have

1 As of March, 2017.
2 As of November, 2016.

contributed many datasets to occurrence databases, most have contributed only a handful. The median number of datasets contributed per investigator to Neotoma is two and the third quantile value is just seven contributed datasets. While specific metadata are scarce, each researcher is likely to use somewhat different equipment, employ different lab procedures, follow different taxonomic guidelines, and utilize different documentation practices, contributing to variation among datasets.

Biodiversity data also face issues of veracity, which are expressed as uncertainty in taxonomic identification or spatiotemporal position. Some sources of uncertainty can be estimated, including spatial or temporal positional uncertainty (Wing et al., 2005) or modeled (Blaauw, 2010). For example, in a random sample of 10,000 records of *Picea* (spruce) from GBIF, over half did not report spatial coordinate uncertainty. Of the 4,519 records that did, the average spatial uncertainty was 305 meters, and the maximum was 1,970 meters. Such uncertainty may be problematic for modeling studies (Beck et al., 2014). In Neotoma, of a sample of 32,341 age controls (e.g., radiocarbon dates, varve counts), only 5,722 reported age uncertainty. The remaining records indicate a mean error of ± 130 years. With respect to taxonomic uncertainty, a recent study of benthic macroinvertebrates suggests that taxonomic identification error may be as high as 21% (Stribling et al., 2008). Other sources of uncertainty, including measurement errors and data loss incurred between field, lab, and database, may also be important. While uncertainty and veracity are entirely scale- and question- dependent, they can adversely affect analyses, particularly at small spatiotemporal scales.

The final piece of the Big Data framework is velocity, which characterizes the analytical sensitivity to time. High-velocity data must be analyzed in real time to produce meaningful insights. For example, tweets from the Twitter microblogging service can be analyzed for trends

as they are posted. Significant effort has been put into developing sophisticated algorithms that can detect clusters and trends in social behavior in real time (Bifet et al., 2011; Kogan, 2014). State-of-the-art warning systems for tornadoes, tsunamis, and earthquakes also involve also time-sensitive analysis (Blewitt et al., 2009). Velocity is perhaps the weakest fit between big data criteria and biodiversity modeling. Unlike many private sector applications, few scientific factors drive biodiversity researchers to immediately analyze new occurrence records. Moreover, automated analyses of distributional data have been warned against, due to heterogeneous data quality (Soberón et al., 2002) and associated uncertainty. However, some kinds of environmental monitoring have a high temporal resolution (e.g. eddy flux towers) and could be in principle leveraged to provide, e.g., high-velocity, near-real-time estimates of biospheric carbon uptake and release.

In summary, ecological occurrence data should be considered big data, because they require advanced, sophisticated techniques to store and analyze (definition 1), and demonstrate high volume, low veracity, and substantial variety (definition 2). To fully and accurately derive value from these databases, novel techniques for working with these data are required, as traditional statistical analyses were not designed to handle big datasets.

2.2 Cloud Computing in the Sciences

In recent years, large technology companies have promoted cloud computing as a way of overcoming the computational challenges associated with big data. The cloud leverages distributed networks of virtualized physical machines to create a computing utility, providing a pay-as-you-go business model and large economies of scale (Armbrust, 2009; Hassan, 2011) that delivers abstract resources and services, in addition to storage and compute resources (Foster et al., 2008). While some organizations and universities have developed ‘private clouds’ -- large

collections of virtualized servers not made available to the general public, similar to computing grids -- many researchers have recognized the potential for incorporating public clouds -- provided as a service by a cloud provider -- into their workflows. With this technology, scientists with little or no computational infrastructure can access scalable and cost-effective computational resources (Hsu et al., 2013). Major federal agencies and scientific organizations in the United States, including the NSF and NASA, have actively promoted cloud computing. Spurred by the U.S. Office of Management and Budget's "25 Point Plan to Reform Federal Information Technology Management" (Kundra, 2010), all federal agencies are now required to adopt a "Cloud First" policy when "contemplating IT purchases and [must] evaluate secure, reliable, and cost-effective cloud computing alternatives when making new IT investments" (Office of the Inspector General, 2013). The federal plan also created programs to help agencies adopt cloud solutions, reducing the effort needed to screen cloud providers for data security policies and enable rapid procurement of cloud services (Kundra, 2010). NSF has launched solicitations for experimenting with and developing new cloud architectures for scientific computing (National Science Foundation, 2012, 2014). Public cloud providers, such as Amazon Web Services and Google Cloud Compute, support scientific enterprise by providing large, open-access datasets for public consumption, including Landsat images, real-time NEXRAD radar, and the 1000 Genomes project, and by soliciting grants for researchers incorporating cloud computing into their research.

Cloud technology, both public and private, has extended into many fields, including bioinformatics (Hsu et al., 2013, Issa et al., 2013; Stein et al., 2007) and climate analytics (Lu et al., 2011; Schnase et al., 2014, 2015). Cloud-based solutions for bioinformatics research relieve the large memory requirements often associated with genomics and drug-design data (Hsu et al.,

2013), and have resulted in low latency, streaming methods for data analysis (Issa et al., 2013) and biology-specific operating systems for protein analysis (Kaján et al., 2013; Schatz et al. 2010). Contemporary climate analytics often requires working with massive datasets too large to be transferred across networks, promoting the development of Climate Analytics as a Service, an effort to integrate data storage and high performance computing to perform data-proximal analytics (Schnase et al., 2014, 2015).

Cloud services have also been used in the environmental sciences, and in ecological modeling problems specifically. Yang et al. (2011a) suggest that many kinds of geoscientific problems are strongly limited by computational ability and argue that the cloud provides a means of overcoming these challenges by leveraging distributed computational resources without increasing the carbon footprint or financial budget of research (see also Yang et al., 2011b). For example, cloud-optimized implementations of numerical models, such as real-time dust storm forecasting, have improved model performance significantly, while reducing cost by only using the intensive computing power required for forecasting during storm events (Yang et al., 2011a). Geoscientific, hydrological, and environmental models can also be run in the cloud (Granell et al., 2013). Applications of cloud computing to biodiversity modeling and species distribution modeling are less common, though some SDM projects are starting to explore this area. For example, Candela et al. (2013) describe a novel platform that enables cloud-based SDM, arguing that a cloud-based approach can aid in data discovery and increase processing capabilities.

2.3 Species Distribution Models (SDMs)

SDMs are a widely used class of statistical models that quantify the relationships between a species and its environmental determinants (Svenning et al., 2011). While these models may sometimes include mechanistic or process components, they usually are correlative models that

use supervised statistical learning algorithms to approximate the functional relationship between species occurrence and environmental covariates (Elith & Leathwick, 2009). Used extensively in both academic and management contexts, SDMs have been shown to provide reliable estimates of climate-driven range shifts when compared to independent datasets (Guisan & Zimmerman, 2000; Guisan et al., 2006). Widespread availability of powerful statistical software and large databases of environmental and occurrence data have led to increased popularity of these techniques in recent years (Franklin, 2010; Svenning et al., 2011). Citations of SDM-focused studies outpaced the field average (National Science Board, 2016) by 3.8% per year between 1997 and 2015, according to an analysis of publications in Web of Science (Fig. 3).

SDMs use a learning algorithm, along with occurrence records and environmental covariates, to approximate the functional form of the species niche that can be used to test ecological hypotheses or to predict to future scenarios. Hutchinson (1957) characterized a species' *fundamental niche* as an *n*-dimensional hypervolume that defines the environmental spaces where the intrinsic population growth rate of the species is positive (Williams & Jackson, 2007). The *realized niche* describes the subset of environmental space that the species actually occupies at some point in time and is smaller than the fundamental niche due to competing biotic interactions with other species. SDMs, through their reliance on observational data, approximate the species' realized niche (Guisan & Zimmerman, 2000; Miller et al., 2007; Soberón & Peterson, 2005). Hence, a key uncertainty associated with SDMs is their possibly incomplete representation of the fundamental niche space and the validity of derived predictions of species distributions under future or past climate changes. The inclusion of fossil data in the model fitting process can increase the likelihood that calibration captures the fundamental niche by

exposing SDMs to states of the climate system not present on Earth today (Veloz et al., 2012; Nogués-Bravo, 2009).

Because of their relative ease of use, SDMs have been widely used by biodiversity conservationists to prioritize habitat protection and to predict species responses to past and future environmental change. SDMs are often used to confirm ecological hypotheses by comparing hindcast projections with the fossil record; for example, supporting hypotheses on the extinction of Eurasian megafauna (Nogués-Bravo et al., 2008; Svenning et al., 2011), identifying late-Pleistocene glacial refugia (Fløjgaard et al., 2009; Keppel et al., 2011; Waltari et al., 2007), and assessing the effect of post-glacial distributional limitations and biodiversity changes (Svenning et al., 2008). SDMs are sometimes combined with genetic, phylogeographic, and other methods to develop a complete assessment of a species' biogeographical history (e.g., Fritz et al., 2013). In the context of contemporary environmental change, SDMs have been used to assess the effectiveness of modern reserve planning (Araújo et al., 2004), predict the distribution of endangered (Thuiller et al., 2005) and invasive species (Ficetola et al., 2007; Václavík & Meentemeyer, 2009; Smith et al. 2013) and ecosystems (Hamann & Wang, 2006), and evaluate the effectiveness of conservation planning for the future (Loiselle et al., 2003).

SDMs rely on three assumptions. First, SDMs assume niche conservatism -- that the niche of the species remains constant across all spaces and times (Pearman et al., 2008). This assumption disregards niche evolution, based in part on evidence that species typically demonstrate niche conservatism on multi-million year time scales (Peterson et al. 1999), although other studies of rapid evolutionary processes may challenge this assumption (Pearman et al. 2008). Second, SDMs assume that species are at equilibrium with their environment (Nogués-Bravo, 2009), being present in all environmentally suitable areas while being absent

from all unsuitable ones. Given dispersal limitations and interactions among species, this may rarely be true. For example, many European tree species appear to be still limited by postglacial migrational lags (Svenning et al. 2008). Finally, SDMs must account for extrapolation to novel climates for which there is no contemporary (or geological) data (Radeloff et al. 2015), which is a challenge given that many future climates are likely to lack current analogs (Williams and Jackson 2007). Inductive learning accuracy declines when predicting cases not within the range of values used in training. Fitting SDMs with fossil data increases the likelihood that climatic assemblages will be included in the training data (Veloz et al., 2012; Nogués-Bravo, 2009), though the problem of projecting models onto novel future climates continues to be a major challenge to their application.

2.3.1 A Taxonomy of Species Distribution Models

SDMs range in complexity from simple algorithms that characterize a ‘climate envelope’ for a species (Guisan & Zimmerman, 2000) to multivariate Bayesian techniques that use Markov Chain Monte Carlo simulations (MCMC) to develop probability distributions around projections and parameters. While all SDMs simulate responses to climatic gradients, SDM algorithms can be broadly grouped into data-driven and model-driven categories (Franklin, 2010). The data-driven/model-driven dichotomy is introduced in Hastie et al. (2009) and differentiates between ‘statistical’ or ‘parametric’ (model-driven) and ‘machine learning’ or ‘nonparametric’ (data-driven) algorithms. Here I add, as a third category, the burgeoning set of methods that employ stochastic, probability-based Bayesian methods because of these models’ structural differences, assumptions, and handling of uncertainty (Table 1). Many studies have assessed variation among models (Araújo & Guisan, 2006; Elith et al., 2006) and parameterizations (Araújo & New, 2007; Thuiller et al., 2008; Veloz et al., 2012).

SDMs, and supervised learning techniques more broadly, must be calibrated against observational data prior to being used for predictions. During the calibration stage, SDMs use a set of training examples, $T=(x_i, y_i), i=1,2,\ldots,n$, where both *x* (environmental covariates) and *y* (species presence) are known, to approximate the real relationship between the two, f, with the learned approximation function, $\hat{f}$. The learned function minimizes a loss function based on the difference between the real and predicted value, $y_i-\hat{f}(i)$. Each training example (x) is composed of a p-dimensional vector of covariates, $x_i=x_{1i}, x_{2i},\ldots,x_{pi}$, $p=1,2,\ldots P$ (Hastie et al, 2009). Model-driven algorithms make *a priori* decisions about the structure of f, while data-driven algorithms can adapt to fit any given design matrix (Hastie et al., 2009; Franklin 2010).

Model-driven SDMs fit parametric statistical models to a dataset, making assumptions about relationships between inputs and outputs, including linearity, error distribution, and independence. While these techniques can make poor predictions if the assumptions are not upheld, they were the first common form of SDM and continue to be widely used because of their strong statistical foundations and ability to realistically model ecological relationships (Austin, 2002). These models include boxcar algorithms, which build multidimensional bounding boxes around species presence in environmental space (Guisan & Zimmerman, 2000), as well as more complex methods, including generalized linear models (Guisan et al, 2002; Vincent & Haworth, 1983) and multiple linear and logistic regression (Franklin, 2010).

An increase in available computing power has spurred the development and application of data-driven learning algorithms, which take a non-parametric approach to approximating f. While not reliant on stringent assumptions about the relationship form, any particular portion of

parameter space depends on only a handful of input points, making the models highly sensitive to small changes in the input data (Hastie et al., 2009). In some cases, these models are shown to outperform their model-driven counterparts (Elith et al., 2006), and include genetic algorithms (Elith et al., 2006), classification and regression trees (Elith et al., 2008), artificial neural networks (Hastie et al., 2009), support vector machines (Drake et al., 2006), and maximum entropy techniques (Elith et al., 2010; Phillips & Dudík, 2008). MaxEnt, a maximum entropy algorithm for SDM and associated Java-based runtime environment is widely used and has been demonstrated to perform consistently, even on small sample sizes (Elith et al., 2010; Phillips & Dudík, 2008; Phillips et al., 2006). A targeted review of recent literature suggests that MaxEnt is the most popular SDM method in use today, appearing in over 20% of all SDM studies published after 2008 (Fig. 4). Recent critiques of MaxEnt, however, suggest that its performance may be questionable, particularly on datasets that cover only a small portion of a species' geographic range (Fitzpatrick et al., 2013). Data-driven models are often more computationally intensive than their model-driven counterparts because they usually take at least two passes over the input dataset to first process the data and then build the model (Hastie et al., 2009). Furthermore, data-driven SDMs are often combined with techniques like bagging -- building a collection of models based on random subsets of the input data -- and boosting -- combining many weakly predictive models into a single, highly predictive ensemble – which can further increase computational intensity (Hastie et al., 2009).

Bayesian methods have also been used to approximate f. Advantages of the Bayesian approach include the ability to include prior ecological knowledge in model formulation (Ellison, 2004) and the ability to estimate model uncertainty without the need for bootstrapping procedures (Dormann et al., 2012; Elith & Leathwick, 2009). With improved computational

infrastructure and better MCMC sampling algorithms, Bayesian methods have become increasingly popular (Clark 2005; Hegel et al., 2010). Golding & Purse (2016), for example, introduce Bayesian SDMs that incorporate Gaussian random fields, which they claim demonstrate both high predictive accuracy and ecologically sound predictions. Clark et al. (2014) use the full joint probability distribution of all taxa in an ecosystem to model both the climatic range limitations of a species and its biotic interactions with other species. Though it can be challenging for ecologists trained in classical statistics to transition to Bayesian approaches (Ellison, 2004; Hegel et al., 2010), software packages now exist for implementing Bayesian SDMs in already-adopted languages such as R (e.g., Vieilledent et al., 2012). Because Bayesian algorithms rely on generating and sampling complex distributions (using, e.g., Gibbs Sampling, No-U-Turn Sampling), they are computationally expensive, though numerical approximations and analytical solutions can sometimes reduce computational burden (Golding & Purse, 2016).

A review of recent literature suggests that the majority of contemporary SDM users employ data-driven models. 2200 of the most recent citations that met the query "*(Species Distribution Model) OR (Ecological Niche Model) OR (Habitat Suitability Model)*", and were published within the last four years, were obtained from the Web of Science in April 2016. 100 of these were randomly sampled using a random number generator and manually coded for the techniques used in the study. A single coder performed the analysis. Of the studies analyzed in this targeted meta-analysis, the overwhelming majority used data-driven models. Of 203 modeling runs described, 131 were data-driven, 38 were model-driven, and 1 was Bayesian (Fig. 4). An additional 33 experiments used unsupervised clustering analyses not suitable for prediction. Of all algorithms, MaxEnt was the most popular (64 runs). Algorithms in the model-driven category included generalized linear models (15), logistic regression (5) and multiple

linear regression (2). Data-driven techniques included boosted regression trees (16), generalized additive models (11), genetic algorithms (11), random forests (8), artificial neural nets (6), and multivariate adaptive regression splines (4). Figure 4 shows the results of the literature meta-analysis and the classification into the taxonomy described here. The citation for each paper reviewed is presented in Appendix A, table A1.

2.3.2 Computational Challenges and Species Distribution Models

Because of the current popularity of data-driven SDMs, I focus my analyses on this class of algorithms. Many authors have alluded to the limitations imposed by computational complexity, though few have estimated or tested those limits explicitly. For example, an often-cited review of novel SDM techniques noted execution times of up to several weeks for some modeling algorithms (Elith et al., 2006). Popular data-driven models were all extremely computationally intensive, including boosted regression trees (80 h), generalized additive models (17h), generalized linear models (17h), and MaxEnt (2.75 h). The authors suggest that performance could be improved if model building was split over multiple processing cores. While processor speeds have increased since 2006, models are still often unable to leverage multiple processors.

Methodological papers often advise against large modeling studies due to computational limitations. For example, Bolker et al. (2009) suggests that, when fitting a generalized linear mixed model (GLMM), if a user encounters insufficient computer memory or time limitations, the user should reduce model complexity, perhaps using a subset of the original dataset. Many authors warn of the computational expense of running SDMs, for example, noting that "considerable computational capacity is necessary for the development of models even for a single species" (Peterson, 2003). Thuiller et al. (2008) cautions "limits to the broad application of

this approach may be posed … by the computational challenges encountered in the statistical fitting of complex models." Modern computing infrastructure in theory can alleviate all of these problems, but in practice, the computational intensity of SDMs often forces a reduction in model complexity or scope.

2.4 Assessing Algorithm Execution Time

It is possible to theoretically estimate the upper, lower, and average run times of an algorithm using *asymptotic complexity analysis* (Knuth, 1976). In this exercise, the first-order term of an algorithm's increase in runtime is determined as the input to the algorithm is increased to infinity. The algorithm that is more efficient asymptotically will typically be the best choice for all but very small inputs (Cormen, 2009). While it is often impossible to produce a robust estimate of the lower-bound on runtime, given an infinite input, an estimate of the slowest or worst-case run time can usually be obtained by inspecting the structure of the algorithm and counting how many operations are required (i.e., *Big-O*; Cormen, 2009). Such theoretical complexity is often considered when considering algorithm scalability, though the actual runtime will vary with real-world inputs (Cormen, 2009; Goldsmith et al., 2007).

