PREDICTING THE OPTIMAL COMPUTING PLAFORM FOR CLIMATE-DRIVEN ECOLOGICAL FORECASTING MODELS

by

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ABSTRACT

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The University of Wisconsin-Madison, 2016

Under the Supervision of Professor John Williams

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# Acknowledgements

# 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-quarter of all species (Thomas, 2010). Species ranges, particularly those of vascular plants, are strongly controlled by climatic factors (Salisbury, 1926; Woodward, 1987), and global changes in climatic gradients is 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 biotic assemblages under different warming scenarios (Clark et al., 2014; Guisan & Thuiller, 2005; Guisan & Zimmerman, 2000; Guisan et al., 2013; Maguire et al., 2015; Thuiller et al., 2008). A growing volume of ecological data is available for modeling species-specific responses to the climate system, both at present and in the geologic past. Environmental monitoring efforts, such as the Long Term Ecological Research program (LTER, Hobbie et al., 2003), the National Ecological Observatory Network (NEON, Schimel et al., 2009), databases of the fossil record, including the Neotoma Paleoecological Database (http://neotomadb.org) and the Paleobiology Database (PBDB, http://paleobiodb.org), and modern biodiversity occurrence databases, like 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 responses to perturbations in the earth system (Brewer et al., 2012; Michener & Jones, 2012). While growing collections of modern and paleo biodiversity data has the potential to improve forecasting studies, data volume and heterogeneity can make successful uptake and implementation challenging for ecologists (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 gain access to configurable and convenient virtual resources (Mell & Grance, 2012). However, little guidance exists for the researcher approaching tradeoffs between model accuracy, performance and cost. The present study develops a method for identifying the optimal configuration on which to run SDMs, describing a flexible and skillful framework that can be used to inform provisioning strategies as well as suggest future priorities for model developers.

With over 700 million modern and historical occurrence records in GBIF and 18 million paleo-occurrence records in Neotoma, traditional statistical methods for analyzing, modeling, and forecasting ecological patterns 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 are unable to 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 techniques to cope with large datasets. As the volume of ecological data increases and the need for accurate, high resolution projections of biotic distributions become more pressing, reducing project scope (e.g., Bolker et al., 2009) can no longer be considered a valid option. Cloud computing provides a platform on which to undertake 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 products 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.

It is unclear when, if ever, the benefits in reduced computing time outweigh the financial costs of a high-performance, cloud-based computing solution, particularly in the context of climate-driven ecological forecasting models. The cloud’s novel expense model of charging users for the use of virtual machines (VMs) rather than the purchase of physical hardware lets consumers scale their resources depending on computational demand (Hassan, 2011). Users are therefore not locked in to a single hardware configuration, and can choose to add or remove different hardware components as the problem changes (Armbrust et al., 2009). While the exact costs of migrating to a cloud environment are difficult to estimate (but see Sun & Li, 2013), the computational time gains achieved by running models on high performance virtual instances can be significant (Yang et al., 2011a).

I hypothesize that, for any SDM modeling experiment, there exists an optimal data-hardware configuration that maximizes SDM accuracy while jointly minimizing the time and cost of modeling. In this thesis, I develop a framework for predicting the optimal configuration for four widely popular SDMs. I gather a large empirical dataset on the cost, runtime, and accuracy under different parameterizations and on different computing hardware. Subsequently, I fit a Bayesian learning model 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. My findings suggest that if SDMs are to benefit from cloud computing, future effort should be directed towards developing models that take explicit advantage of parallelism and distributed computing frameworks.

# Background and Previous Work

## Big Data in Ecology

The contemporary influx of massive datasets, including geonomic sequences, long term monitoring projects, phylogenetic histories, and biodiversity occurrence data, has required the development robust, expressive and quantitative methods in the biological sciences, and is promoting 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). Significant challenges, including the inability to move datasets across networks, increased metadata requirements for storage and data discovery, and the need to support novel uses for the data, are common (Schnase et al., 2014).

Ecological occurrence data -- spatiotemporally-explicit records of presence, absence, or abundance of individuals of a species or higher taxonomic grouping -- 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. Since the early 1990s, the Internet and an increased willingness to share primary data between scientists 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 derive from the literature or in the field (Beck et al., 2014; Grimm et al., 2013). Entire new fields, namely ‘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 primary data regarding life now housed in biodiversity databases (Soberón & Peterson, 2004).

The term Big Data is typically used to describe very large datasets, whose volume is often accompanied by lack of structure and a need for real-time analysis. Big Data, while posing significant management and analysis challenges, can provide new insights into difficult problems not tractable with smaller datasets (Chen et al., 2014). Though the precise definition of Big Data is loose, there are two prominent frameworks for discriminating Big Data from traditional 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, the Bigness of the data is specific to both the time 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 with time or as technology advances. Furthermore, the criteria for what constitutes Big Data can vary between problem domains (Chen et al., 2014), the size of datasets common that domain, and the software tools that are commonly used in that industry (Manyika et al., 2015). While Big Data most often refers to datasets between terabytes and petabytes (240 to 250 bytes), recent development of complex relational databases that store spatiotemporal occurrence records and their metadata suggests that traditional methods of data handling were not sufficient for modern ecological analyses (Grimm et al. 2013). Further developments, like 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). While not of the size common in popular commercial applications, new, custom-built tools to store, analyze, visualize, and use ecological occurrence data are required.

A second framework by which to assess Big Data is the ‘Four V’s Framework’. First introduced by IBM and used by large technological companies in the early 2000’s to characterize their data, it is now a popular and flexible framework under which to evaluate data Bigness. Here a dataset is described by its Volume, Variety, Veracity, and Velocity. Yang & Huang (2013) describe this framework by suggesting that “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).

Since the late 1990s, the scale of biodiversity information has become challenging to manage. Figures 1a and 1b track the growth in collections of Neotoma and GBIF, respectively, through time. In 1990, only 2 of the datasets now stored in Neotoma were in digitized collections. Today, there are over 14,000 datasets containing more than 18 million individual occurrence records, and associated spatial, temporal, and taxonomic metadata, corresponding to an average growth rate of 1,825 occurrences per day for the past 27 years. Nearly all records in Neotoma are derived from sediment coring or other fossil extraction efforts -- techniques that require large expenditures of time and effort (Davis, 1963; Glew et al., 2002). GBIF houses digital records of well over 700 million observations, recorded specimens (both fossil and living), and reports in the scientific literature. Since its conception in the early 2000s, the facility’s holdings have grown nearly 300%, from about 180 million records in 2001 to over 700 million records in 2016. GBIF’s efforts to digitize existing specimens allow its holdings to precede its origin in 2001.

Biodiversity data is also highly diverse and has many complicated interrelationships. As shown in Figure 2a, Neotoma’s holdings feature 23 dataset categories, including X-ray fluorescence (XRF) and isotopic measurements, macrofossils of both vertebrates and plants, modern and fossil microfossils, including pollen and non-marine diatoms and ostracodes. GBIF delineates 9 record classes, including human observations, living and fossil specimens, literature review, and machine measurements (Figure 2b). Though the records coexist in the databases, they are distinctly different, derived using different protocols by different communities of researchers. Moreover, the data is both spatial and temporal. All of Neotoma’s records and 87.6% of GBIF’s records are georeferenced[[1]](#footnote-1). 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. While controlled vocabularies and defined data structures help to efficiently assimilate large numbers of records, nearly every record was collected, analyzed, and published by a different scientist. While some scientists have contributed many datasets to occurrence databases, most have contributed only a handful. The median number of datasets contributed to Neotoma is 2 and the third quantile value is just 7 datasets. While specific metadata is scarce, each researcher is likely to use different equipment, employ different lab procedures, and utilize different documentation practices, contributing to a high variation between datasets.

Biodiversity data also has high levels of uncertainty associated with it. Some of the sources of uncertainty in the data, including spatial or temporal positional uncertainty can be estimated (Wing et al., 2005) or modeled (Blaauw, 2010). Both Neotoma and GBIF show high levels of quantifiable uncertainty. Of a random sample of 10,000 records of the genus *Picea* 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). Temporal uncertainties in Neotoma is also large. Out of a sample of 32,341 age controls (e.g., radiocarbon dates, varve counts) in the database, only 5,722 reported any age uncertainty at all. The remaining records indicate a mean uncertainty of ± 130 years of the actual date. Other sources of uncertainty have yet to be quantified, such as inter-researcher identification differences, measurement errors, and data loss incurred between field, lab, and database. Expert elicitation was recently used to quantify differences between known events in a pollen record. High variability was seen between researchers, suggesting that “expert knowledge of the region and the late-Holocene history of the site” is an important factor in making conclusions from the data (Dawson et al., 2016).

The final piece of the Big Data framework is the dataset’s velocity, which characterizes the dataset’s sensitivity to time. High velocity data must be analyzed in real time as a stream to produce meaningful insights. Tweets from the popular microblogging service Twitter (http://twitter.com), for example, are analyzed for trends as they are posted. Users are drawn to participation in up-to-the minute discussion and significant effort has been put towards the development of sophisticated algorithms that can detect clusters and trends in real time (Bifet et al., 2011; Kogan, 2014). Unlike many private sector applications, there is little incentive for biodiversity researchers to immediately analyze new occurrence records. Moreover, automated analyses of distributional data have been warned against, due to the overall poor data quality (Soberón et al., 2002) and high uncertainty.

While not time sensitive, ecological occurrence data requires advanced, sophisticated techniques to store and analyze, and demonstrates high volume, low veracity, and substantial variety, and should therefore be considered Big Data. To fully and accurately derive value from new data being added to these databases, novel techniques for working with this data are required, while traditional statistical analyses may begin to suffer because they were not designed to handle Big datasets.

## 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 2010 “25 Point Plan to Reform Federal Information Technology Management” (Kundra, 2010), federal agencies are now required to adopt a “Cloud First” policy when “contemplating IT purchases and evaluate secure, reliable, and cost-effective cloud computing alternatives when making new IT investments” (“NASA’s Progress in adopting cloud-computing technologies,” 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). In 2013, the NSF announced a $20 million dollar solicitation for supporting “research infrastructure that enables the academic research community to develop and experiment with novel cloud architectures addressing emerging challenges, including real-time and high-confidence systems”[[2]](#footnote-2). 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 Geonomes project, and by soliciting grants for researchers incorporating cloud computing into their research. Amazon Web Service’s website claims that many prominent research institutions, including the NASA Jet Propulsion Laboratory, rely heavily on their products and services[[3]](#footnote-3).

Cloud technology, both public and private, has been extensively lauded for its application in 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., 2015; Schnase et al., 2014). Cloud-based solutions for bioinformatics research relieve the large memory requirements often present in geonomics 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. Schnase et al. (2014) describes 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., 2015; Schnase et al., 2014).

Cloud services have also been used in the geosciences, and in ecological modeling problems specifically. Yang et al. (2011a) suggest that 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 (Yang et al., 2011b). In practice, cloud-optimized implementations of numerical models, such as real-time dust storm forecasting, have improved model performance significantly (Yang et al., 2011a). Environmental models can also be run in the cloud (Granell et al., 2013). Indeed, 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.