Empirical complexity studies have attempted to bridge the gap between asymptotic theory and real programs (Cannon et al., 2007). These studies use observations of algorithm runtime under different parameterizations and inputs to build models that predict the run time of future applications of the algorithm, seeking a method "with the generality of a Big-O bound by measuring and statistically modelling the performance … across many workloads" (Goldsmith et al., 2007, p. 395). Brewer (1995) describes an initial attempt to develop a statistical model for the run and compile time of algorithms in a C library. While many statistical and pattern recognition techniques have been attempted, simple linear regression between input size and execution time

has been shown to perform well in some cases (Fink, 1998). Empirical complexity models have become an important subfield of artificial intelligence and have important applications to algorithm selection (Hutter et al., 2014). Algorithms for solving very difficult (NP -Hard/ NP -Complete) combinatorial problems can exhibit high runtime variance among different problem instances. Empirical models can be used to select the algorithms that will most efficiently reach a solution (Hutter et al., 2014; Leyton-Brown et al., 2003; Hutter et al., 2013). Hutter et al. (2014) outline a comprehensive analysis of strategies and methods for empirical runtime models in the context of algorithm portfolio optimization. Parameterized algorithms can be treated the same way as nonparametric algorithms, by including model parameters as input features in the execution time model (Hutter et al., 2014). Nonlinear, tree-based methods for empirical performance modeling, such as random forests and additive trees, were shown to be superior to other methods because of their ability to group similar inputs together and fit local responses, so that some large outliers do not interfere with the predictions of other groups (Hutter et al., 2014, 2013).

Concurrently running programs, operating system tasks, and other processes may affect the execution time of a real computer program at any point in time. Changes in dynamic system state are stochastic and can cause unpredictable, non-linear and non-additive changes in program runtime (Jones & Kalibera, 2013; Lilja, 2009). Random variation in system state makes deterministic statistical modeling of hardware's influence on execution time difficult. These variations result from the way in which memory access patterns differ in space and time when small changes are made to the operating system state, timing device, or algorithm and its inputs (Lilja, 2009), and few attempts have been made to model them explicitly. However, several recent studies that took dynamic system state into account as a predictor of algorithm runtime

performed well when considering data center optimization (Sadjadi et al., 2008; Wu & Datla, 2011).

Models based on benchmarked runtime may provide an accurate estimate of an upper bound of execution time, though due to potentially large, nondeterminstic, system-induced variance in empirical results, it is important to perform the benchmarking experiment many times (Jones & Kalibera, 2013). However, failing to properly characterize the workload, running benchmarks that are too simplistic, or running benchmarks in inconsistent environments can lead to meaningless results (Dongarra et al., 1987).

3. General Problem Formulation

In the present study, I use benchmarking and empirical performance modeling to develop computation performance models (CPMs) for optimizing SDM workflows. The following framework presents an SDM workflow consisting of a series of steps that advance the SDM user towards her goal of obtaining scientific insight from a dataset. I assume the SDM modeler is a rational consumer in a supply- and demand-driven computing market and that the modeler has imperfect information regarding the species environment relationship. In this framework, the modeler will undertake several steps, including model computation, to minimize her costs, in both runtime and financial terms, and to maximize her utility, represented here as proximity to the knowledge of the true functional relationship, f, between environment and species presence. This proximity between f and $\hat{f}$ is measured as SDM accuracy (Simon, 1986). These steps are as follows:

1. Consider a pool of computing resources, H, that is characterized by multiple possible hardware configurations consisting of memory, CPUs, and any other component that influences computing power.

2. In a cloud computing market driven by supply and demand consumers face costs that are priced by the hour as a function of the computing power provided: $C_{Compute} = f(H)$. For example, Google's infrastructure-as-a-service (IaaS) cost surface closely tracks memory and CPUs (Fig. 5). Conversely, traditional, non-cloud computing, which tends to have more fixed hardware configurations and costs, with less consumer flexibility.
3. Costs associated with modeling application are multidimensional and are not limited to monetary costs. Additional costs may include the runtime of the model.
4. Every user of a modeling application has a particular set of goals for using it in the first place (Norman, 1984). Hence, we can conceptualize, for any given SDM, a finite set of use cases that fall within the bounds of existing or expected use (Carroll, 1999; Rosson, 2002). Let U be a vector of characteristics that fully describe the user's goals in these possible use cases. The components of U include user traits, such as experience with the model and interface, motivation, skill, and desired accuracy, as well as the number and parameterizations of each modeling run required ($E¿$.
4. Assume, in addition to computing the model, the user must also undertake a number of other pre- and post-processing steps in a scientific workflow. The total time elapsed during this workflow can be expressed as

$$T_{model} = T_{Input} + T_{Prep} + T_{Compute} + T_{Output} + T_{Interp}$$

Where T_{Input} represents the portion of time that is spent by user gathering the resources needed to model, such as time needed to find and download occurrence points and covariates. T_{Input} is a function of user expertise, the computing resources available to the user (how fast can data be discovered and downloaded?), and the experiment (what is the data?). T_{Prep} represents time required by the modeler to prepare the data for entry into an

algorithm, including data cleaning, projection, and conversion. T_{Prep} can vary widely among modelers, data source and quality, and user skill and motivation (Elith et al. 2006). $T_{compute}$ is the time spent computing the model and predicting to future climate scenarios. T_{Output} represents time needed to transfer the output from the location of the computation to the user, which may be non-trivial if the model is run remotely and large-volume outputs are transferred over a network. Finally, T_{Interp} represents the amount of time spent by the user evaluating model output and determining whether her goals were met during the modeling process. Like T_{Prep}, this term will be highly variable between model users and applications.

5. Single experiments can be combined together to form workflows, so that a user's time-to-goal for a workflow of N modeling experiments can be expressed as a function of the experiments and the computing resources on which they are run.

$$T_g = \sum_{i=1}^{N} T_{Model}(E_i, H)$$

6. Combining equations (2) and (5), the total time for a set of modeling experiments is the sum of total time of spent modeling, while the total monetary cost is the cost of provisioning computing resources for this length of time. The total workflow cost is then a function of the user and their set of required modeling experiments, the computing resources, and the cost surface that dictates the cost of these resources. Therefore, a multivariate cost function for all potential user activities is:

$$C(U, H) = f(T_g(U, H), C_{Compute}(H))$$

7. Each individual scenario, *u*, in *U*, the set of all possible scenarios, will have its own multidimensional cost curve that is subject to both the particular characteristics of the workflow and the cost surface imposed by the computing provider. If we select one specific

element of U and call it $u*$¿ , we obtain a unique cost function for this workflow that depends only on the computing resources used to fit the model. The minimum along this curve in multidimensional space corresponds to the optimal hardware configuration for use in the modeling scenario.

8. Multiple experiments may meet the user's goals, but have different costs. The optimal workflow for a user to pursue is that which jointly maximizes model accuracy while minimizing modeling costs. This corresponds to the lowest of all potential *u** minima. These costs include both the runtime of the model and monetary costs of provisioning the resources for the time required. If desired, a set of weights could be applied to preferentially weight accuracy, monetary cost, runtime, or other dimensions. Additionally, if a user faces constraints on time (e.g., latency requirements) or money (e.g., budget requirements), these can be incorporated to find the optimal configuration within the allowable space.

4. HYPOTHESES

The remainder of this thesis addresses three hypotheses based on this framework. Specifically, I hypothesize that:

1. for any SDM, there exists an optimal configuration of data and hardware that maximizes SDM accuracy while jointly minimizing the time and cost of modeling;
2. choice of hardware configuration will affect SDM runtime, but not the accuracy; and
3. data volume will affect both the runtime and accuracy of the SDM.

In the study, I characterize *data* as the number of training examples and the number of environmental covariates used to fit the model. I characterize *hardware* as the number of CPUs and amount of memory, in gigabytes (GB), of the VM on which the SDM is run. I use four data-driven SDM algorithms that are widely used and have shown competitive accuracy results in the

literature: multivariate adaptive regression splines (MARS, Leathwick et al., 2006), gradient boosted regression trees (GBM-BRT, Elith et al., 2008; Friedman, 2001; Natekin, 2013), generalized additive models (GAM, Guisan et al., 2002; Yee & Mitchell, 1991), and Random Forests (RF, Breiman, 2006; Elith & Graham, 2009). Random forests were specifically chosen because they are embarrassingly parallel, and are therefore expected to behave differently than their sequential (non-parallel) counterparts. Specifically, GBM-BRT, GAM, and MARS are all sequential algorithms that execute one instruction after another, and are not expected to experience significant execution time reduction on multiple cores. Random forests, on the other hand, are capable of building decision trees across multiple processors, and are therefore likely to be impacted by the number of CPU cores available for model fitting. Maxent is excluded because (1) it is written in Java, with only R bindings linking it to the R platform and (2) it is not open source, being instead distributed as a black-box algorithm. The experimental design is meant to mimic actual use cases and is therefore performed using popular implementations of the algorithms in R.

5. METHODS

5.1 DATA COLLECTION

5.1.1 SDM DATA PREPARATION

Systematic, controlled observation of SDM run time and accuracy on a complete set of data and hardware configurations was completed using the R statistical environment (R Core Team, 2016). Each SDM was fit with the standard R package for that model. Specifically, GBM-BRT models were fit using the *dismo* package version 1.1-1 (Hijmans et al., 2016), GAMs using the *gam* package, version 1.12 (Hastie, 2015), MARS using the *earth* package version 4.4.4

(Milborrow, 2016), and RF using the *randomforest* package version 4.6-12 (Liaw & Wiener, 2002).

Each SDM was fit using fossil pollen occurrence data obtained from the Neotoma Paleoecology Database in April 2016. Neotoma was selected as the provider of occurrence data due to its rich coverage in space and time in North America since the last glacial maximum. However, Neotoma is just one instance of occurrence data and similar analyses could be undertaken with other databases, such as GBIF or PBDB. All records for the genera *Picea* (spruce), *Quercus* (oak), *Tsuga* (Hemlock), and *Betula* (birch) were downloaded in R using the neotoma package (Goring et al., 2015), and filtered to include only those records dated to within the last 22,000 years and located in North America. For each record, the latitude, longitude, age, and relative abundance of the taxon was retained and stored in comma-separated text format.

Climatic covariates were obtained from downscaled and debiased Community Climate System Version 3 (CCSM3) model simulations for North America (Lorenz et al., 2016). Post-processed model output was obtained in NetCDF format with a 0.5-degree spatial resolution and decadal temporal resolution for the last 22,000 years. Bioclimatic variables (BV, O'Donnell & Ignizio, 2012) were calculated for each timestep using the biovars function in the dismo R package (Hijmans et al. 2016). BV values were then extracted for the space-time location of each fossil occurrence. The dataset was then filtered to include only the six least correlated BV covariates, using the variance inflation factor as a metric of multicollinearity (VIF, Obrien, 2007). The variables retained were BV2 (mean diurnal temperature range), BV7 (annual temperature range), BV8 (mean temperature of wettest quarter), BV15 (precipitation seasonality), BV17 (precipitation of warmest quarter), and BV18 (precipitation of driest quarter).

Downscaled future climate layers for the year 2100 CE were obtained for the HadCM3 climate model (Lorenz et al. 2016), for the CMIP5 RCP 8.5 scenario, which assumes high population, moderate economic growth, and a sustained dependence on fossil fuels (Riahi et al., 2011). These layers were processed as above.

5.1.2 Computing Infrastructure

Google Cloud Compute Engine (GCE) cloud-based virtual machines (VMs) were used for all model runs. Google's platform was chosen over other public cloud vendors because of its ability to create custom hardware configurations that adhere to user-defined specifications. Other vendors (e.g., Amazon Web Services) provide more predefined instance types, but do not support the creation of an instance with arbitrary hardware.

The experimental system is illustrated in full in Appendix B. In brief, a master node-compute node infrastructure was devised so that a single server monitored the progression through the experimental design and controlled the provisioning of computing nodes. The master node (i.e., a single cloud-based VM) ran a python control script attached to a centralized MySQL relational database via a Node.js API. The database contained the parameters for all the experiments to be undertaken, including both hardware requirements and algorithm parameters. The control script drew rows at random from the database and executed the initialization of a computing node (i.e., a separate cloud-based VM) with the corresponding hardware configuration using the GCE API. In many cases, to facilitate experiment efficiency, many computing nodes were simultaneously online, though concurrency was limited due to GCE account limitations. The computing nodes all ran Debian Linux 8. All experimental data (e.g., occurrence records, environmental layers, application code) required to compute the SDM were stored in a private GitHub repository and were transferred to the fresh VM using Git. Once

booted and provided with data, the computing node automatically ran the SDM using the assigned algorithm. Upon completion, the node communicated the runtime and accuracy back to the central database on the master node, then was released and decommissioned.

5.2 Estimating and Modeling SDM Runtime, Cost, and Accuracy

Once the hardware configuration (CPUs and memory) and the data parameters (number of covariates and number of training examples) were communicated to the computing node, the set of pre-processed occurrence points was partitioned into a testing set (20%) and a training set (80%) of the total number of training points. Environmental covariates were selected at random from the five potential layers.. An SDM was fit to the training data, assessed for accuracy, and then projected to the modeled future climate. The covariates randomly entered the model, eliminating any ordering effect that might be present if a single order was used Accuracy was evaluated using the testing set and quantified using the Area Under the Curve (AUC) statistic. Runtime (in seconds) was estimated within R using the proc.time function. No database I/O was done inside the timing script, so network connection speed is not expected to have influenced the results.

In total, 26,730 experimental trials were made, with each trial consisting of a particular combination of CPU cores, server memory, number of training examples, number of environmental covariates, and number of cells in the prediction layers. Configurations were chosen to maximize the parameter space covered in the analysis while maintaining at least three replicates per configuration. Where feasible (see “Limitations”), more replicates were made.

Once data collection was completed, SDM runtime and accuracy were modeled using Bayesian additive regression trees (BART), fit with the bartMachine R package, version 1.2.3 (Kapelner & Bleich, 2016). This Bayesian learning model fits a probability distribution for the

response at each leaf node, rather than the standard single maximum likelihood estimate, as in traditional regression tree implementations. A boosted ensemble size of 50 trees was used, and models were fit using default priors on the parameters and hyperparameters as suggested by Kapelner and Bleich (2016) (described in detail in Appendix C). Runtime and accuracy were modeled separately for each SDM. Runtime was modeled on a log scale (log-seconds), which improves predictive skill for on high-variance datasets (Hutter et al., 2014). The observed runtime and accuracy data for each SDM was randomly split into a training set (80%) and testing set (20%) for evaluation. 1250 MCMC iterations were performed, each of which built an entire additive model ensemble of 50 trees. The first 250 iterations were discarded as burn-in, leaving 1000 posterior samples to analyze and evaluate.

The predictive skill of the runtime and accuracy models was evaluated using the mean squared error (MSE), the r^2 statistic between observed and predicted values from the mean of the posterior distribution, and the standard deviation of the prediction posterior. Model results were also visually assessed by plotting the predicted values against the observed data and qualitatively assessing deviations from the y=x line.

The influence of each predictor in the runtime and accuracy models was evaluated by leave-one-out cross-validation, in which models were separately built using four of the five predictors. Each predictor was left out of a model in turn, and the r^2 of the subset model was evaluated and compared to the r^2 of the full model. The reduction in r^2 was interpreted as the predictive strength of the left-out variable.

5.3 Optimal Prediction

Prediction of the optimal data-hardware configuration for each SDM followed a four-step process (Fig. 6). First, the accuracy model was used to identify the data configuration that

maximized accuracy. Second, the performance model was used to predict the execution time of the accuracy-maximizing model run under various hardware configurations. Third, multidimensional hierarchical clustering was used to assemble groups of configurations. Finally, the hardware cluster with the lowest runtime, cost, and uncertainty was selected as optimal.

For the first step, the accuracy model was used to predict the accuracy of 500 regularly spaced configurations for a given SDM. These configurations included training dataset sizes between 0 and 10,000 occurrences at an interval of 100 and covariates between one and five. Hardware configurations were chosen between 1 and 24 CPU cores at an interval of 1 core (24 conditions) and 1 and 24 GB of memory at an interval of 2 GB (12 conditions), resulting in 288 unique CPU and memory configurations. Predictions were sorted, first by descending order of accuracy, then by ascending order of training dataset size, and finally by ascending number of covariates. Once ordered, the first configuration was chosen. Hence, given equal accuracy, the configuration that requires the smaller training dataset was preferentially chosen.

In the second step, the accuracy-maximizing data configuration, and thus expected accuracy, was held constant and used as an input for the performance model. The performance model was used to predict the runtime of an SDM experiment for the set of 288 configurations. Candidate configurations were chosen from GCE-allowed custom instance types, and covered the parameter space between 1 and 24 cores and 1 and 24 GB of memory. Each runtime prediction was evaluated as 1000 samples from the posterior distribution provided by bartMachine. The mean of the distribution was used to calculate runtime cost, using GCE rates (Cost = $0.03492*CPU + $0.00468*GB; Google, Inc, 2017), and the standard deviation was used as a measure of prediction uncertainty. The dataset was subsequently scaled and centered using the R function scale.

The runtime predictions were then clustered using complete linkage hierarchical clustering on three axes: runtime, run cost, and prediction uncertainty. The results were plotted as a dendrogram and demarcated into clusters using the silhouette rule for maximizing within-cluster homogeneity while maximizing out-of-cluster variance (Rousseeuw, 1987).

Finally, the clusters were plotted in time-cost-uncertainty space. The hypothetical ideal scenario would involve no time, no cost, and no uncertainty, which occurs at the origin of these three axes. The Euclidean distance between the centroid of each cluster and the origin was calculated and the cluster with the smallest distance to the origin was identified as the optimal set of hardware configurations for that SDM. The Euclidean distance metric normalizes each dimension by its mean and standard deviation, eliminating the problem of optimizing using data with different units and variances.

6. RESULTS

6.1 OPTIMAL DATA CONFIGURATION

For most SDMs, the simulations with the highest predictive accuracies have large training datasets and many covariates (Fig. 10). In contrast to other SDMs, MARS achieves its highest predicted accuracy with only 1000 training examples, and only the addition of more covariates can increase accuracy. However, for all SDMs, additional covariates continued to increase accuracy up to the five covariates included here.

6.2 CPM PERFORMANCE

Predictive models of runtime were skillful when compared to a holdout testing set (Table 2, Fig. 7). While results varied across SDM classes, the models for each SDM explained more than 50% of the variance in the runtime data ($r^2>0.5$¿ . The CPMs with the highest skill were

for GBM-BRT and MARS, with r^2 values of approximately 0.96, and an MSEs of approximately 0.05 log-seconds. The estimates from the runtime models were tightly constrained, with low mean standard deviation of the prediction posteriors, ranging between 0.01 and 0.035 log-seconds, suggesting low uncertainty in the predictions.