## Species Distribution Models

Species Distribution Models (SDMs) are a widely used class of statistical models that quantify the relationships between a species and its environmental range determinants (Svenning et al., 2011). While these models may sometimes include mechanistic or process components, they most often refer to correlative models (Elith & Leathwick, 2009) that use supervised statistical learning algorithms to approximate the functional relationship between species occurrence and environmental covariates. 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 lead 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 (Figure 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. Most scholars argue that SDMs approximate the species’ realized niche (Guisan & Zimmerman, 2000; Miller et al., 2007; Soberón & Peterson, 2005), though the inclusion of fossil data in the model fitting process can increase the likelihood that calibration captures the fundamental niche by exposing the model to states of the climate system not present on Earth today (Veloz et al., 2012).

SDMs rely on three important assumptions. First, as a fundamental justification for applying predictions across space and time, SDMs assume niche conservatism -- that the niche of the species remains constant across all spaces and times (Pearman et al., 2008). Though niche evolution is not accounted for, Peterson et al. (1999) suggest that species typically demonstrate niche conservatism on multi-million year time scales. Second, SDMs rely on the assumption 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 biotic interactions between species, this may rarely be the case. For example, Svenning et al. (2008) showed that many European tree species are still limited by postglacial migrational lag. Finally, SDMs must account for extrapolation to novel and no-analog climates for which there is no modern or fossil data. Inductive learning is severely impacted when it is used to predict onto future cases not within the range of values used in training. Williams & Jackson (2007) note the high likelihood of encountering novel and no-analog climates in the near future. Fitting the models with fossil data increases the likelihood that climatic assemblages will be included in the training data, however, given rapid and highly uncertain climate change, the problem of projecting models onto unseen climates is a major limitation on their application.

Despite strong assumptions, SDMs have been used in many paleo and contemporary studies of geographic and environmental distribution. 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), 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 both 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).

### 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 aim to model responses to climatic gradients, (Franklin, 2010) suggests a meaningful way of grouping algorithms into data-driven and model-driven categories. The data-driven/model-driven dichotomy is introduced in Hastie et al. (2009) and is often employed when differentiating between ‘statistical’ or ‘parametric’ (model-driven) and ‘machine learning’ or ‘nonparametric’ (data-driven) algorithms. I add, as a third category, the burgeoning set of methods that employ stochastic, probability-based Bayesian methods to this taxonomy due to their recent uptake, high accuracy, and explicit modeling of uncertainty. No individual method or class of methods has consistently outperformed any other (Araújo & New, 2007; Elith et al., 2006; Veloz et al., 2012), though many scholars have attempted to assess variation between 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 in general, use a set of training examples, , where both *x* (environmental covariates) and *y* (species presence) are known, to approximate the real relationship between the two, , with the learned approximation, . The learned function is the relationship that minimizes a loss function based on the difference between the real and predicted value, . Each training example () is composed of a -dimensional vector of covariates, , . Model-driven algorithms make *a priori* decisions about the structure of , while data-driven algorithms can adapt to fit any given design matrix.

Model-driven learners fit parametric statistical models to a dataset, making assumptions about how inputs and outputs are related, including linearity and error distribution. While these techniques can make poor predictions if the assumptions are not upheld, they were the first to see substantial use in SDM applications 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 . While not reliant on stringent assumptions about the form of the relationship, any particular portion of parameter space depends on only a handful on input points, making the models highly sensitive to small changes in the input data (Hastie et al., 2009). In some cases, these models been shown to out perform their model-driven counterparts (Elith et al., 2006), and include genetic algorithms (Elith et al., 2006), classification and regression trees (Elith, Leathwick, & Hastie, 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). 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. Recent critiques of the approach, however, suggest that its performance may be questionable (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 process the data and build the model (Hastie et al., 2009). Furthermore, data-driven learners 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.

Bayesian methods have also been used to approximate . 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 in recent years (Hegel et al., 2010). Golding & Purse (2016) introduce SDMs that incorporate Gaussian processes, 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 the frequentist perspective to transition to a Bayesian approach (Ellison, 2004; Hegel et al., 2010), software packages are in development for implementing Bayesian SDMs in languages like R (e.g., Vieilledent et al., 2012). MCMC methods are computationally very 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. Of 100 randomly sampled recent publications in Web of Science that met the query “*(Species Distribution Model) OR (Ecological Niche Model) OR (Habitat Suitability Model)*”, the overwhelming majority used data-driven models. Of 203 modeling runs described, 131 were data-driven, 38 were model-driven, and 1 was Bayesian (Figure 4). 33 additional 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.

### Computational Challenges and Species Distribution Models

Because of the overwhelming propensity of scholars to employ methods in the data-driven category, 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. Elith et al. (2006) recorded the execution time of the runs they used in their often-cited review of novel SDM techniques, noting execution times of up to several weeks for some modeling algorithms. Popular learning models, including boosted regression trees (80 h), generalized additive models (17h), generalized linear models (17h), and MaxEnt (2.75 h), were all shown to be extremely computationally intensive. The authors suggest that performance could be improved if model building was split over multiple processing cores. While processor speeds have increased since their 2006 analysis, models are still often unable to leverage multiple processors.

Methodological papers often advise against large modeling studies due to computational limitations. A 2009 review 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 (Bolker et al., 2009). 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 may alleviate some of these problems, but often, the computational intensity of SDMs forces a reduction model complexity or scope.

## Assessing Algorithm Execution Time

It is possible to theoretically estimate the upper, lower, and average run times of an algorithm using asymptotic complexity analysis. In this exercise, the order of growth of an algorithm’s runtime is determined as its input is increased to infinity, so that only first order terms are relevant (Knuth, 1976). The algorithm that is more efficient asymptotically will typically be the best choice for all but very small inputs (Cormen, 2009). An estimate of the slowest run time (Big-O), can usually be obtained by inspecting the structure of the algorithm and counting how many operations are required when the inputs is sufficiently large (Cormen, 2009). Such theoretical complexity is often considered when considering 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). Brewer (1995) describes an initial attempt to develop a statistical model for the run and compile time of algorithms in a C library. While most contemporary empirical runtime models use data-driven pattern recognition, linear regression between input size and execution time has been shown to perform well in some cases (Fink, 1998). Empirical complexity models have recently become an important subfield of artificial intelligence and have important applications to algorithm selection (Hutter et al., 2014). Algorithms for solving very difficult (-Hard/-Complete) combinatorial problems, can exhibit high runtime variance between different problem instances. Empirical models can be used to select the model 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, including random forests, 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; Hutter et al., 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).

Jones & Kalibera (2013) suggest that 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. Dongarra et al., (1987) warn that a failure to properly characterize the workload, running benchmarks that are too simplistic, or running benchmarks in inconsistent environments can lead to meaningless results.

# Theoretical Problem Formulation

In the present study, I use benchmarking and empirical performance modeling to develop predictive models useful in optimizing SDM workflows. The following framework presents an SDM workflow – a series of steps that advance the model user towards her goal of obtaining scientific insight from a dataset. As a rational consumer in a supply and demand driven computing market, and with imperfect information regarding the covariate-species presence relationship, the modeler will undertake several steps, including model computation, to minimize her costs, in both time and model, to maximize her utility, represented here as proximity to the knowledge of the true functional relationship, , between environment and species presence, and measured as SDM accuracy (Simon, 1986).

1. Consider a pool of computing resources, , that is characterized by its hardware capabilities, including memory, CPUs, and any other component that affects effective computing power.
2. Consumers of computing services are part of a market driven by supply and demand, and face costs set by computing providers that are a function of the computing power provided: For example, Google’s infrastructure-as-a-service (IaaS) cost surface is clearly a function of memory and CPUs (Figure 5). While traditional, non-cloud computing has a fixed cost model, total purchase price can be converted to an hourly rate if several assumptions about computer use and lifespan are considered.
3. Every user of a modeling application has a particular set of goals for using it in the first place (Norman, 1984). We can conceptualize, for any given model, a finite set of use cases that fall within the bounds of existing or expected use (Carroll, 1999; Rosson, 2002). Let be a vector of characteristics that fully describe the user’s goals in the scenario. The components of 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 (
4. Assume, in addition to computing the model, the user must also undertake a number of other pre- and post-processing steps. The total time elapsed during a modeling experiment can be expressed as

Where 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, and is a function of the computing resources available to the user (how fast can data be downloaded?) and the experiment (what is the data?). represents time required by the modeler to prepare the data for entry into an algorithm, including data cleaning, projection, and conversion, and can vary widely between modelers, data source and quality, and user skill and motivation. For example, Elith et al. (2006) note the potential impact of user experience on the modeling time and results. is the time spent computing the model. represents time needed to transfer the output from the source of computation to the user, which may be non-trivial if the model is run on a set of remote resources and network downloads are included. Finally, represents the amount of time spent by the user evaluating model output and determining whether her goals were met during the modeling process. Like , this term may be highly variable between model users and applications.

1. Single experiments can be combined together to form workflows, so that a user’s time-to-goal for a workflow of modeling experiments can be expressed as a function of the experiments and the computing resources on which they are run.
2. Combining equations from (2) and (5), the total time for a modeling experiment is the sum of total time of spent modeling and the total monetary cost is the cost of provisioning computing resources for this time. The total workflow cost is then a function of the user and their 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:
3. Let *U* be the set of all possible scenarios. Each individual scenario, *u*, will have its own cost curve that’s subject to both the particular characteristics of the workflow and the cost surface imposed by the computing provider. If select one and call it , we can 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 corresponds to the optimal hardware for use in this modeling scenario.
4. 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 the cost of provisioning the computing resources for the time required. A set of weights could be applied to preferentially weight one or more of these 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.

# Hypotheses

The remainder of this thesis addresses several 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. hardware will affect the runtime of the SDMs, but not the accuracy;
  3. data volume will affect both the runtime and accuracy of the SDM; and
  4. SDMs will be differentially affected by data and hardware

In the study, I will characterize data as the number of training examples and the number of environmental covariates used to fit the model. I will characterize hardware as the number of CPUs and amount of memory, in gigabytes (GB), of the VM on which the SDM is run. I will use four SDM algorithms that 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 (Breiman, 2006; Elith & Graham, 2009). The experimental design was meant to mimic actual use cases, and performed using popular implementations of the algorithms in R.

# Methods

## Data Collection

### 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 package for that model for use with SDM. 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 Paleoecological Database in April 2016. 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 using a comma separated value format file.

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 (VIF, Obrien, 2007). The variables retained were BV2 (mean diurnal temperature range), BV7 (annual temperature range), BV8 (mean temperature of wettest quarter), BV15 (precipitation of warmest quarter), BV17 (precipitation of warmest quarter), and BV18 (precipitation of driest quarter).

Future climate layers for the year 2100 were obtained from the CMIP project, HadCM3 climate model. These layers represent modeled climate variables under the UN IPCC RCP 8.5, a scenario that assumes high population, moderate economic growth, and a sustained dependence on fossil fuels (Riahi et al., 2011). These layers were processed as above.

### Computing Infrastructure

Google Cloud Compute Engine (GCE) cloud-based virtual machines were used for all model runs. Google’s platform was chosen over other public cloud vendors because of its ability to create ‘custom’ instance types that adhere to user-defined specifications of hardware configuration. Other vendors (e.g., Amazon Web Services) provide a larger number of predefined instance types, but do not support the creation of an instance with arbitrary hardware. VMs running Debian Linux 8 were provisioned and released as needed. Git was used to transfer required files to computing nodes. Experimental results were stored in a MySQL relational database for further analysis. Automation was facilitated by using a combination of master-compute node architecture, a Node.js database API, a python control script, and a set of MySQL database tables holding the specification for each required trial. The system is illustrated in Appendix B.