For the runtime models, GAM and RF had lower r^2 values than the other two models. Interestingly, however, the GAM runtime model had a relatively low MSE (0.01 log-s) compared to the other models, while RF had the highest MSE of all models (0.64 log-s). Several factors likely contributed to the lower explanation of variance by GAM and RF. The GAM trials tended to converge within several seconds (maximum 10.3s), regardless of data or hardware configuration, exposing these trials to a stronger influence by low-level system processes not explicit in the runtime model and resulting in a higher-variance dataset with lower predictive power. In contrast, the other three SDMs took minutes to hours to terminate (maximum: GBM-BRT, 5285.0s). Secondly, the GAM (training set size = 2,636) and RF (2,861) models are fit with smaller datasets than the GBM-BRT (9,256) and MARS (6,632) models, which may partially explain their relatively lower predictive skill. Nonetheless, all models explained a majority of the variance in SDM runtime. Note that the difference in training set size was due to the time and financial pressure described in the “Limitations” section.

The accuracy models were generally more skillful than the runtime models in terms of r^2 (Table 3, Fig. 8). While ensemble size, tree depth, and other hyper parameters, not included in this modeling exercise, can affect learning accuracy (Hastie et al., 2009), the models included here without those parameters still proved skillful. The RF accuracy models was the best performing of the four, with an r^2 of of 0.98 and an MSE < 3.5×10^{-5} AUC. The lowest performing accuracy model was the GBM-BRT, with an r^2 of 0.87 and an MSE of 2.45×10^{-4}

AUC. All accuracy models indicate low uncertainty and well-constrained posterior estimates, with posterior standard deviations ranging from 0.0006 to 0.005 AUC. GAM predictions have the highest uncertainty associated with them (0.005 AUC), again perhaps due to small training set size.

6.3 Controls on SDM Runtime and Accuracy

The factors that control SDM runtime vary widely among algorithms (Table 4). One of the most important contributions is the number of training examples with which the algorithm is fit. The influence of this term on GBM-BRT, GAM, and RF runtime is large (>0.36 reduction in r^2). As data-driven algorithms, these SDMs rely heavily on creating structure from the given input dataset, and their runtime should be tied asymptotically to the number of training examples (Hastie et al., 2009). The number of environmental covariates does not seem to be an important predictor of runtime for any SDM; only GBM-BRT is influenced by this predictor, and only slightly. This finding is surprising because theoretical complexity suggests that learning algorithms are often asymptotically influenced by both training examples and covariates (Hastie et al, 2009; Cormen 2009). However, under real workloads, it appears that the number of covariates does not strongly influence runtime. In contrast to other SDMs, GAM runtime was weakly influenced by number of training examples and strongly controlled by the number of cells on which to predict the fitted model. This SDM's learning time, as described above, is quick; nearly all of the total time during each experiment was spent in the prediction phase.

Among SDMs, RF shows the strongest sensitivity to number of CPU cores, with 5.55% of variance explained (Table 4). For GAM, GBM-BRT, and MARS, CPU capacity accounts for less than 1% of total variance. The higher sensitivity of RF is consistent with SDM model structure: RF models build many independent trees and so can take advantage of parallel

computing configurations. The RF algorithm has diminishing marginal returns when run on increasing numbers of processors (Figure 11). The difference between a model run sequentially (one core) and one run with two cores is large, while the marginal benefit of adding the 16th or 24th core is comparatively small. RF efficiencies vary by the number of training examples, but range between 0.05 and 0.4 at 25 cores.

SDM model accuracy is also closely tied to training dataset size (Table 4).The number of training examples and covariates together accounted for >50% of the predictive skill in all SDMs. Indeed, for RF and GBM-BRT, training data volume accounted for nearly 80% of the model's total predictive skill. As seen in the runtime model, GAM differs from the other three SDMs, and is only sensitive to the number of covariates in the training set. As hypothesized, hardware configuration has little influence on SDM accuracy.

6.4 Hardware Optimization

The optimization analyses suggest that SDMs require few CPU cores (Fig. 9, 12). GBM-BRT is best suited to only one CPU core, while the GAM optimum lies at 3 CPUs. As suggested by moderate dependence on CPU cores, the optimal configuration for RF is between four and seven CPU cores.

Memory requirements are generally low (Fig. 9, 12). RF and GBM-BRT are both optimized at only one gigabyte of memory. Hence, the optimal configuration for RF should include time on several cores but relatively little memory. GAMs are best suited to one to 20 GB. The GAM clustering suggests very little memory dependence; one GB of memory is as suitable for GAM as 25 GB.

The MARS optimization procedure yielded strange and as yet unexplained results. The optimization analyses suggested that MARS require anywhere between 1 and 24 cores, and 16

GB of memory. A first working hypothesis was that an error in sampling design had oversampled some hardware configurations, potentially causing an artificial bias. To test this hypothesis, the MARS hardware configurations used to train the runtime CPM were subsampled into a dataset with one observation per configuration. This reduced the dataset size from 6,632 observations to 617 observations.

However, upon fitting the reduced CPM and rerunning the optimization routine, an optimal configuration of 16 GB of memory and between 1 and 25 cores was still reported. These results are peculiar for two reasons. First, the assessment of the CPM drivers suggests that the CPM does not depend on memory to make predictions (Table 4). Indeed, information about the amount of memory of the configuration yields only 1.7% increase in CPM skill. Second, the optimization does not sequentially favor hardware configurations with higher amounts of memory; rather, configurations with less or more than 16 GB of memory are found to be suboptimal, and only those with exactly 16 GB are found to be optimal. Should memory be of true importance, it would be logical to expect that the configurations would become closer to optimal as additional memory is added to the configuration. At the present time, it is unclear why this odd preference for 16 GB memory is occurring, and only in the MARS model. For this reason, this finding will be left as unexplained, and more work is needed to uncover the reason for this strange behavior.

7. Discussion

7.1 Overview

These findings show how the general optimization framework developed here can be applied to identify the optimal data-hardware configuration for biodiversity modeling. As

biodiversity database growth continues and cloud computing gains popularity among researchers, more work is needed to optimize computing platforms. A key finding of this work is that many of the most accurate and widely used SDMs are not well structured to harness the flexible computing power enabled by cloud computing. The optimization framework is general, and could be applied to other ecological models.

These results support all three of the hypotheses developed at the outset of this thesis. First, for each model, after finding the configuration that maximizes model accuracy, there is an optimal region for which financial and runtime costs are jointly minimized. Second, hardware configuration appears to minimally influence model accuracy. Finally, data volume, in both number of training examples and number of environmental covariates, influences both the time required to fit SDMs and SDM accuracy. The dependence of both runtime and model accuracy on data volume therefore creates a tradeoff among data volumes that support more accurate SDMs versus faster SDMs.

7.2 R-Based Biodiversity Models and High Performance VMs

These findings suggest that many current R implementations are generally insensitive to the high performance hardware made available by cloud computing. The R implementations of GAM, GBM-BRT[3], and MARS are all fit sequentially, one instruction after another, on a single processor. The algorithms underlying the corresponding R functions are not easy to parallelize, because the model building process involves loops over the entire dataset, a procedure not easily split into smaller tasks suitable for multiple processors (Hastie et al., 2009). A sequential model should theoretically have little dependence on CPU cores, since R may use only one core during

3 The GBM-BRT code in the Ridgeway (2015) gbm package underlies the implementation of boosted regression trees in the dismo package, common in SDM applications (Hijmans et al., 2016). A review of the gbm code suggests that model validation can use multiple processing cores, but model fitting is done sequentially.

model building. Empirical results support this claim, showing that the number of CPU cores explains less than one percent of the variance in these three SDMs' runtimes. Both GBM-BRT and GAM have clearly defined optimal configurations at a low number of CPU cores. In both cases, higher CPU configurations provide no advantage .

Conversely, the RF algorithm can be easily split across into small subtasks, and so can easily leverage additional cores in powerful hardware configurations. Specifically, individual tree building is done in parallel on multiple cores, after which the model ensemble is assembled and evaluated on a single processor. The maximum expected accuracy is approximately that of GBM-BRT, but can be achieved in a fraction of the time. Both SDMs achieve maximal accuracy with 10,000 training examples and 5 covariates. However, when parallelized, random forests can be fit in between 10% and 30% of the time to fit a GBM-BRT model with the same data. Thus, the economically rational researcher would therefore be best served by employing an RF, run in parallel across many cores, rather than waiting for the GBM-BRT to converge.

The RF optimal hardware configuration demonstrates the tradeoff between monetary cost and time. Because the algorithm can effectively use of additional CPU cores, configurations with additional cores have decreased execution time, but are charged a higher rate. Conversely, VMs with fewer cores take additional time to fit, but have a lower rate. When taken together, the two balance out -- illustrating the tension between cost and time when considering hardware provisioning for parallel algorithms.

RF, like other algorithms designed for parallel computation, is subject to diminishing speed returns as it is spread across additional cores (Gustafson, 1988). All algorithms must run, at least in part, sequentially, e.g., during setup and/or ensemble combination. Because of the portion of code executed on a single processor, it is impossible to obtain an infinite speedup,

even across infinite processors (Amdahl's Law, Amdahl, 1967). Inter-core communication increases as additional processors are added -- eventually causing the benefits of parallelization to be offset by the extra overhead. This phenomenon is typically measured in an algorithm's parallel efficiency, the ratio of serial (T_1) to parallel (T_N) runtimes of the algorithm, divided by the number of cores (N), given as:

$$E = \frac{\frac{T_1}{T_N}}{N}$$

Furthermore, no SDM responds to increased memory allocations on the VM. Although not tested rigorously, datasets exceeding 100MB, or several hundred thousand training examples, caused fatal crashes in R. R is known for poor memory management. Specifically, functions often create multiple copies of data objects in both built-in and external packages (Johnson, 2012). When data size becomes large, making in-memory copies is not possible without exceeding total allocation, resulting in program crashes. While packages exist to handle datasets too large to fit into an instance's main memory (https://cran.r-project.org/web/views/HighPerformanceComputing.html accessed October 10, 2016), SDM functions in popular packages (e.g., dismo) require significant modification before they can incorporate these tools. As data volume and memory requirements increase, SDM model developers should consider porting algorithms from R to more memory efficient software, such as standalone Java- or C-based applications, either on a desktop (e.g., Maxent) or in the cloud.

7.3 Extensions of the Optimization Approach

The unconstrained maximization routine is useful when neither data nor runtime are externally limited. However, in many real-world situations, data availability or runtime requirements may constrain acceptable model performance. Indeed, many SDM analyses

consider datasets with less than 100 occurrences (Wisz et al. 2008). Constrained optimization, either on runtime or data volume can be useful in these situations. In this analysis, the space of potential data configurations would first be truncated to include only those configurations possible under the constraint (i.e., configurations with less training examples than the number in the dataset). The accuracy-maximizing point is then selected from the subspace, rather than the full space, to reflect a point feasible within the data limitations. The optimization then continues as above.

One can also place a hard maximum bound on SDM execution time or cost. For example, consider a cloud-based SDM application that computes SDMs for arbitrary datasets remotely and returns the results to a client over the Internet. Users of interactive web applications are apt to lose interest and turn their attention elsewhere if the application takes more than several seconds to respond (Roth, 2013). If a maximum-accuracy experiment for GBM-BRT is requested, the client faces a response time of over 1 hour and would quickly stop interacting with the application. It would benefit the application developer, then, to limit the time it takes to complete the model run so that (a) their costs are minimized and (b) they retain the user's interest and business. To accomplish this, a large set of potential configurations is generated and the runtime for each is predicted using the performance model. Those configurations that have predicted runtimes that fall within the constraint are fed into the accuracy model. These results are then sorted by accuracy to yield an estimate of the highest-accuracy configuration that would fall below the runtime threshold. By constraining the optimal with a hard maximum bound on the time it takes to compute the model, the management can provision the cheapest resources, return results of high accuracy, and keep their audience engaged.

This approach could also be extended to preferentially weight run time, run cost, or prediction uncertainty. However, a given researcher may care differently about each factor. For example, she may care most about achieving low cost, next about prediction uncertainty, and finally about modeling runtime. Weighting each axis would allow the user customize the optimization to meet her own needs.

7.4 Limitations of the Framework

This approach has several important limitations. Perhaps most importantly, while a real SDM workflow contains various pre- and post-processing steps (eq. 1), the analyses here focus only on computing time ($T_{Compute}$). Overall workflow time depends on many factors that may be difficult or impossible to model, including data availability and user skill and motivation. Future work could focus on modeling these factors in a form that could be incorporated into this predictive modeling framework. Furthermore, the hardware analysis includes only two components, CPU cores and memory. Other hardware components, such as CPU clock rate, may improve model results, but are difficult to manipulate experimentally.

A second limitation of the approach described here is that these analyses are limited to virtual computing instances hosted on Google Cloud Compute Engine (GCE), rather than real-world physical machines, limiting the conclusions that can be drawn about optimization solutions for physical hardware configurations. Nonetheless, this uniform experimental design strengthens the benchmark estimates of computing time, by providing a consistent computing environment unaffected by other tasks or concurrent programs (Dongarra et al., 1987). Similarly, using GCE VM instances limits this experiment to only the processors provided by Google, which may be changed in the future. At the current time, GCE provides only one processor type for the VMs I used, a 2.6 GHz Intel Xeon E5 processor.

This work is limited to the analysis of data-driven SDMs, because systematic literature review suggests that a majority of SDM users use these methods. Similarly, there are known limitations to the language design and speed of R (e.g., Morandat, 2012), the platform is the most widely used for SDM analysis, so this analysis focuses on the most popular R implementations of these SDMs.

A final limitation was computational cost. In order to gather enough data and replicates to develop predictive models of SDM runtime and accuracy, I limited the number of models running longer than several hours and the number of replicates. Similarly, experiments on VMs with expensive hardware configurations were limited to allow for more experimentation on less costly instances. More data collected in all portions of configuration space, particularly on larger training datasets and VMs with high memory and many CPUs, may improve the robustness of the results presented here.

Most importantly, the specific estimates of runtime, accuracy, and optimal computing configuration are likely to quickly become outdated as hardware capabilities continue to improve and pricing schemes change. The optimization framework (Figure 6), however, is general and robust to both changing hardware capabilities and costs. To incorporate new hardware configurations, additional data can be collected using methods similar to those described here, the models refit, and the predictions re-run. If other parameters (e.g., processor speed) remain the same, new data can be directly appended to the existing dataset. If not, an entirely new dataset should be collected. To incorporate new pricing schemes, only the third and fourth steps of the optimization (clustering and distance calculations) would need to be re-run using the new cost surface. Furthermore, the results presented here are likely to be robust between different cloud service providers. Because the data was collected on hardware dedicated to running the SDMs

with no concurrently running programs, VMs with similar specifications are expected to behave similarly, regardless of provider. However, because cloud instances are only partitions of physical hardware, total load on the shared physical server may influence model runtime. Two potentially interesting hypotheses are (1) to assess whether the time of day influences runtime, to assess whether times of high system usage, e.g., morning, evening, have significantly different runtime and (2) to assess whether the results vary among different cloud providers (e.g., Google, Amazon, Microsoft). Further work should consider these factors when implemented this framework.

Although these results are specific to the SDMs, parameterizations, and implementations described here, the framework could be applied to any predictive modeling workflow. This approach relies on algorithm inputs and hardware capabilities and has no intrinsic relationship to SDM. To extend the framework to additional algorithms or hardware or data components, a new set of empirical trials would be required to gather a dataset of runtime and accuracy. Care must be paid to completely and evenly covering the full parameter space. Even models with many parameters could be incorporated, by treating algorithm parameters as additional components (Hutter et al., 2014).

7.5 Cloud Computing in Biodiversity Modeling: Recommendations and Prospects

The observations collected here are primarily for models with fairly short runtimes and very low costs. Even the longest observations of runtime are only several hours, far short of the several weeks reported by Elith et al. (2006). However, as data volumes grow and modeling approaches to biodiversity problems become more common, even these short runtimes become formidable. Many studies now model hundreds or even thousands of species (e.g., Rezende et al., 2015). Some projects attempt to model entire biotas; for example, Candela et al. (2013) describe

routinely modeling and mapping distributions of over 11,000 marine species. Most contemporary SDM studies use multiple model classes, predict to multiple time periods, and use multiple climate scenarios. When fitting multiple models for thousands of taxa, spending several hours for each model becomes costly. Therefore, while the individual results presented here quickly add up for all but the smallest modeling activities typical in contemporary SDM literature.

The relatively minor contributions of hardware to SDM execution time, suggest that the sequential SDMs may not be good candidates for a transition to the pay-as-you-go, utility model of cloud computing. Because GAM, GBM-BRT, and MARS are all optimized with configurations of few cores and low memory, it may not benefit the SDM user to cloud-enable these SDMs. Rather, the user is likely better off using the lowest-cost hardware available. Provisioning additional cores or memory is unlikely to bring returns in execution time, reduce modeling cost, or increase prediction certainty. For these models, to achieve performance gains in a cloud-based system, a system would need to be developed that simultaneously provisioned multiple, isolated VM instances to run independently, each fitting a single SDM. To make this work automatically, efficiently, and without error would be difficult and require a significant amount of technical prowess.

RF, however, may be a good candidate for incorporation into a cloud-based runtime environment because of its native support for multiple-CPU parallelism. Because RF efficiency scales with training set size, it is well suited to the scalability provided by the cloud. The ability to scale the number of CPUs based on problem-specific features would be helpful to model users interested in reducing model runtime. Public cloud providers make scalability easily, allowing users to put code and programs onto a virtual hard disk and scaling the underlying hardware configuration up or down. In the context of SDM, researchers could configure their virtual

hardware and scale it to an efficient hardware configuration once an experiment has been designed. It should be noted that virtual machines like those provisioned through GCE often leverage hyperthreading -- logical partitioning of physical hardware – that may reduce the marginal benefit of each virtual core when compared to the additional of a physical core.

Of course, even for RF, the difficulty of the transition to a cloud-based solution may outweigh any benefits, particularly for small workflows. It is not a trivial task to provision and configure virtual hardware and install and prepare modeling software effectively on a cloud instance. However, for large modeling workflows with thousands of species and many prediction scenarios, for researchers experienced with cloud-based VMs, or for server-based SDM geoprocessing (e.g, Souza Muñoz et al., 2009) as a service (e.g., Granell, 2013), cost and time optimization will be helpful.

The framework developed here provides a well-grounded foundation for future study. Specifically, the framework could be used in testing bigger datasets. While the datasets in this paper conformed to the typical dataset size for SDM studies, occurrence datasets are becoming larger, and a study that applied the optimization framework to massive datasets would be beneficial in characterizing computational limitations and opportunities for very large datasets. Moreover, this framework could be used to test multiple cloud providers. Amazon Web Services, Google Cloud Engine, and Microsoft Azure all offer platform-as-a-service (PaaS) products that allow researchers to spin up virtual hardware of given specifications. While the technical specifications of the VMs are the same, it may be that these providers differ in their quality of service, due to load balancing and the underlying physical hardware. A study that investigated differences among public cloud providers would be beneficial for ecologists interested in migrating their workflows into the cloud. Finally, a study that examined a large suite of SDM

algorithms, such as all of those shown in Figure 4, would be interesting, to determine similarities and differences between data-driven, model-driven, and Bayesian SDM algorithms in terms of their optimal data-hardware configuration, accuracy, and runtime.