### SDM Model Protocol

For each hardware configuration (CPUs and memory), data parameters (number of covariates and number of training examples) were communicated to the node via a configuration file. Pre-processed occurrence points were partitioned into a testing set (20%) and a training set (80%) of the total number of teaching examples (i.e., occurrence points). An SDM was fit to the training data, projected to the modeled future climate, and assessed for accuracy. Accuracy was evaluated using the testing set and quantified using the Area Under the Receiver Operator Curve (AUC) statistic. Learning (hyper)parameters were initially evaluated as a potential predictor, but were discarded as uninformative, though have been noted to substantially change learning accuracy (Hastie et al., 2009 ) Timing was done within R using the proc.time function for timing arbitrary pieces of code. No database I/O was done inside of the timing script, so network connection speed is not expected in influence the results. The timing script is publicly available on the code-sharing platform Github (http://github.com/scottsfarley93/thesis-scripts).

In total, 26,730 experimental trials were made. Data-hardware configurations were chosen to maximize the parameter space covered in the analysis while maintaining at least three replicates per configuration. Where feasible (see “Assumptions and Limitations”), more replicates were made.

## Modeling Performance and Accuracy

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). The Bayesian model fits a probability distribution for the response at each leaf node, rather than the standard single maximum likelihood estimate. An boosted ensemble size of 50 trees was used, and models were fit using default priors on the parameters and hyperparameters as suggested by the authors (Appendix C). For more details about the model and its implementation, see Kapelner & Bleich (2016). Runtime and accuracy were modeled separately for each SDM. Runtime was modeled on a log scale (log-seconds), which has been shown to improve prediction 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. The first 250 iterations were discarded as burn-in, leaving 1000 posterior samples to analyze and evaluate.

## Model Evaluation

The predictive skill of each model was evaluated using the mean squared error (MSE), the statistic between observed and predicted values from the mean of the posterior distribution, and the standard deviation of the prediction posterior. Visual assessment of model results was done by plotting the predicted values against the observed data and qualitatively assessing deviations from the y=x line.

Strength of model drivers was evaluated by cross validating the performance of a separately built model using four of the five model predictors. Each predictor was left out of a model in turn, and the of the subset model was evaluated and compared to the of the full model. The reduction in is interpreted as the predictive strength of the left-out variable.

## Optimal Prediction

Prediction of the optimal data-hardware configuration for an SDM consisted of a four-step process (Figure 6). First, the accuracy model was used to identify the accuracy-maximizing data configuration. Second, the performance model was used to predict the execution time of the accuracy-maximizing model run on a large set of hardware configurations. Third, multidimensional hierarchical clustering was used to assemble groups of configurations similar to one another. Finally, the hardware cluster with the lowest runtime, cost, and uncertainty was selected as optimal. The spatial region and extent (number of grid cells in the prediction) is chosen *a priori* by the researcher, and is not included in optimization.

To predict the accuracy-maximizing data configuration for an SDM, the accuracy model corresponding to that SDM was used to predict the accuracy of a 500 of regularly spaced data configurations. This set of predictions included every 100 training examples between 0 and 10,000 and every number of covariates between one and five. Hardware configuration was included, as I hypothesize that hardware should not affect SDM accuracy (see Table 3). Predictions were sorted, first by descending order of accuracy, then by ascending order of number of training examples, and finally by ascending number of covariates. Training examples are costly in time, therefore, given equal accuracy, the configuration that requires the least number of training examples was preferentially chosen.

The accuracy-maximizing data configuration, and thus expected accuracy, was held constant and used as an input for the performance model. This model was used to predict the runtime of an experiment with the given data configuration on a set of 288 CPU and memory configurations. Candidate configurations were chosen from GCE allowable custom instance types, and covered the parameter space between 1 and 25 cores and 1 and 25 GB of memory. Each runtime prediction was evaluated as 1000 samples from the posterior distribution. The mean of the distribution was used to calculate runtime cost, using GCE custom instance type rates[[4]](#footnote-4), and the standard deviation was used as a measure of prediction uncertainty.

The runtime predictions were then clustered using complete linkage hierarchical clustering on runtime, run cost, and prediction uncertainty. Prior to clustering, the dataset was centered and scaled using the R scale function. 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.

## Extensions

Several extensions to this optimization are possible, including weighted optimization and constrained optimization. The optimization described above weights each dimension equally, assuming equal importance for run time, run cost, and model uncertainty. However, the routine could easily accommodate user-specific weighting on these components by using multipliers applied after the runtime predictions have been made. This would allow a user to preferentially increase or decrease the effect of a component during further analysis.

Two forms of constrained optimization are also possible as modifications to the procedure described here: data-constraint and time-constraint. The unconstrained analysis above assumes infinitely large datasets are available to the model user, which is rarely the case. Indeed, many SDM analyses consider datasets of less than 100 occurrences (Wisz et al., 2008). A data constrained optimization would allow such small datasets to be considered under the same framework. In the constrained analysis, the space of potential data configurations is first subset to include only those for which data exists. 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.

A second form of constrained optimization is a time-constrained optimization, where runtime must fall below a certain threshold to meet user-defined standards. First, a large set of realistic configurations is selected and the runtime for each experiment 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.

# Limitations

This approach has several important limitations. Perhaps most importantly, while a real SDM workflow contains terms other than those directly related to model computation, I focus here on only computing time. User skill and motivation and can depend on many factors that may be difficult or impossible to model. While excluding terms improves the tractability of the problem, predictions of the true optimal value are no longer possible. Future work could be pointed towards modeling these factors in a form that could be incorporated into this predictive model framework. Furthermore, I limit my analysis to include only two hardware components, CPU cores and memory, to keep the project to a manageable scope. Other hardware components may improve model results, but are difficult to manipulate experimentally.

A second limitation of the approach described here is that my analysis is limited to virtual computing instances hosted on Google Cloud Compute Engine (GCE), rather than real-world physical machines, limiting the conclusions I am able to draw about the relative benefits of physical hardware and virtual machines. However, this experimental design adds validity to the benchmarks of computing time, by providing them with a consistent environment unaffected by other tasks or concurrent programs (Dongarra et al., 1987). Nonetheless, because real-world machines do have many concurrent and interacting processes running at any one time, this may bias the results. Moreover, by using GCE, I am unable to experimentally vary the CPU clock rate as a hardware component. By using GCE VM instances, I am limited to only the processors provided by Google, which may be updated or changed at their discretion. At the current time, GCE provides only one processor type for the VMs I used, a 2.6 GHz Intel Xeon E5 processor. Fortunately, my results will not be biased by non-experimental manipulation of CPU rates, as might be the case if I collected data on physical machines instead of virtual instances.

I limit my work to the analysis of data-driven SDMs, as systematic literature review suggests that a majority of SDM users use these methods. Furthermore, I focus on the most popular R implementations of these SDMs. While 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. 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, it is distributed as a black-box algorithm.

A final limitation was computational cost. In order to gather enough data to develop a predictive model that covered the realistic parameter space, I limited the number of models running longer than several hours and the number of replicates. Similarly, I limited my experimentation on virtual servers with expensive hardware configurations to allow for more experimentation on less costly servers. More data collected in all areas, particularly on virtual instances with high memory and many CPUs may improve the robustness of the results presented here.

The utility of the results may be limited, as they will become outdated as the computing landscape changes and computing providers change their pricing schemes. Hardware capabilities continue to improve, yielding faster processors, better cores, and higher-performance memory. Furthermore, prices for computing resources continue to decrease, particularly as cloud computing gains popularity. The optimization framework, however, is robust to both changing hardware capabilities and costs. To incorporate new hardware, 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 a new pricing scheme, the dataset could be left unchanged, and only the third and fourth steps of the optimization (clustering and distance calculation) would need to be re-run using the new costs.

## Framework Extensibility

Though 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). Furthermore, I argue that 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, further work should be directed at confirming this hypothesis.

# Results

## Model Performance

Predictive models of performance and accuracy were skillful when compared to a holdout testing set. While results varied across SDM classes, the models for each SDM explained more than 50% of the variance in the runtime data ( and more than 87% of the variance in the accuracy data (). The most explanative performance models were for GBM-BRT and MARS, with values of approximately 0.96, and an MSEs of approximately 0.05 log-seconds2. The estimates from all models were tightly constrained, with low mean standard deviation of the prediction posteriors. The mean posterior SD for GAM, GBM-BRT, and MARS were all between 0.01 and 0.035 log-seconds, suggesting high certainty in the predictions. Performance model evaluation statistics are presented as Table 1 and shown in Figure 7.

Both GAM and RF models were less explanatory than the other two SDMs, both shown to have lower values than the other two models. It is likely that several factors contributed to this lack of predictive skill. The observed GAM trials tended to converge within several seconds (maximum 10.3s), regardless of data or hardware configuration, potentially exposing it to a stronger influence by low-level system processes not explicit in the model and resulting in a higher variance dataset with lower predictive power. In contrast, the other three SDMs take minutes to hours to terminate (maximum in training: GBM-BRT, 5285.0 s). Secondly, both 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. While the parameter space appears to be relatively well covered for these models, additional data, including more replications and parameterizations, may enhance model skill. Nonetheless, all models explained a majority of the variance in SDM runtime. While stochastic variance in system processes is often suggested as an impediment to modeling algorithm execution time, the results shown here indicate that a skillful model can be produced without accounting for this source of error.

The accuracy models were more skillful than the performance models, despite the large number of hyperparameters suggested to enhance SDM accuracy, including the shrinkage parameter and tree depth (GBM-BRT) and ensemble size (RF) (Hastie et al, 2009). The RF accuracy models was the best performing of the four, with an of of 0.98 and a MSE of less than 3.5x10-5 AUC. Moreover, all of the accuracy models indicate low uncertainty and well-constrained posterior estimates on their predictions. GAM predictions have the highest uncertainty associated with them, again perhaps due to small training set size. The full accuracy assessment is presented in Table 2 and shown in Figure 8.

## Model Drivers

As hypothesized, factors that control runtime of SDM vary between algorithms (Table 3). One of the most important contributions to SDM runtime 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 ). 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). However, surprisingly, the number of environmental covariates is not shown to be an important predictor of runtime for any SDM; only GBM-BRT is influenced by this predictor, and only slightly. Theoretical complexity suggests that learning algorithms are often asymptotically influenced by both training examples and covariates. However, under real workloads, it appears that the number of covariates does not have a strong influence on run time. GAM, interestingly, is quite strongly controlled only by the number of cells on which to predict the fitted model. This SDM’s convergence time, as described above, is often trivial; nearly all of the total time during each experiment was spent predicting the model onto the novel climate scenario grid.

Importantly, with the exception of RF, the computing variables, memory and CPUs, have relatively little influence on execution time. For GAM, GBM-BRT, and MARS, CPU capacity accounts for less than 1 percent of the total variance. Similarly, for all models, memory accounts for less than 3% of the structure in the data. Random forests, as expected due to their ability to be built in parallel, show a slight dependence on CPU cores (~5.55%). However, the overall trend of low dependence on hardware capabilities is surprising, indicating that, without additional optimization, SDMs run at roughly the same speed on computers of all hardware configurations.