The sensitivity of SDM execution time to training dataset size suggests that popular SDM algorithms like those examined here may be unable to cope with the large datasets possible as biodiversity database size grows. Austin (2007) argues that a solid foundation of ecological theory is the most essential factor in correctly predicting species ranges and testing hypotheses with SDMs. Indeed, he claims that the ecological underpinnings of the statistics may be even more important than the statistical method itself. Elith & Leathwick (2009) follow, suggesting that additional improvements in species distribution modeling will come not from novel learning algorithms, but from the incorporation of more ecologically relevant information into the statistical modeling process, claiming, “further advances in SDM are more likely to come from better integration of theory, concepts, and practice than from improved methods per se.”

Due to rapidity of database growth, I contend that modelers should focus their effort not only on the incorporation of ecological realism, but also on optimizing existing and novel models to take advantage of parallelism, high performance libraries, and cloud computing. While ecological datasets may not have been “big” in the past, they are now, and scholars working with this data should take this into account when considering research priorities. New collaborations among ecological researchers, big data experts, and computer scientists, will prove fruitful in developing new technologies to better support biodiversity research. Specifically, both projects that implement low-level optimizations and higher level efforts that facilitate utilization of advanced computing technology by ecological models are important in improving the ability of forecasting models to leverage computation resources. New SDM model development efforts

should be undertaken to modify existing models to effectively leverage high performance computing infrastructure, multiple computing cores, effective memory management strategies, and scalability; for example, refactoring traditionally sequential data-driven algorithms to in parallel across multiple CPU cores simultaneously (GBM-BRT, Tyree et al., 2011). However, the development of new R-packages is only one step in advancing the landscape of cyberinfrastructure for ecological forecasting. The development of entirely new learning methods that are explicitly designed to work with big datasets and the complexities of ecological data is also a priority. Improvements at the computer-code interface, while not traditionally considered by ecologists, will have a large impact on the efficiency of biodiversity modeling. Together, these projects are key in improving the inference garnered from growing data streams; and allow scientists and managers to more effectively understand and prepare for biotic shifts in the coming decades.

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FIGURES

Figure 1: This figure tracks the growth in collection size of community biodiversity databases through time, for the Global Biodiversity Information Facility (A, left) and the Neotoma Paleoecology Database (B, right). A record is a single data point denoting presence, absence, or abundance of a taxonomic group at a spatiotemporal location. Date of accession (Neotoma) is the date that record was formally incorporated into the Neotoma Database. Date of record (GBIF) is the date the record was made, which may be prior to GBIF's incorportation in 2001, due to efforts to digitize existing observational accounts.

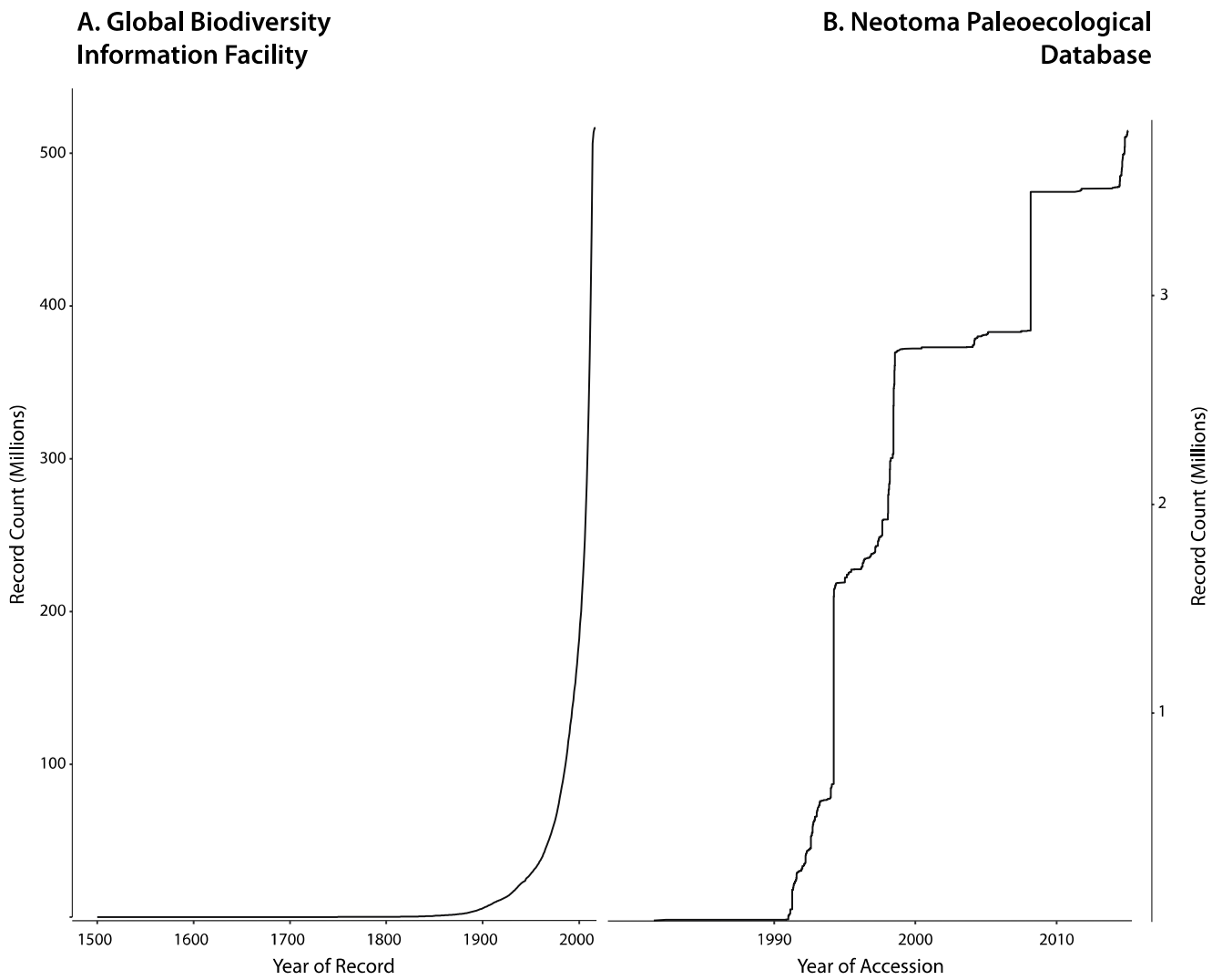


Figure 2: This figure shows the diversity of record types in the Global Biodiversity Information Facility (A, left) and the diversity of datasets in the Neotoma Paleoecology Database (B, right). The vertical axis in panel A shows millions of occurrence records, while the axis in panel B shows numbers of datasets, due to the different data models of the two databases. Due to the larger scope of the GBIF project, the categorization of database records (horizontal axis) is more general in A than in B.

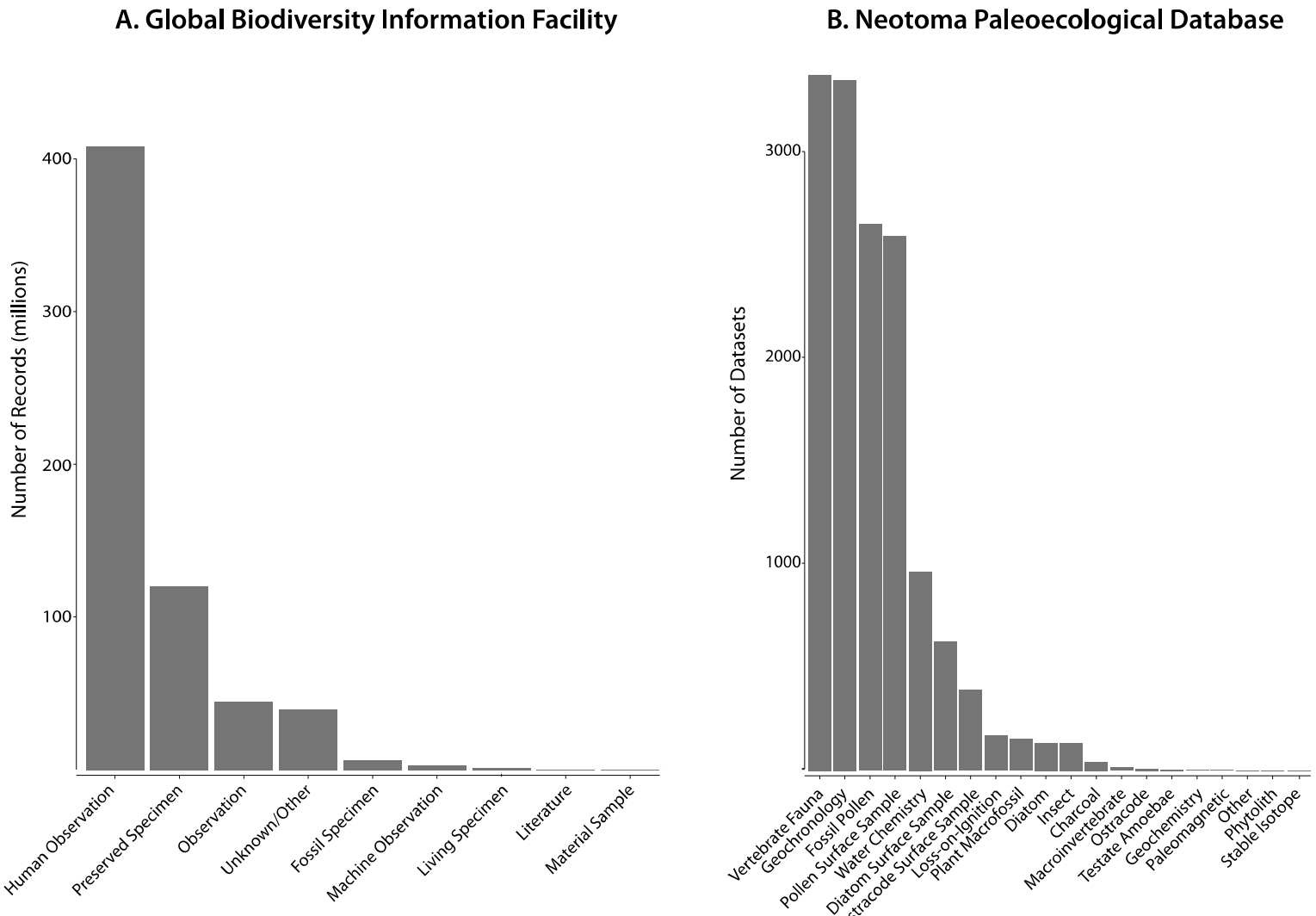

A. Global Biodiversity Information Facility
Number of Records (millions)
400
300
200
100
Human Observation
Preserved Specimen
Observation
Unknown/Other
Fossil Specimen
Machine Observation
Living Specimen
Literature
Material Sample
B. Neotoma Paleoecological Database
Number of Datasets
3000
2000
1000
Vertebrate Fauna
Geochronology
Fossil Pollen
Pollen Surface Sample
Water Chemistry
Diatom Surface Sample
Ostracode Surface Sample
Loss-on-Ignition
Plant Macrofossil
Diatom
Insect
Charcoal
Macroinvertebrate
Ostracode
Testate Amoebae
Geochemistry
Paleomagnetic
Other
Phytolith
Stable Isotope

Figure 3: Time series of the number of papers returned in a Web of Knowledge search for query “Species Distribution Model*” (blue), compared with average annual citation growth in science and engineering, as reported by the U.S. National Science Board (2016) (black).

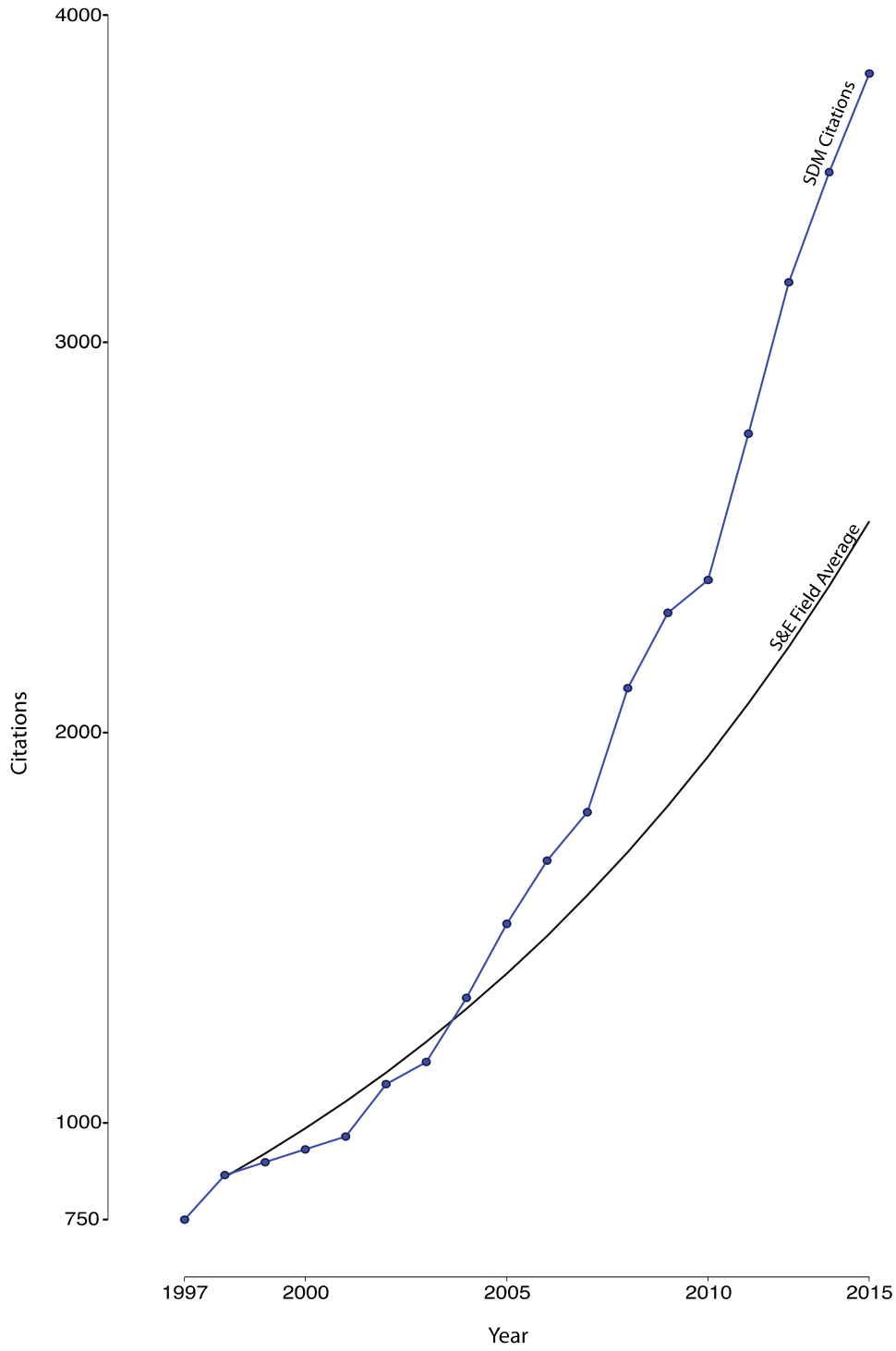

4000
3000
2000
1000
750
Citations
SDM Citations
S&E Field Average
1997
2000
2005
2010
2015
Year

Figure 4: This figure presents the classification of 100 recent SDM-focused studies into data-driven, model-driven, and Bayesian model types. Candidate studies were identified using a query to the Web Knowledge on (“Species Distribution Model*” OR “Ecological Niche Model*” Habitat Suitability Model*”), from which randomly chosen subset of 100 studies used for scoring. Scoring was based on Hastie et al. (2009), Franklin (2009), and Elith et al. (2006) and studies were scored their use of parametric/statistical methods, non-parametric/machine-learning models, Bayesian predictive models. Many studies employed multiple SDM runs, yielding more than 100 scored algorithm applications. Studies that used unsupervised modeling routines were scored into a separate category, because they cannot be used in prediction tasks.

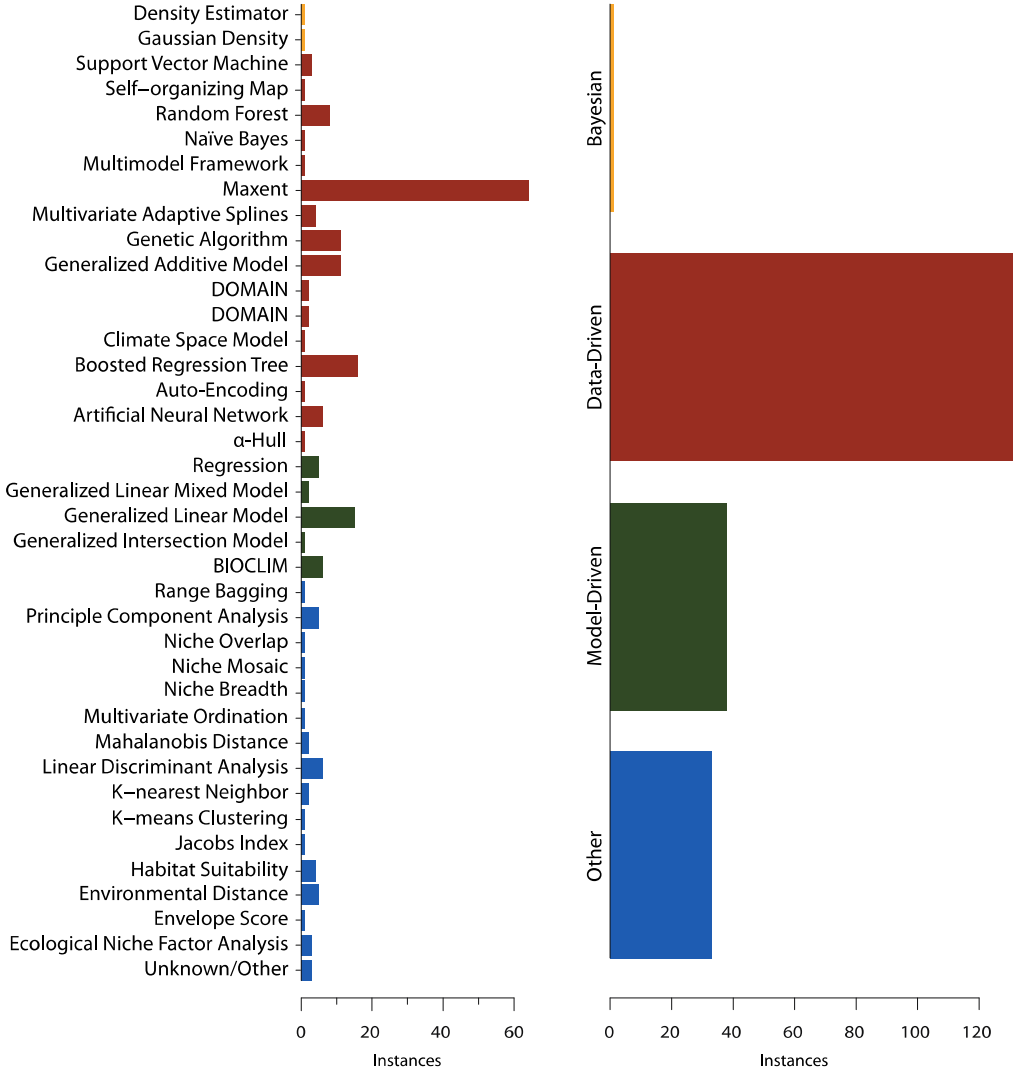


Figure 5: Plot of the Google Cloud engine custom virtual machine (VM) pricing scheme, showing the price surface faced by consumers of computing utilities as a function of the VM hardware configuration. Number of cores refers to the number of CPU cores dedicated to the VM. Memory refers to the amount of virtual memory dedicated to the VM, measured in gigabytes (GB).

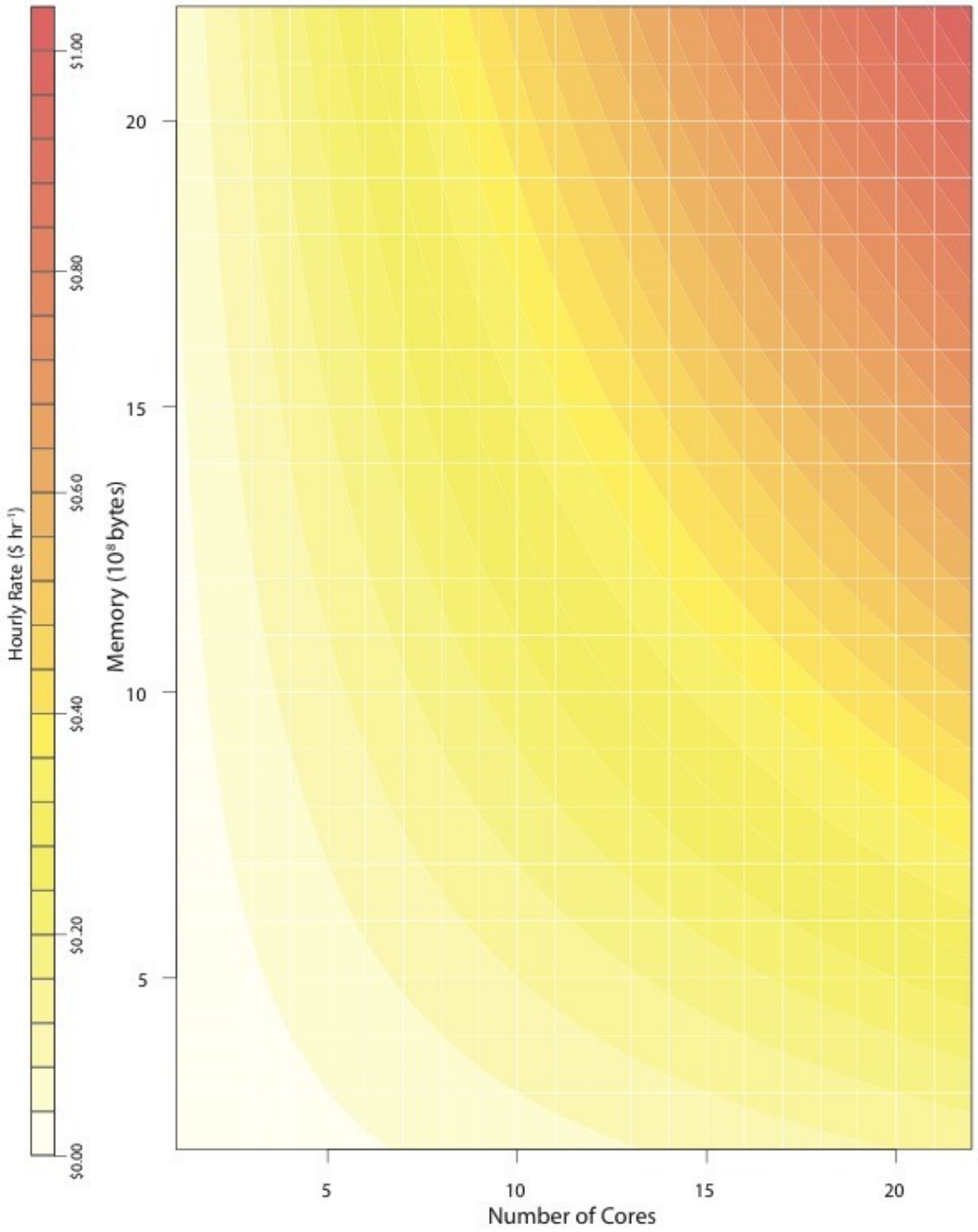
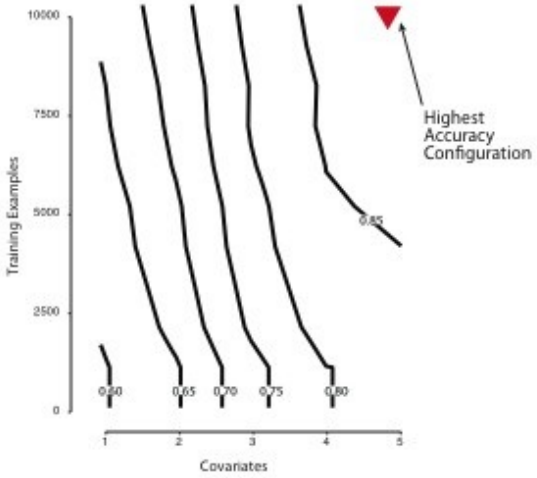
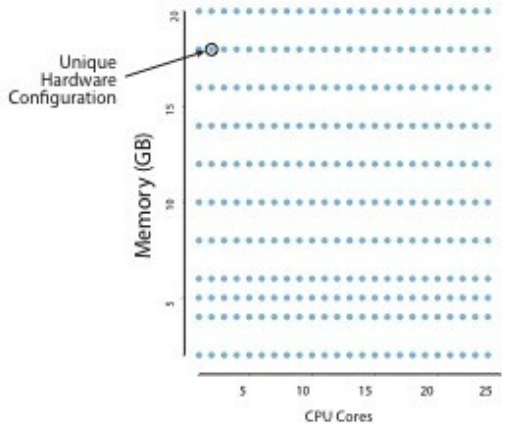

Hourly Rate ($ hr^{-1})
$0.00
$0.20
$0.40
$0.60
$0.80
$1.00
Memory (10^8 bytes)
5
10
15
20
Number of Cores
5
10
15
20

Figure 6: The general framework for optimizing the data-hardware configuration for an SDM forecasting model. 1. The configuration of training examples and environmental covariates that maximizes model accuracy is selected from a set of candidate configurations. 2. Using the runtime model, the execution time of that model run is predicted on a set of candidate hardware configurations, limited to VM instance types allowed on the Google Cloud Engine. 3. Complete linkage hierarchical clustering was performed on three axes: run time, run cost, and standard deviation of the prediction posterior. 4. The theoretical optimal hardware configuration would involve no time, no cost, and no uncertainty; therefore, the cluster whose multidimensional center is closest to the origin (0,0,0), is selected as the optimal set of hardware configurations.

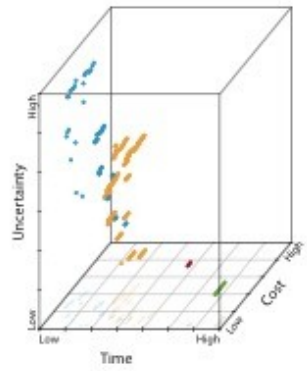
1. Identify accuracy-maximizing **data configuration**



2. **Predict runtime** of accuracy-maximizing data on different hardware configurations



3. Perform **hierarchical clustering**



Dimensions:
- Run Time
- Run Cost
- Prediction Uncertainty

4. Choose **minimum distance** from origin

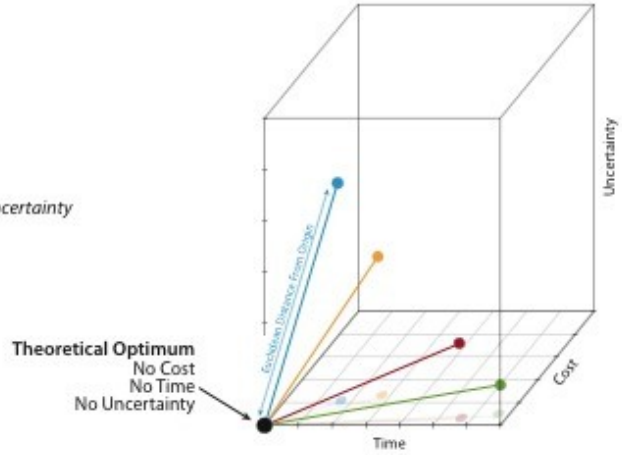


Figure 7: Plots of observed SDM runtime against the predicted SDM runtime for four species distribution models (GBM-BRT, MARS, GAM, RF) and the holdout testing set of observed runtime. R^2 values indicate the percent variance explained by each runtime model, as calculated by the correlation between predicted and observed values. The black line shows the y=x line expected for a perfectly-predictive model. All plots are displayed on logarithmic axes.

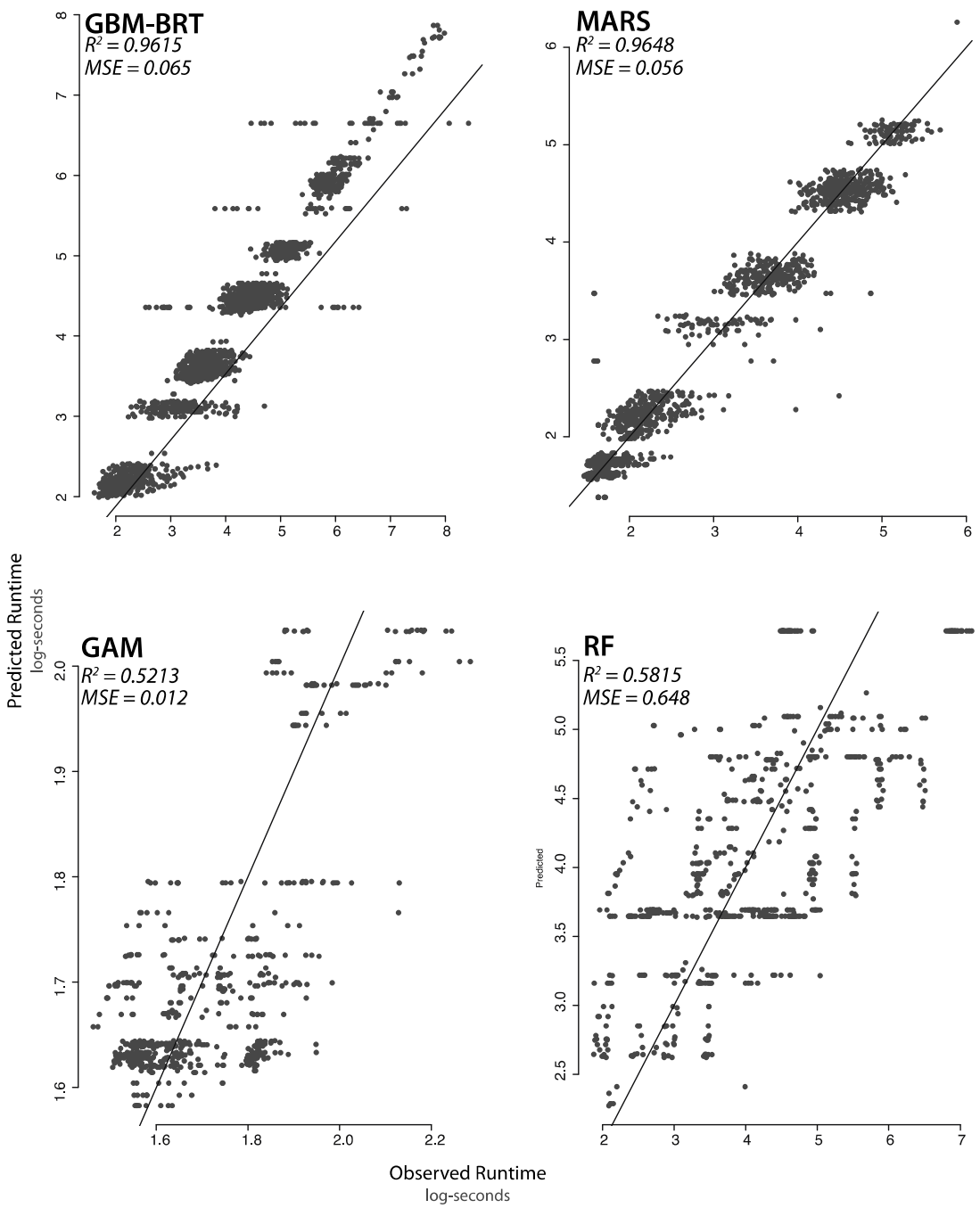

GBM-BRT
$R^2 = 0.9615$
MSE = 0.065
MARS
$R^2 = 0.9648$
MSE = 0.056
GAM
$R^2 = 0.5213$
MSE = 0.012
RF
$R^2 = 0.5815$
MSE = 0.648
Predicted Runtime
log-seconds
Observed Runtime
log-seconds
Predicted

Figure 8: Plots of expected SDM accuracy, measured by the AUC statistic, against the AUC predicted by the accuracy model. Figure design follows that of Figure 7.

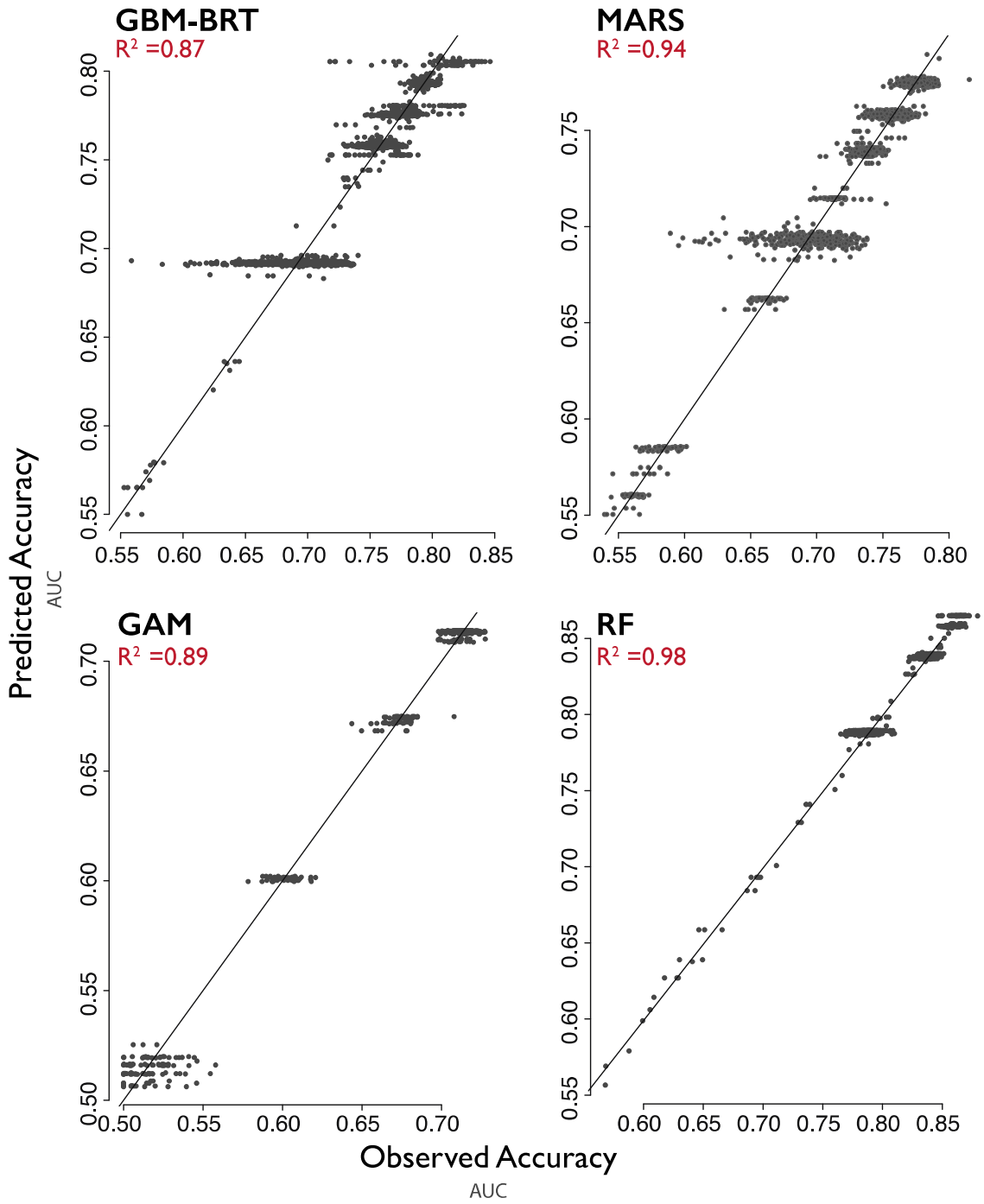

GBM-BRT
R² =0.87
MARS
R² =0.94
GAM
R² =0.89
RF
R² =0.98
Predicted Accuracy
AUC
Observed Accuracy
AUC

Figure 9: Plot of the optimal hardware configuration, based on the accuracy-maximizing experiments, for each SDM type. Note that the findings from the MARS models are peculiar, and should be interpreted with caution.