MARS shows a surprising and strong dependence on memory. Upon further investigation, I suggest that an error in sampling design incorrectly weighted some portions of the parameter space and may have artificially biased model results. Nearly ten times as many experimental trials were run on two VM instances -- a one core, 4 GB memory VM and a four core, 16 GB memory VM -- than other instance types. While the full parameter space was explored, I believe that the additional influence of these data points may have caused biased results, indicated in the model drivers and seen in the optimized hardware below.

SDM model accuracy is closely tied to the amount of data being used to fit the model. Together, the configuration of training examples and covariates accounted for over 50% of the model skill in all models. Indeed, for RF and GBM-BRT, data volume accounted for nearly 80% of the model’s total predictive skill. As seen in the runtime model, GAM is different than the other three SDMs, and is only strongly controlled by the number of covariates in the training set. As I hypothesized, model driver evaluation suggests that hardware and cells have very little influence on SDM accuracy.

## Optimization

An unconstrained optimization was undertaken to determine the optimal data-hardware configuration assuming infinitely large datasets and arbitrary computing resources.

### Data Configuration

The accuracy surface of each model was fully evaluated, and the point that resulted in the highest accuracy with the least data was selected. Most of the accuracy-maximizing points lie close to the top right of the space; requiring all available data, as expected from both theory and empirical analysis of model drivers. The total possible number of training examples and covariates was limited due to in the experimental design, so supplying additional data may further increase SDM accuracy. However, literature suggests that typical SDM workflows often use less than 10,000 training examples and five covariates. Interestingly, the MARS achieves its highest predicted accuracy with only 1000 training examples, rather than 9000 or more for all other SDM types. The MARS accuracy surface is interesting in that after ~1000 training examples, in which accuracy increases quite quickly, only the addition of more covariates can increase accuracy (see Figure 10). In all cases, additional covariates continued to increase accuracy up to the five covariates included in this analysis, while additional training examples alone were not guaranteed to improve accuracy.

### Hardware Configuration

The optimal configuration of hardware for each SDM was calculated using the unconstrained optimization routine. Figure 9 shows the location of the cluster of optimal configurations in CPU-memory space. In general, this analysis suggests SDMs require few CPU cores. GBM-BRT is best suited to only one CPU core, while the GAM optimal lies at 3 CPUs. As suggested by moderate dependence on CPU cores in the runtime model and the ability to build ensemble members on separate cores, random forests are best suited to between four and seven CPU cores. MARS require anywhere between 1 and 25 cores, however, due to the sampling issues described above, this result should be interpreted carefully.

Memory requirements are generally low. RF and GBM-BRT are both optimized at only one gigabyte of memory. GAMs are best suited to between one and 20 GB. Because of the clustering, each of members of the optimal cluster is statistically identical, suggesting very little dependence at all on memory for GAM -- one GB of memory is as suitable for running these models as 25 GB. Looking back at the contributors to the runtime of this model confirms that virtually no structure in the data is explained by VM memory. Therefore, this SDM can be interpreted as requiring only one GB of memory. Finally, MARS is optimized at 16 GB of RAM, though again, this result should be discarded or interpreted with caution. Since there is no incremental increase in SDM runtime between 1 and 16 GB of memory, I suggest that these results are not correct. Furthermore, optimization analysis suggests that the second best cluster (not shown) is at only 1 GB of memory, further implicating biased observational data.

# Discussion

## Relative Location of the Accuracy Maximizing Point

The position of the data configuration that maximizes accuracy within the space of training examples and covariates yields an interesting perspective on the maximization of SDM accuracy. One might suggest that additional covariates and training examples would uniformly enhance model prediction and its ability to characterize future examples. However, observational results suggest otherwise. While GBM-BRT and RF require all available data, both GAM and MARS require less than the full dataset to maximize accuracy, needing less training examples. Moreover, a given accuracy may be achieved by several unique data configurations, suggesting that an accuracy substitution rate (ASR) may be used to characterize the amount of one input that can be substituted to get to the accuracy obtained by an increase in the other input. The ASR is dynamic and changes across models and across the configuration space. ASR curves for each SDM are shown in Figure 10.

All SDMs show a rapid increase in accuracy with the addition of the first 1000 training examples, after which the number of covariates dominates an increase accuracy. GAM, GBM-BRT, and MARS all show nearly vertical ASR curves after approximately 2500 training examples, indicating that additional occurrence observations are unlikely to significantly affect model accuracy. Instead, more covariates must be included to increase accuracy. RF shows an interesting oblique pattern of accuracy contours throughout, indicating that training examples can be easily substituted for covariates, and visa versa, if sufficient data exists. Like GBM-BRT, a flattening of the ASR contours indicates that eventually, many thousands of training examples are needed to substantially increase accuracy, while adding more covariates is unlikely to affect accuracy.

The ASR is important to evaluate for three reasons. First, it provides the model user with the tools to predict maximum accuracy with their given data, before a model is run. While the accuracy may be low, knowing the character of the accuracy surface informs the model user of estimated accuracy before they begin the modeling process. Second, it can be used to identify when garnering additional data is no longer necessary or where additional data collection efforts should be pointed. Depending on the SDM, effort could be put preferentially into finding additional covariates or training examples. In a data-limited situation, for example, when modeling a rare species, a researcher weigh the relative return in accuracy of identifying additional occurrence points against the expected effort of finding them. Moreover, for some models, additional data will not result in any increased accuracy. For example, beyond 1000 training examples with MARS, no additional accuracy will be achieved despite additional training examples. The time and effort going to collecting these training examples could, in this case, be better spent identifying additional covariates. Third, the performance models respond differently to training examples and covariates. Knowing the ASR may enable the research to improve the execution time of the SD, for example, if a similar accuracy may achieved either covariates or training examples, the configuration with fewer training examples should be selected. The ASR effectively describes the tradeoffs between the two parameters so that the choice can be quantitatively modeled.