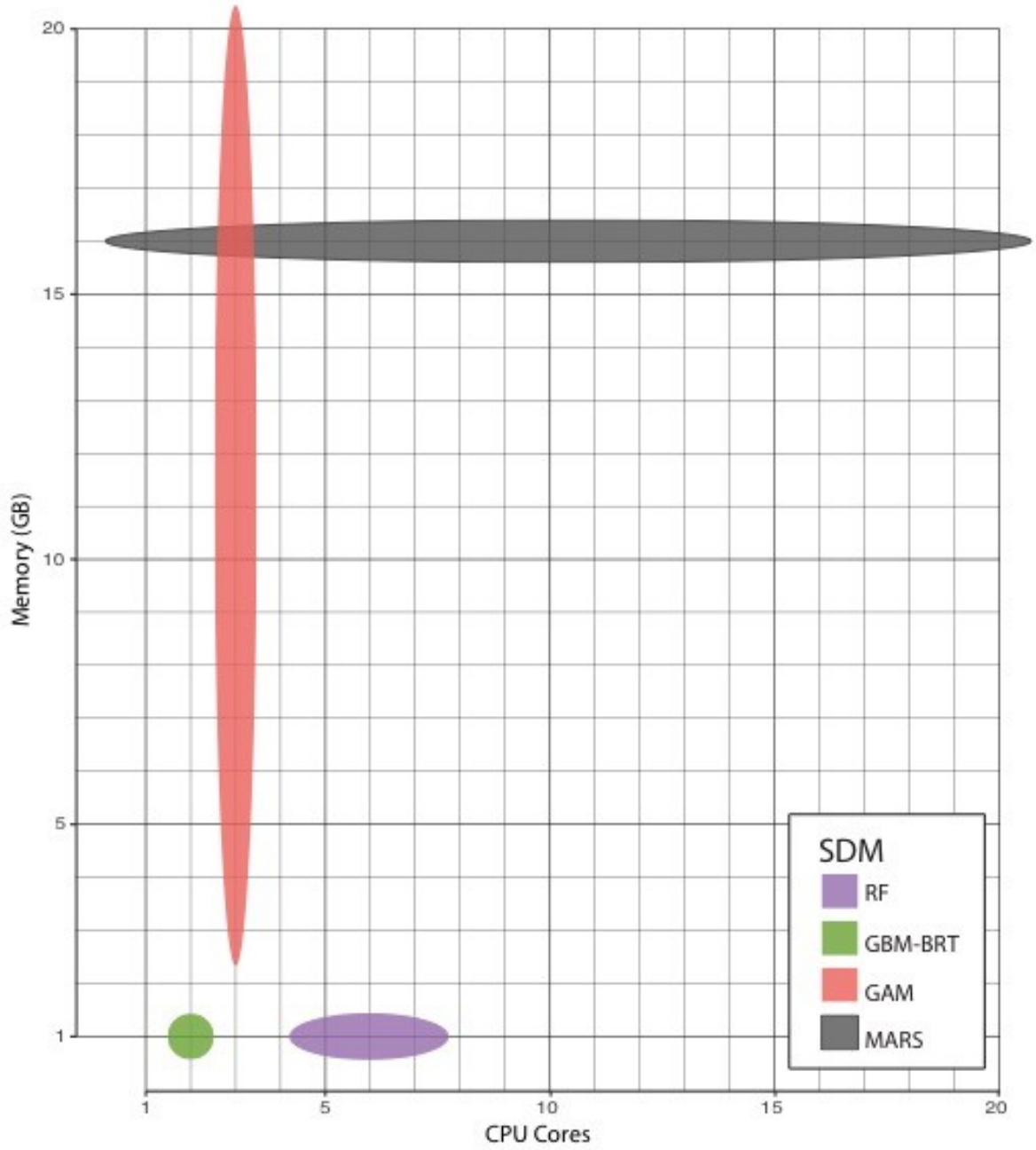


Figure 10: This contour plot shows, for each SDM algorithm, lines of constant accuracy as a function of training dataset volume and number of covariates. The substitution rate shows the relative tradeoff between number of training examples and number of covariates required to maintain a given accuracy. Contour interval is 0.01 AUC. AUC values of 1 indicate a perfect fit, while an AUC of 0.5 indicates a fit between model and data that is no better than random. For GBM-RT, MARS, and GAM, AUC is insensitive to training dataset volumes above 2500 samples, while AUC continues to improve with increasing training set size for RF.

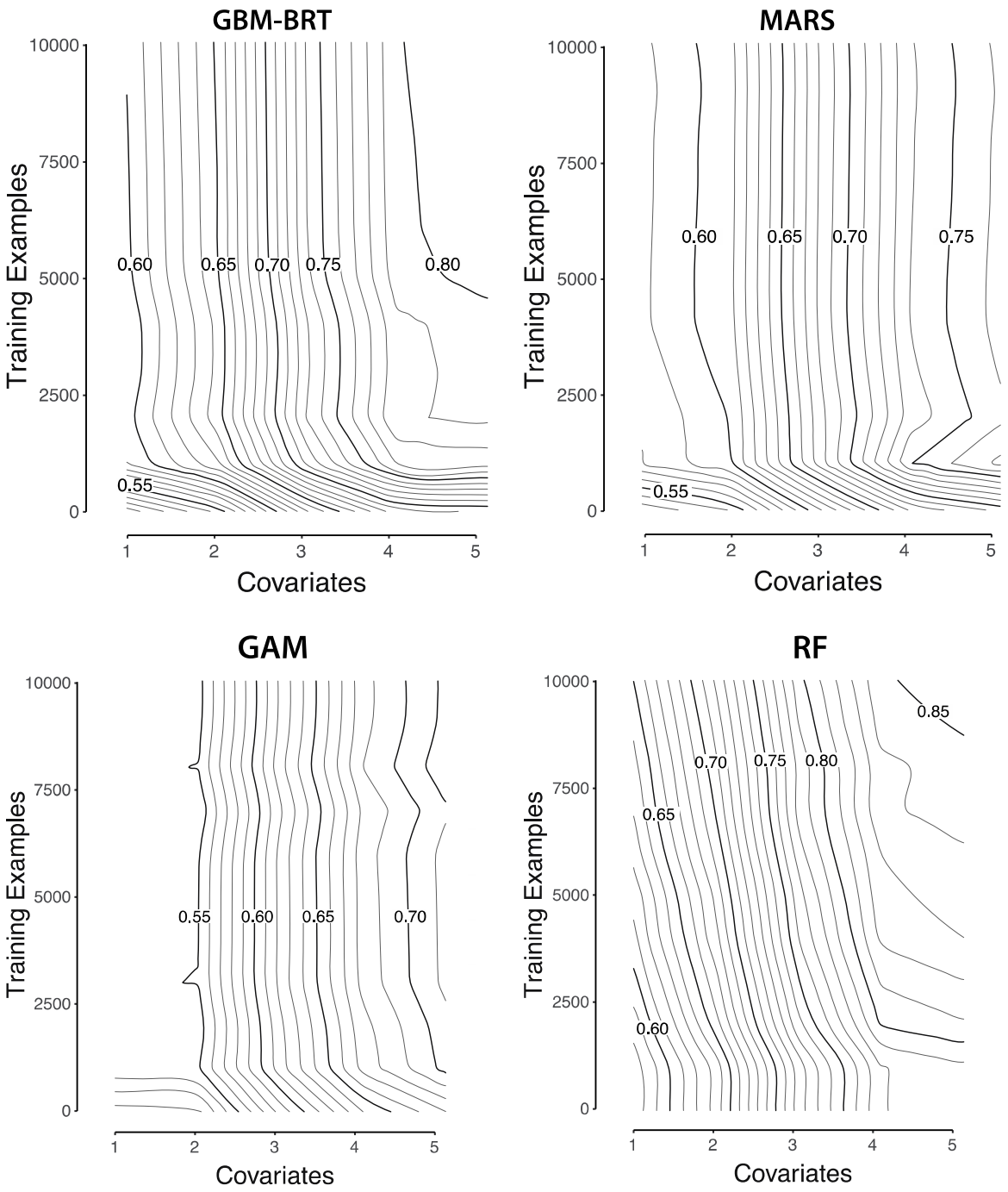

GBM-BRT
MARS
GAM
RF
Training Examples
Covariates
10000
7500
5000
2500
0
1
2
3
4
5
0.55
0.60
0.65
0.70
0.75
0.80
0.85

Figure 11: This figure shows the parallel efficiency of the RF SDM on datasets with different numbers of training examples. Parallel efficiency is calculated by dividing the ratio of the runtime on multiple cores to the runtime on a single core by the number of cores used. Efficiency can be interpreted as the marginal return gained by provisioning additional cores on which to run the algorithm. Higher efficiencies are obtained for larger training datasets, but efficiency necessarily decreases as the numbers of cores increases. The perfect efficiency line is shown, although this is impossible to achieve under real circumstances (Amdahl, 1967).

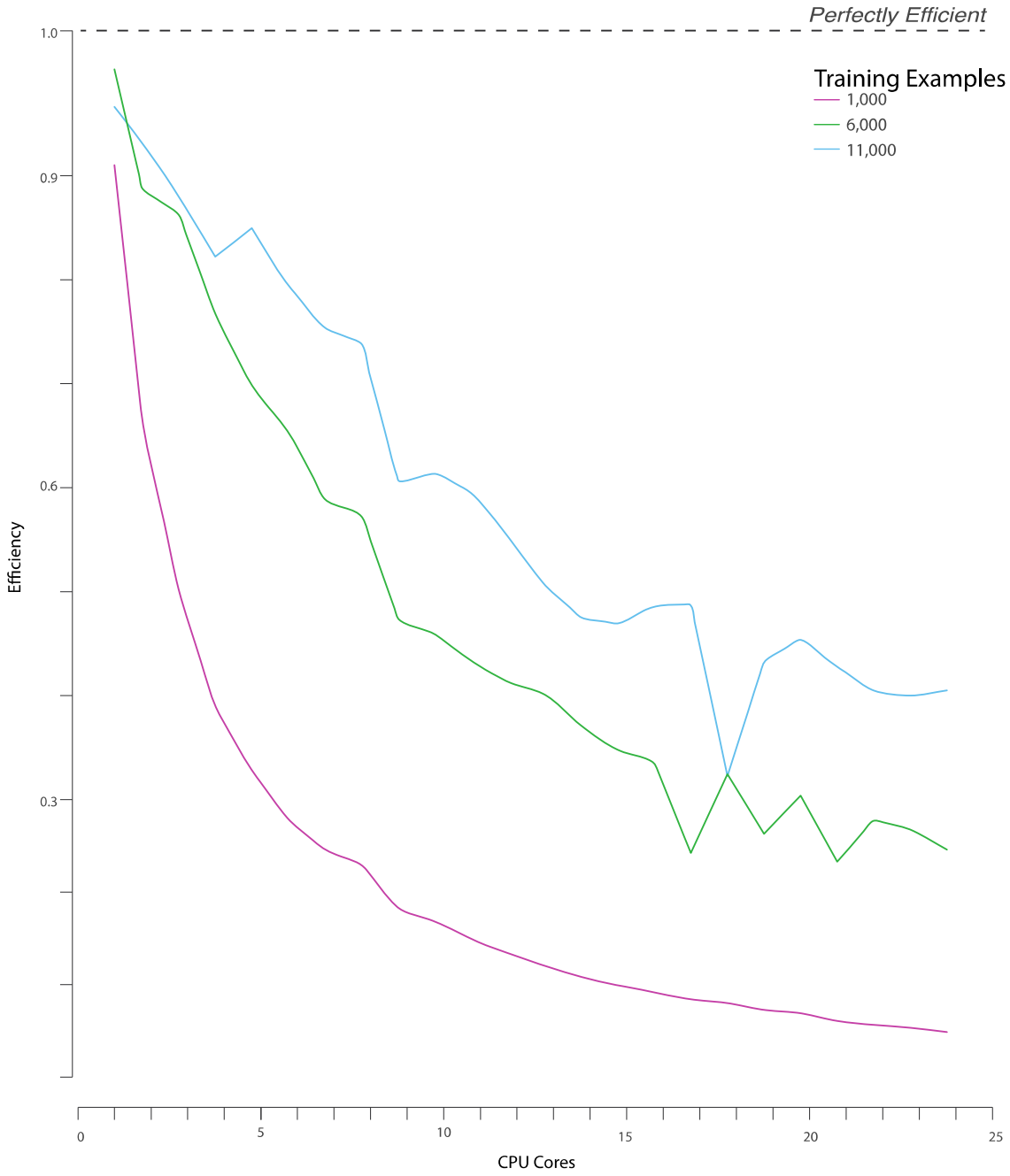
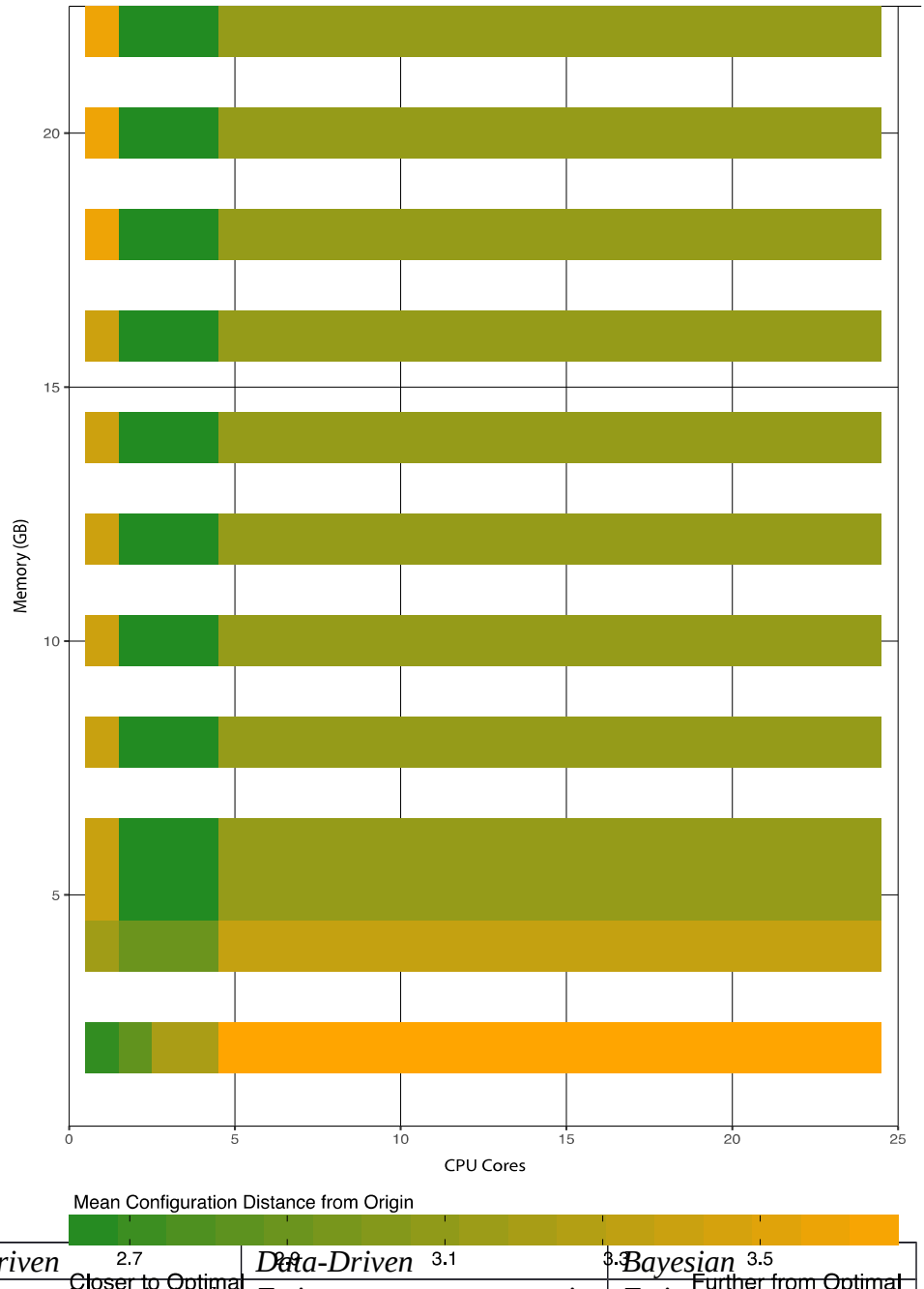

Perfectly Efficient
Training Examples
1,000
6,000
11,000
1.0
0.9
0.6
0.3
Efficiency
0
5
10
15
20
25
CPU Cores

Figure 12: This figure shows the mean distance of each hardware configuration from the origin over the GBM-BRT, GAM, and RF SDMs, in which distance is calculated as Euclidean distance from the origin of time, cost, and prediction uncertainty. Each configuration's distance to the origin was averaged over all SDM types to generate a mean configuration position. Green indicates lower distances and hardware configurations that are closer to optimal for these SDMs, while orange indicates larger distances and hardware configurations that are further from optimal. MARS was omitted from this analysis, due to its potentially misleading results and spurious dependence on memory. Note the large portion of the space far from the origin (orange), which suggests that many hardware configurations are suboptimal for running SDMs.

TABLES

Table 1: A comparison between data-drive, model-driven, and Bayesian modeling approaches. Method describes the way in which models approach the estimation of the relationship between inputs and outputs. Stability refers to the robustness of the model to small changes in the input dataset. Assumptions describe the relative number of assumptions that must be made in applying the model. Several common examples of each class are also shown.



	Model-Driven	*Data-Driven*	*Bayesian*
Method	*Fit a parametric statistical model to the dataset*	*Estimate a non-parametric function from the data*	*Estimate the relationship between inputs and outputs using a probability model*
Stability	*High*	*Low*	*High*
Assumptions	*Many (e.g., linearity, error*	*None/Few*	*Some (e.g.,*

	distribution)		*probability model)*
Examples	*Linear Regression* *Logistic Regression* *Generalized Linear Models*	*Boosted Regression Trees* *MaxEnt* *Multivariate Adaptive Regression Splines* *Support Vector Machines* *Random Forests*	*Gaussian Random Fields* *Generalized Joint Attribute Modeling*

Table 2: Performance model evaluation statistics. Training denotes the number of observations used to fit the runtime model. Testing represents the number of observations that were reserved for evaluation of the model (approximately 20% of the total dataset). MSE is the mean squared prediction error of the runtime model. r^2 is the coefficient of determination between observed and predicted values, and is interpreted as fraction of explained variance. Posterior SD is the mean standard deviation of the prediction posteriors, measured in log-seconds.

SDM	Training	Testing	MSE (log-seconds)	r^2	Posterior SD (log-seconds)
GBM-BRT	9256	2314	0.0646	0.9615	0.0257
GAM	2636	659	0.0121	0.5213	0.01069
MARS	6632	1657	0.0561	0.9648	0.03397
RF	2861	715	0.64824	0.5851	0.10174

Table 3: Accuracy Model Evaluation Statistics. Fields are as in Table 2.

SDM	Training	Testing	MSE (AUC)	r^2	Posterior SD (AUC)
GBM-BRT	9256	2314	0.000245	0.8748	0.0012
GAM	2636	659	0.000718	0.8993	0.004998
MARS	6632	1657	0.000168	0.9418	0.001421
RF	2861	715	0.000034	0.9818	0.00062

Table 4: Controls on SDM runtime and accuracy, calculated as the reduction in explanatory power when a predictive factor is removed, for the execution time model (top) and accuracy model (bottom). All values are expressed as percentage change in r^2 values for reduced model relative to full model. Note that the MARS values are from the reduced model that fixes a potential sampling issue.

Runtime Model	RF	MARS	GBM-BRT	GAM
Number of Covariates	-0.03%	3.07%	-1.67%	0.25%
CPU Cores	-5.55%	3.00%	-0.04%	-0.63%
GB Memory	-0.65%	-1.70%	-0.12%	0.08%
Number of Training Examples	-38.36%	-34.90%	-71.74%	-1.22%
Number of Predictive Cells	0.01%	-1.81%	-5.69%	-33.67%
Accuracy Model	RF	MARS	GBM-BRT	GAM
Number of Covariates	-34.39%	-26.31%	-16.40%	-50.45%
CPU Cores	-0.09%	0.04%	-0.07%	0.01%
GB Memory	-0.02%	-0.01%	-0.30%	0.00%
Number of Training Examples	-45.72%	-26.36%	-67.84%	-0.34%
Number of Predictive Cells	0.00%	0.14%	-0.03%	0.01%

Table 5: Accuracy-maximizing points for each SDM, calculated during optimization. Fixed accuracy is the estimated accuracy given the corresponding number of training examples and covariates for that model. Training examples is the number of training examples that optimize SDM accuracy, during the unconstrained optimization procedure. Covariates is the optimized number of environmental covariates with which to fit the model.

Model	Fixed Accuracy	Training Examples	Covariates
GAM	0.7131	9000	5
GBM-BRT	0.8087	10000	5
MARS	0.7722	1000	5
RF	0.8523	10000	5

APPENDICES

APPENDIX A: LITERATURE META-ANALYSIS

TABLE A1: STUDIES EVALUATED IN THE ANALYSIS

Authors	Title	Journal	Issue	Number	Pages	DOI	Year
Diniz-Filho, Jose Alexandre F; Rodrigues, Hauanny; Telles, Mariana Pires De Campos; De Oliveira, Guilherme; Terribile, Levi Carina; Soares, Thannya Nascimento; Nabout, Joao Carlos	Correlation between genetic diversity and environmental suitability: taking uncertainty from ecological niche models into account	Molecular Ecology Resources	15	5	1059-1066	**10.5061/DRYAD.3CP3T**	2015
Khoury, Colin K.; Castaneda-Alvarez, Nora P.; Achicanoy, Harold A.; Sosa, Chrystian C.; Bernau, Vivian; Kassa, Mulualem T.; Norton, Sally L.; van der Maesen, L. Jos G.; Upadhyaya, Hari D.; Ramirez-Villegas, Julian; Jarvis, Andy; Struik, Paul C.	Crop wild relatives of pigeonpea [Cajanus cajan (L.) Millsp.]: Distributions, ex situ conservation status, and potential genetic resources for abiotic stress tolerance	BIOLOGICAL CONSERVATION	184		259-270	10.1016/j.biocon.2015.01.032	2015
Chust, Guillem; Castellani, Claudia; Licandro, Priscilla; Ibaibarriaga, Leire; Sagarminaga, Yolanda; Irigoien, Xabier	Are Calanus spp. shifting poleward in the North Atlantic? A habitat modelling approach	ICES JOURNAL OF MARINE SCIENCE	71	2	241-253	10.1093/icesjms/fst147	2014
Davis, Edward Byrd; McGuire, Jenny L.; Orcutt, John D.	Ecological niche models of mammalian glacial refugia show consistent bias	ECOGRAPHY	37	11	1133-1138	10.1111/ecog.01294	2014
Yang, Xuejun; Huang, Zhenying; Venable, David L.; Wang, Lei; Zhang, Keliang; Baskin, Jerry M.; Baskin, Carol C.; Cornelissen, Johannes H. C.	Linking performance trait stability with species distribution: the case of Artemisia and its close relatives in northern China	JOURNAL OF VEGETATION SCIENCE	27	1	123-132	10.1111/jvs.12334	2016
Ananjeva, Natalia B.; Golynsky, Evgeny E.; Lin, Si-Min; Orlov, Nikolai L.; Tseng, Hui-Yun	MODELING HABITAT SUITABILITY TO PREDICT THE POTENTIAL DISTRIBUTION OF THE KELUNG CAT SNAKE Boiga kraepelini STEINEGER, 1902	RUSSIAN JOURNAL OF HERPETOLOGY	22	3	197-205		2015
Chlond, Dominik; Bugaj-Nawrocka, Agnieszka	Model of potential distribution of Platymeris rhadamanthus Gerstaecker, 1873 with redescription of species.	Zoological Studies	53		1-14		2014

Miller, Matthew J.; Lipshutz, Sara E.; Smith, Neal G.; Bermingham, Eldredge	Genetic and phenotypic characterization of a hybrid zone between polyandrous Northern and Wattled Jacanas in Western Panama	BMC EVOLUTIONARY BIOLOGY	14			10.1186/s12862-014-0227-7	2014
Fernandez-Mazuecos, Mario; Jimenez-Mejias, Pedro; Rotllan-Puig, Xavier; Vargas, Pablo	Narrow endemics to Mediterranean islands: Moderate genetic diversity but narrow climatic niche of the ancient, critically endangered Naufraga (Apiaceae)	PERSPECTIVES IN PLANT ECOLOGY EVOLUTION AND SYSTEMATICS	16	4	190-202	10.1016/j.ppees.2014.05.003	2014
Tainio, Anna; Heikkinen, Risto K.; Heliola, Janne; Hunt, Alistair; Watkiss, Paul; Fronzek, Stefan; Leikola, Niko; Lotjonen, Sanna; Mashkina, Olga; Carter, Timothy R.	Conservation of grassland butterflies in Finland under a changing climate	REGIONAL ENVIRONMENTAL CHANGE	16	1	71-84	10.1007/s10113-014-0684-y	2016
Oke, Oluwatobi A.; Thompson, Ken A.	Distribution models for mountain plant species: The value of elevation	ECOLOGICAL MODELLING	301		72-77	10.1016/j.ecolmodel.2015.01.019	2015
Tsuyama, Ikutaro; Nakao, Katsuhiro; Higa, Motoki; Matsui, Tetsuya; Shichi, Koji; Tanaka, Nobuyuki	What controls the distribution of the Japanese endemic hemlock, Tsuga diversifolia? Footprint of climate in the glacial period on current habitat occupancy	JOURNAL OF FOREST RESEARCH	19	1	154-165	10.1007/s10310-013-0399-9	2014
Yen, Shih-Ching; Wang, Ying; Ou, Heng-You	Habitat of the Vulnerable Formosan sambar deer Rusa unicolor swinhoii in Taiwan	ORYX	48	2	232-240	10.1017/S0030605312001378	2014
Hertzog, Lionel R.; Besnard, Aurelien; Jay-Robert, Pierre	Field validation shows bias-corrected pseudo-absence selection is the best method for predictive species-distribution modelling	DIVERSITY AND DISTRIBUTIONS	20	12	1403-1413	10.1111/ddi.12249	2014
Patrao, Claudia; Assis, Jorge; Rufino, Marta; Silva, Goncalo; Jordaens, Kurt; Backeljau, Thierry; Castilho, Rita	Habitat suitability modelling of four terrestrial slug species in the Iberian Peninsula (Arionidae: Geomalacus species)	JOURNAL OF MOLLUSCAN STUDIES	81		427-434	10.1093/mollus/eyv018	2015
Del Toro, Israel; Silva, Rogerio R.; Ellison, Aaron M.	Predicted impacts of climatic change on ant functional diversity and distributions in eastern North American forests	DIVERSITY AND DISTRIBUTIONS	21	7	781-791	10.1111/ddi.12331	2015
Voda, Raluca; Dapporto, Leonardo; Dinca, Vlad; Vila, Roger	Why Do Cryptic Species Tend Not to Co-Occur? A Case Study on Two Cryptic Pairs of Butterflies	PLOS ONE	10	2		10.1371/journal.pone.0117802	2015
Laube, Irina; Graham, Catherine H.; Boehning-Gaese, Katrin	Niche availability in space and time: migration in Sylvia warblers	JOURNAL OF BIOGEOGRAPHY	42	10	1896-1906	10.1111/jbi.12565	2015

Askeyev, Oleg; Askeyev, Igor; Askeyev, Arthur; Monakhov, Sergey; Yanybaev, Nur	River fish assemblages in relation to environmental factors in the eastern extremity of Europe (Tatarstan Republic, Russia)	ENVIRONMENTAL BIOLOGY OF FISHES	98	5	1277-1293	10.1007/s10641-014-0358-0	2015
Meseguer, Andrea S; Lobo, Jorge M; Ree, Richard; Beerling, David J; Sanmartin, Isabel	Data from: Integrating fossils, phylogenies, and niche models into biogeography to reveal ancient evolutionary history: the case of Hypericum (Hypericaceae)	Dryad				**10.5061/DRYAD.5845B**	2014
Soto-Centeno, J. Angel; O'Brien, Margaret; Simmons, Nancy B.	The importance of late Quaternary climate change and karst on distributions of Caribbean mormoopid bats	AMERICAN MUSEUM NOVITATES	3847				2015
Blanchard, Ryan; O'Farrell, Patrick J.; Richardson, David M.	Anticipating potential biodiversity conflicts for future biofuel crops in South Africa: incorporating spatial filters with species distribution models	GLOBAL CHANGE BIOLOGY BIOENERGY	7	2	273-287	10.1111/gcbb.12129	2015
Paudel, Prakash Kumar; Hais, Martin; Kindlmann, Pavel	Habitat suitability models of mountain ungulates: identifying potential areas for conservation	ZOOLOGICAL STUDIES	54			10.1186/s40555-015-0116-9	2015
Hsu, Chorng-Bin; Hwang, Gwo-Wen; Lu, Jane-Fuh; Chen, Chang-Po; Tao, Hsiao-Hang; Hsieh, Hwey-Lian	Habitat Characteristics of the Wintering Common Teal in the Huajiang Wetland, Taiwan	WETLANDS	34	6	1207-1218	10.1007/s13157-014-0581-7	2014
Henrys, P. A.; Bee, E. J.; Watkins, J. W.; Smith, N. A.; Griffiths, R. I.	Mapping natural capital: optimising the use of national scale datasets	ECOGRAPHY	38	6	632-638	10.1111/ecog.00402	2015
Becker, Nina I.; Encarnacao, Jorge A.	Silvicolous on a Small Scale: Possibilities and Limitations of Habitat Suitability Models for Small, Elusive Mammals in Conservation Management and Landscape Planning	PLOS ONE	10	3		10.1371/journal.pone.0120562	2015
Drake, John M	Range bagging: a new method for ecological niche modelling from presence-only data.	Journal of the Royal Society, Interface / the Royal Society	12	107		10.1098/rsif.2015.0086	2015
Masin, Simone; Bonardi, Anna; Padoa-Schioppa, Emilio; Bottoni, Luciana; Ficetola, Gentile Francesco	Risk of invasion by frequently traded freshwater turtles	BIOLOGICAL INVASIONS	16	1	217-231	10.1007/s10530-013-0515-y	2014
Ficetola, Gentile Francesco; Cagnetta, Massimo; Padoa-Schioppa, Emilio; Quas, Anita; Razzetti, Edoardo; Sindaco, Roberto; Bonardi, Anna	Sampling bias inverts ecogeographical relationships in island reptiles	GLOBAL ECOLOGY AND BIOGEOGRAPHY	23	11	1303-1313	10.1111/geb.12201	2014

Segurado, Pedro; Branco, Paulo; Avelar, Ana P.; Ferreira, Maria T.	Historical changes in the functional connectivity of rivers based on spatial network analysis and the past occurrences of diadromous species in Portugal	AQUATIC SCIENCES	77	3	427-440	10.1007/s00027-014-0371-6	2015
Zhao, C. S.; Yang, S. T.; Liu, C. M.; Dou, T. W.; Yang, Z. L.; Yang, Z. Y.; Liu, X. L.; Xiang, H.; Nie, S. Y.; Zhang, J. L.; Mitrovic, S. M.; Yu, Q.; Lim, R. P.	Linking hydrologic, physical and chemical habitat environments for the potential assessment of fish community rehabilitation in a developing city	JOURNAL OF HYDROLOGY	523		384-397	10.1016/j.jhydrol.2015.01.067	2015
Roger, Erin; Duursma, Daisy Englert; Downey, Paul O.; Gallagher, Rachael V.; Hughes, Lesley; Steel, Jackie; Johnson, Stephen B.; Leishman, Michelle R.	A tool to assess potential for alien plant establishment and expansion under climate change	JOURNAL OF ENVIRONMENTAL MANAGEMENT	159		121-127	10.1016/j.jenvman.2015.05.039	2015
Poulos, Davina E.; Gallen, Christopher; Davis, Tom; Booth, David J.; Harasti, David	Distribution and spatial modelling of a soft coral habitat in the Port Stephens-Great Lakes Marine Park: implications for management	MARINE AND FRESHWATER RESEARCH	67	2	256-265	10.1071/MF14059	2016
Lira-Noriega, Andres; Peterson, A. Townsend	Range-wide ecological niche comparisons of parasite, hosts and dispersers in a vector-borne plant parasite system	JOURNAL OF BIOGEOGRAPHY	41	9	1664-1673	10.1111/jbi.12302	2014
Olsson, Ola; Bolin, Arvid	A model for habitat selection and species distribution derived from central place foraging theory	OECOLOGIA	175	2	537-548	10.1007/s00442-014-2931-9	2014
Lee, Chang-Bae; Yun, Soon Jin; œÌÈTÖ	Effects of climate change on the geographic distribution of Quercus acuta Thunb.	Journal of Agriculture & Life Science	49	6	47-56	10.14397/jals.2015.49.6.47	2015
Skov, Henrik; Heinanen, Stefan; Thaxter, Chris B.; Williams, Adrian E.; Lohier, Sabine; Banks, Alex N.	Real-time species distribution models for conservation and management of natural resources in marine environments	MARINE ECOLOGY PROGRESS SERIES	542		221-234	10.3354/meps11572	2016
Afkhami, Michelle E.; McIntyre, Patrick J.; Strauss, Sharon Y.	Mutualist-mediated effects on species' range limits across large geographic scales	ECOLOGY LETTERS	17	10	1265-1273	10.1111/ele.12332	2014
Mimet, Anne; Maurel, Noelie; Pellissier, Vincent; Simon, Laurent; Julliard, Romain	Towards a unique landscape description for multi-species studies: A model comparison with common birds in a human-dominated French region	ECOLOGICAL INDICATORS	36		19-32	10.1016/j.ecolind.2013.06.029	2014

Owens, Hannah L.	Evolution of codfishes (Teleostei: Gadinae) in geographical and ecological space: evidence that physiological limits drove diversification of subarctic fishes	JOURNAL OF BIOGEOGRAPHY	42	6	1091-1102	10.1111/jbi.12483	2015
Rato, Catarina; Harris, David James; Perera, Ana; Carvalho, Silvia B.; Carretero, Miguel A.; Roedder, Dennis	A Combination of Divergence and Conservatism in the Niche Evolution of the Moorish Gecko, Tarentola mauritanica (Gekkota: Phyllodactylidae)	PLOS ONE	10	5	-	10.1371/journal.pone.0127980	2015
Munoz, Antonio-Roman; Jimenez-Valverde, Alberto; Luz Marquez, Ana; Moleon, Marcos; Real, Raimundo	Environmental favourability as a cost-efficient tool to estimate carrying capacity	DIVERSITY AND DISTRIBUTIONS	21	12	1388-1400	10.1111/ddi.12352	2015
Ortego, Joaquin; Gugger, Paul F.; Sork, Victoria L.	Climatically stable landscapes predict patterns of genetic structure and admixture in the Californian canyon live oak	JOURNAL OF BIOGEOGRAPHY	42	2	328-338	10.1111/jbi.12419	2015
Latif, Quresh S.; Saab, Victoria A.; Mellen-Mclean, Kim; Dudley, Jonathan G.	Evaluating Habitat Suitability Models for Nesting White-Headed Woodpeckers in Unburned Forest	JOURNAL OF WILDLIFE MANAGEMENT	79	2	263-273	10.1002/jwmg.842	2015
Branco, Paulo; Segurado, Pedro; Santos, Jose M.; Ferreira, Maria T.	Prioritizing barrier removal to improve functional connectivity of rivers	JOURNAL OF APPLIED ECOLOGY	51	5	1197-1206	10.1111/1365-2664.12317	2014
Callen, Steven T.; Miller, Allison J.	Signatures of niche conservatism and niche shift in the North American kudzu (Pueraria montana) invasion	DIVERSITY AND DISTRIBUTIONS	21	8	853-863	10.1111/ddi.12341	2015
Alberdi, Antton; Gilbert, M. Thomas P.; Razgour, Orly; Aizpurua, Ostaizka; Aihartza, Joxerra; Garin, Inazio	Contrasting population-level responses to Pleistocene climatic oscillations in analpine bat revealed by complete mitochondrial genomes and evolutionary history inference	JOURNAL OF BIOGEOGRAPHY	42	9	1689-1700	10.1111/jbi.12535	2015
Rezende, Vanessa Leite; de Oliveira-Filho, Ary T.; Eisenlohr, Pedro V.; Yoshino Kamino, Luciana Hiromi; Vibrans, Alexander Christian	Restricted geographic distribution of tree species calls for urgent conservation efforts in the Subtropical Atlantic Forest	BIODIVERSITY AND CONSERVATION	24	5	1057-1071	10.1007/s10531-014-0721-7	2015
Fresia, Pablo; Silver, Micha; Mastrangelo, Thiago; De Azeredo-Espin, Ana Maria L.; Lyra, Mariana L.	Applying spatial analysis of genetic and environmental data to predict connection corridors to the New World screwworm populations in South America	ACTA TROPICA	138		S34-S41	10.1016/j.actatropica.2014.04.003	2014
Mod, Heidi K.; le Roux, Peter C.; Guisan, Antoine; Luoto, Miska	Biotic interactions boost spatial models of species richness	ECOGRAPHY	38	9	913-921	10.1111/ecog.01129	2015

le Roux, Peter C.; Luoto, Miska	Earth surface processes drive the richness, composition and occurrence of plant species in an arctic-alpine environment	JOURNAL OF VEGETATION SCIENCE	25	1	45-54	10.1111/jvs.12059	2014
Razgour, Orly; Salicini, Irene; Ibanez, Carlos; Randi, Ettore; Juste, Javier	Unravelling the evolutionary history and future prospects of endemic species restricted to former glacial refugia	MOLECULAR ECOLOGY	24	20	5267-5283	10.1111/mec.13379	2015
Belmaker, Jonathan; Zarnetske, Phoebe; Tuanmu, Mao-Ning; Zonneveld, Sara; Record, Sydne; Strecker, Angela; Beaudrot, Lydia	Empirical evidence for the scale dependence of biotic interactions	GLOBAL ECOLOGY AND BIOGEOGRAPHY	24	7	750-761	10.1111/geb.12311	2015
Wrege, Marcos Silveira; Coutinho, Enilton Fick; Pantano, Angelica Prela; Jorge, Rogerio Oliveira	POTENCIAL DISTRIBUTION OF OLIVE IN BRAZIL AND WORLDWIDE	REVISTA BRASILEIRA DE FRUTICULTURA	37	3	656-666	10.1590/0100-2945-174/14	2015
Dong, Xiaoli; Grimm, Nancy B.; Ogle, Kiona; Franklin, Janet	Temporal variability in hydrology modifies the influence of geomorphology on wetland distribution along a desert stream	JOURNAL OF ECOLOGY	104	1	18-30	10.1111/1365-2745.12450	2016
Liu, Canran; Newell, Graeme; White, Matt	On the selection of thresholds for predicting species occurrence with presence-only data	ECOLOGY AND EVOLUTION	6	1	337-348	10.1002/ece3.1878	2016
Recio, Mariano R.; Seddon, Philip J.; Moore, Antoni B.	Niche and movement models identify corridors of introduced feral cats infringing ecologically sensitive areas in New Zealand	BIOLOGICAL CONSERVATION	192		48-56	10.1016/j.biocon.2015.09.004	2015
Tocchio, Luana J.; Gurgel-Goncalves, Rodrigo; Escobar, Luis E.; Peterson, Andrew Townsend	Niche similarities among white-eared opossums (Mammalia, Didelphidae): Is ecological niche modelling relevant to setting species limits?	ZOOLOGICA SCRIPTA	44	1	1-10	10.1111/zsc.12082	2015
Guo, Chuanbo; Lek, Sovan; Ye, Shaowen; Li, Wei; Liu, Jiashou; Li, Zhongjie	Uncertainty in ensemble modelling of large-scale species distribution: Effects from species characteristics and model techniques	ECOLOGICAL MODELLING	306		67-75	10.1016/j.ecolmodel.2014.08.002	2015
Yin, Hengxia; Yan, Xia; Shi, Yong; Qian, Chaoju; Li, Zhonghu; Zhang, Wen; Wang, Lirong; Li, Yi; Li, Xiaoze; Chen, Guoxiong; Li, Xinrong; Nevo, Eviatar; Ma, Xiao-Fei	The role of East Asian monsoon system in shaping population divergence and dynamics of a constructive desert shrub Reaumuria soongarica	SCIENTIFIC REPORTS	5			10.1038/srep15823	2015
Huang, Jen-Pan	Modeling the effects of anthropogenic exploitation and climate change on an endemic stag beetle, Lucanus miwai, of Taiwan	Dryad				**10.5061/DRYAD.8MP13**	2014

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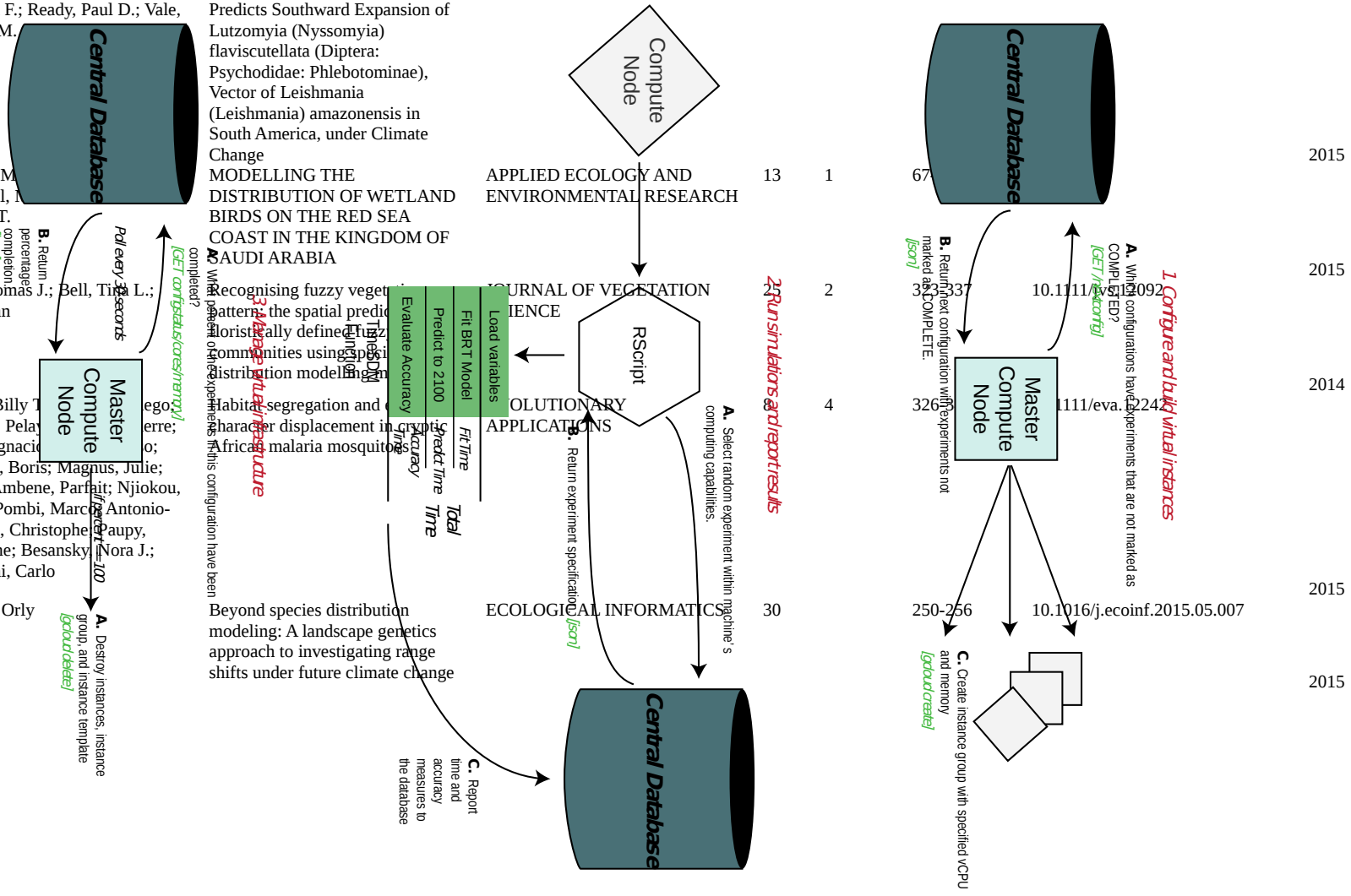
Naczk, Aleksandra M; Kolanowska, Marta	Glacial Refugia and Future Habitat Coverage of Selected Dactylorhiza Representatives (Orchidaceae).	PloS one	10	11	e0143478-e0143478	10.1371/journal.pone.0143478	2015
Maher, Sean P.; Randin, Christophe F.; Guisan, Antoine; Drake, John M.	Pattern-recognition ecological niche models fit to presence-only and presence-absence data	METHODS IN ECOLOGY AND EVOLUTION	5	8	761-770	10.1111/2041-210X.12222	2014
Carolan, Kevin; Ebong, Solange Meyin A.; Garchitorena, Andres; Landier, Jordi; Sanhueza, Daniel; Texier, Gaetan; Marsollier, Laurent; Le Gall, Philipe; Guegan, Jean-Francois; Lo Seen, Danny	Ecological niche modelling of Hemipteran insects in Cameroon; the paradox of a vector-borne transmission for Mycobacterium ulcerans, the causative agent of Buruli ulcer	INTERNATIONAL JOURNAL OF HEALTH GEOGRAPHICS	13			10.1186/1476-072X-13-44	2014
Moraes R, Monica; Rios-Uzeda, Boris; Rene Moreno, Luis; Huanca-Huarachi, Gladis; Larrea-Alcazar, Daniel	Using potential distribution models for patterns of species richness, endemism, and phytogeography of palm species in Bolivia	TROPICAL CONSERVATION SCIENCE	7	1	45-60		2014
Lim, Haw Chuan; Zou, Fasheng; Sheldon, Frederick H.	Genetic differentiation in two widespread, open-forest bird species of Southeast Asia (Copsychus saularis and Megalaima haemacephala): Insights from ecological niche modeling	Current Zoology	61	5	922-934		2015
Caouette, J. P.; Steel, E. A.; Hennon, P. E.; Cunningham, P. G.; Pohl, C. A.; Schrader, B. A.	Influence of elevation and site productivity on conifer distributions across Alaskan temperate rainforests	CANADIAN JOURNAL OF FOREST RESEARCH	46	2	249-261		2016
Manuel Alvarez-Martinez, Jose; Suarez-Seoane, Susana; Stoorvogel, Jetse J.; de Luis Calabuig, Estanislao	Influence of land use and climate on recent forest expansion: a case study in the Eurosiberian-Mediterranean limit of north-west Spain	JOURNAL OF ECOLOGY	102	4	905-919	10.1111/1365-2745.12257	2014
Pabijan, Maciej; Brown, Jason L.; Chan, Lauren M.; Rakotondravony, Hery A.; Raselimanana, Achille P.; Yoder, Anne D.; Glaw, Frank; Vences, Miguel	Phylogeography of the arid-adapted Malagasy bullfrog, Laliostoma labrosum, influenced by past connectivity and habitat stability	MOLECULAR PHYLOGENETICS AND EVOLUTION	92		11-24	10.1016/j.ympev.2015.05.018	2015

Obolenskaya, Ekaterina V.; Lissovsky, Andrey A.	Regional zoogeographical zoning using species distribution modelling by the example of small mammals of South-Eastern Transbaikalia	Russian Journal of Theriology	14	2	171-185		2015
Zeng, Qing; Zhang, Yamian; Sun, Gongqi; Duo, Hairui; Wen, Li; Lei, Guangchun	Using Species Distribution Model to Estimate the Wintering Population Size of the Endangered Scaly-Sided Merganser in China	PLOS ONE	10	2		10.1371/journal.pone.0117307	2015
de Castro Pena, Joao Carlos; Yoshino Kamino, Luciana Hiromi; Rodrigues, Marcos; Mariano-Neto, Eduardo; de Siqueira, Marinez Ferreira	Assessing the conservation status of species with limited available data and disjunct distribution	BIOLOGICAL CONSERVATION	170		130-136	10.1016/j.biocon.2013.12.015	2014
Collevatti, Rosane G.; Terribile, Levi C.; Rabelo, Suelen G.; Lima-Ribeiro, Matheus S.	Relaxed random walk model coupled with ecological niche modeling unravel the dispersal dynamics of a Neotropical savanna tree species in the deeper Quaternary	FRONTIERS IN PLANT SCIENCE	6			10.3389/fpls.2015.00653	2015
Wang, Lifei; Jackson, Donald A.	Shaping up model transferability and generality of species distribution modeling for predicting invasions: implications from a study on Bythotrephes longimanus	BIOLOGICAL INVASIONS	16	10	2079-2103	10.1007/s10530-014-0649-6	2014
Paiva, Vitor H.; Geraldes, Pedro; Rodrigues, Isabel; Melo, Tommy; Melo, Jose; Ramos, Jaime A.	The Foraging Ecology of the Endangered Cape Verde Shearwater, a Sentinel Species for Marine Conservation off West Africa	PLOS ONE	10	10		10.1371/journal.pone.0139390	2015
Aguirre-Gutierrez, Jesus; Serna-Chavez, Hector M.; Villalobos-Arambula, Alma R.; Perez de la Rosa, Jorge A.; Raes, Niels	Similar but not equivalent: ecological niche comparison across closely-related Mexican white pines	DIVERSITY AND DISTRIBUTIONS	21	3	245-257	10.1111/ddi.12268	2015
Tererai, Farai; Wood, Alan R.	On the present and potential distribution of Ageratina adenophora (Asteraceae) in South Africa	SOUTH AFRICAN JOURNAL OF BOTANY	95		152-158	10.1016/j.sajb.2014.09.001	2014
Costa, Henrique C.; de Rezende, Daniella T.; Molina, Flavio B.; Nascimento, Luciana B.; Leite, Felipe S. F.; Fernandes, Ana Paula B.	New Distribution Records and Potentially Suitable Areas for the Threatened Snake-Necked Turtle Hydromedusa maximiliani (Testudines: Chelidae)	CHELONIAN CONSERVATION AND BIOLOGY	14	1	88-94		2015

Costa, J.; Dornak, L. L.; Almeida, C. E.; Peterson, A. T.	Distributional potential of the Triatoma brasiliensis species complex at present and under scenarios of future climate conditions.	Parasites and Vectors	7	238			2014
Saupe, Erin E.; Hendricks, Jonathan R.; Peterson, A. Townsend; Lieberman, Bruce S.	Climate change and marine molluscs of the western North Atlantic: future prospects and perils	JOURNAL OF BIOGEOGRAPHY	41	7	1352-1366	10.1111/jbi.12289	2014
Alves, Joana; da Silva, Antonio Alves; Soares, Amadeu M. V. M.; Fonseca, Carlos	Spatial and temporal habitat use and selection by red deer: The use of direct and indirect methods	MAMMALIAN BIOLOGY	79	5	338-348	10.1016/j.mambio.2014.05.007	2014
Qi, Xin-Shuai; Yuan, Na; Comes, Hans Peter; Sakaguchi, Shota; Qiu, Ying-Xiong	A strong "filter" effect of the East China Sea land bridge for East Asia's temperate plant species: inferences from molecular phylogeography and ecological niche modelling of Platycrater arguta (Hydrangeaceae)	TreeBASE					2014
Alexander, Neil; Medlock, Jolyon; Morley, David; Wint, Willy	A first attempt at modelling red deer (Cervus elaphus) distributions over Europe	Figshare	1			10.6084/M9.FIGSHARE.1008334	2014
de Andrade, Andrey Jose; Gurgel-Goncalves, Rodrigo	New record and update on the geographical distribution of Pintomyia monticola (Costa Lima, 1932) (Diptera: Psychodidae) in South America.	Check List	11	2	1566-1566		2015
van Andel, T. R.; Croft, S.; van Loon, E. E.; Quiroz, D.; Towns, A. M.; Raes, N.	Prioritizing West African medicinal plants for conservation and sustainable extraction studies based on market surveys and species distribution models	BIOLOGICAL CONSERVATION	181		173-181	10.1016/j.biocon.2014.11.015	2015
Burger, J.; Edler, B.; Gerowitt, B.; Steinmann, H. H.	Predicting weed problems in maize cropping by species distribution modelling.	Julius-Kuhn-Archiv	443	379	386-		2014
Sanchez-Montes, Sokani; Espinosa-Martinez, Deborah V.; Rios-Munoz, Cesar A.; Berzunza-Cruz, Miriam; Becker, Ingeborg	Leptospirosis in Mexico: Epidemiology and Potential Distribution of Human Cases	PLOS ONE	10	7		10.1371/journal.pone.0133720	2015
Williams, K. A.; Richards, C. S.; Villet, M. H.	Predicting the geographic distribution of Lucilia sericata and Lucilia cuprina (Diptera: Calliphoridae) in South Africa	AFRICAN INVERTEBRATES	55	1	157-170		2014

Wang, Hsiao-Hsuan; Koralewski, Tomasz E.; McGrew, Erin K.; Grant, William E.; Byram, Thomas D.	Species Distribution Model for Management of an Invasive Vine in Forestlands of Eastern Texas	FORESTS	6	12	4374-4390	10.3390/f6124374	2015
Pouteau, Robin; Meyer, Jean-Yves; Larrue, Sebastien	Using range filling rather than prevalence of invasive plant species for management prioritisation: the case of Spathodea campanulata in the Society Islands (South Pacific)	ECOLOGICAL INDICATORS	54		87-95	10.1016/j.ecolind.2015.02.017	2015
Carvalho, Bruno M.; Rangel, Elizabeth F.; Ready, Paul D.; Vale, Mariana M.	Ecological Niche Modelling Predicts Southward Expansion of Lutzomyia (Nyssomyia) flaviscutellata (Diptera: Psychodidae: Phlebotominae), Vector of Leishmania (Leishmania) amazonensis in South America, under Climate Change	PLOS ONE	10	11		10.1371/journal.pone.0143282	2015
Almalki, M O'Connell, Szekely, T.	MODELLING THE DISTRIBUTION OF WETLAND BIRDS ON THE RED SEA COAST IN THE KINGDOM OF SAUDI ARABIA	APPLIED ECOLOGY AND ENVIRONMENTAL RESEARCH	13	1	67		2015
Duff, Thomas J.; Bell, Tina L.; York, Alan	Recognising fuzzy vegetation patterns: the spatial predictability of floristically defined fuzzy communities using species distribution modelling	JOURNAL OF VEGETATION SCIENCE	25	2	323-337	10.1111/jvs.12092	2015
Fossog, Billy T Acevedo, Pelay Mebuy, Ignacio Makanga, Boris; Magnus, Julie; Awono-Ambene, Parfait; Njiokou, Flobert; Pombi, Marco; Antonio-Nkondjio, Christophe; Paupy, Christophe; Besansky, Nora J.; Costantini, Carlo	Habitat segregation and character displacement in cryptic African malaria mosquitoes	EVOLUTIONARY APPLICATIONS	8	4	326-3	1111/eva.12242	2014
Razgour, Orly	Beyond species distribution modeling: A landscape genetics approach to investigating range shifts under future climate change	ECOLOGICAL INFORMATICS	30		250-256	10.1016/j.ecoinf.2015.05.007	2015



Appendix B: Data Collection Protocol

Figure B1: Conceptual Flowchart of Distributed System Used for Automated SDM

APPENDIX C: BAYESIAN MODEL PRIORS
MODEL NAME: Bayesian Additive Regression Trees

IMPLEMENTATION: bartMachine version 1.2.3

Adam Kapelner, Justin Bleich (2016). bartMachine: Machine Learning with Bayesian Additive Regression Trees. Journal of Statistical Software, 70(4), 1-40. doi: 10.18637/jss.v070.i04

MODEL STRUCTURE:

$$\boldsymbol{Y} = f(\boldsymbol{X}) + \boldsymbol{\varepsilon} \approx \mathcal{T}_1^{\mathcal{M}}(\boldsymbol{X}) + \mathcal{T}_2^{\mathcal{M}}(\boldsymbol{X}) + \ldots + \mathcal{T}_m^{\mathcal{M}}(\boldsymbol{X}) + \boldsymbol{\varepsilon}, \qquad \boldsymbol{\varepsilon} \sim \mathcal{N}_n\left(\mathbf{0}, \sigma^2 \boldsymbol{I}_n\right), \qquad (1)$$

$$\begin{aligned} \mathbb{P}\left(\mathcal{T}_1^{\mathcal{M}}, \ldots, \mathcal{T}_m^{\mathcal{M}}, \sigma^2\right) &= \left[\prod_t \mathbb{P}\left(\mathcal{T}_t^{\mathcal{M}}\right)\right] \mathbb{P}\left(\sigma^2\right) = \left[\prod_t \mathbb{P}\left(\mathcal{M}_t \mid \mathcal{T}_t\right) \mathbb{P}\left(\mathcal{T}_t\right)\right] \mathbb{P}\left(\sigma^2\right) \\ &= \left[\prod_t \prod_\ell \mathbb{P}\left(\mu_{t,\ell} \mid \mathcal{T}_t\right) \mathbb{P}\left(\mathcal{T}_t\right)\right] \mathbb{P}\left(\sigma^2\right), \end{aligned}$$

MODEL PRIORS:

1. Node Depth Prior: P(Tt) ~ $\alpha(1+d)^{-\beta}$ where $\alpha \in (0, 1)$ and $\beta \in [0, \infty]$
2. Leaf-Value Prior: P(Mt | Tt) = $\mu_l \sim N(\mu_\mu / m, \sigma_\mu^2)$
   - $\mu\mu$ is picked to be the range center, $\mu\mu = \frac{y_{min} + y_{max}}{2}$
   - σ_μ^2 is empirically chosen so that the range center plus or minus k =2 variances cover 95% of the provided response values in the training set
3. Error Variance Prior: $\sigma^2 \sim$ InvGamma(ν/2, νλ/2)
   - λ is determined from the data so that there is a q = 90% a priori chance (by default) that the BART model will improve upon the RMSE from an ordinary least squares regression.
4. Response likelihood: mean of response in leaf in given MCMC iteration with variance: $y_i \quad N\left(\mu_i, \sigma^2\right)$

5. Default hyperparameters:
   - α: 0.95
   - β: 2
   - k: 2
   - ν: 3
   - q: 90%