## Sequential Model Hardware Responses

R implementations of GAM, GBM-BRT[[5]](#footnote-5), 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, as 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 model building. Empirical results support this claim, showing that less than one percent of the variance in these three SDMs’ runtimes is explained by the number of CPU cores on the VM. While MARS shows a wide range of CPU core preferences, both GBM-BRT and GAM have clearly defined optimal configurations at a low number of CPU cores. In both cases, there is no demonstrated advantage of a higher CPU configuration.

Furthermore, no SDM, except MARS, responds to increased memory allocations on the VM. The GAM and GBM-BRT optimal configurations both require very small amounts of memory, consistent with the fact that even large the training sets fit well within the VM’s main memory. As noted above, MARS is optimized at 16GB of RAM, though there is no reason for greater memory requirements than the other sequential algorithms. Anecdotal observational evidence suggests that SDMs may fail under very large dataset sizes. Although not tested rigorously, datasets exceeding 100MB, or several hundred thousand training examples, caused fatal crashes in R. The R language 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.

It is important to evaluate the expected accuracy against the expected execution time of these runs. While GAM typically converges much faster than GBM-BRT, its predicted maximum accuracy is also lower. Of course, along with increased processing time, GBM-BRT models have higher costs as well, with several observed data-hardware configurations costing more than $5. While more expensive, GBM-BRT may result in an increase in AUC of nearly 0.15, associated with a transition from ‘fair’ to ‘good’ in a qualitative assessment of the AUC statistic (Araújo et al., 2005; Swets, 1988). The specific application and individual modeler may dictate whether or not the tradeoff between an increase in accuracy is worth the order of magnitude increase in execution time and cost.

## Random Forest Model Hardware Responses

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. Given the approximately equal accuracy, 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 well the trade off between monetary cost and time. Because the algorithm can make effective use of additional CPU cores, configurations with additional cores are associated with 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, for example, during setup and ensemble combination. Because of the portion of code executed on a single processor, it is impossible to obtain an infinite speedup across infinite processors (Amdahl’s Law, Amdahl, 1967). Inter-core communication increases as addition 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 difference between parallel (*TN*) and serial (*T*1) runtimes of the algorithm, divided by the number of cores (*N*), given as:

Figure 11 demonstrates the diminishing marginal returns of the RF algorithm when run on multiple processors and on dataset with different numbers of training examples. The difference between a model run sequentially and one run in parallel with just two cores is large, while the marginal benefit of adding the 16th or 24th core is comparatively small. An infinitely parallel algorithm (E=1), incurs no diminished returns as additional cores are added. RF efficiencies vary by the number of training examples, but range between 0.05 and 0.4 at 25 cores. Importantly, workloads with more training examples, are better suited to parallelization -- have higher efficiency -- than small modeling problems with few training examples. For example, SDM runs with 10,000 training examples experience a much slower decline in efficiency than runs with 1,000 training examples. Biodiversity database size trends suggests that much more data will be available to researchers in fitting SDMs over the next decade. Therefore, parallel SDMs, like random forests, are likely to see increased benefits of running in a cloud-based environment, because the hardware can be easily scaled to meet problem needs and optimize efficiency.

## Utility of Constrained Optimization and Weighted Optimization

The unconstrained maximization routine is useful when neither data nor runtime is externally limited. However, in many real-world situations, scenarios when neither of these factors is limited are unlikely. Constrained optimization, either on runtime or data volume can be useful in these situations. For example, a constraint on the number of training examples or covariates available to the researcher seems probable, as the low-friction availability of biodiversity records in databases like Neotoma and GBIF if more data were available, it would be incorporated.

It can also be useful to place a hard maximum bound on the execution time or cost of the SDM. For example, consider a cloud-based SDM application that computes SDMs for arbitrary datasets remotely and returns the results to the client over the Internet. Users of interactive web applications are apt to loose interest and turn their attention to other tasks 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 using the application. It would benefit the application developer, then, to limit the time it takes to complete the model so that (a) their costs are minimized and (b) they retain the user’s interest and business. 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 continue to keep their audience engaged.

Another potential extension of this work is weighted optimization to preferentially influence one or two of the three components included in the determination of the optimal clusters. In a standard optimization, run time, run cost, and prediction uncertainty are all weighted equally. However, a given researcher may care different amounts about each of these axes. For example, she may care most about achieving low-cost, next about the level of certainty on the prediction, and finally about the time it takes to complete the modeling. Weighting each axis would allow the user customize the optimization to meet her own needs.

## Cloud Computing’s Role

The relatively minor contributions of hardware to model execution time, suggest that the sequential models 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 model 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, fitting its own SDM experiment. To make this work automatically, efficiently, and without error would be difficult and require a significant amount of technical skill.

RF, however, is a good candidate SDM for incorporation into a cloud-based runtime environment that supports 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.

Of course, even for RF, the difficulty of the transition to a cloud-based solution may outweigh its 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.

## Future Model Development

The sensitivity of SDM execution time to the number of training examples suggests that popular SDM algorithms like those examined here may be unable to cope with large training datasets possible as biodiversity database size increases. 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 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” (Elith & Leathwick, 2009).

Due to rapidity of database growth, I contend that modelers should focus their effort not only on the incorporation of ecological realism, but 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. New model development efforts should be undertaken to advance models that effectively leverage high performance computing infrastructure, multiple computing cores, effective memory management strategies, and scalability. While some attempts to refactor traditionally sequential models to run in parallel have been successful, these studies used entirely novel implementations of the traditional techniques (GBM-BRT, Tyree et al., 2011). Together the incorporation of additional ecological relevant information will help to strengthen the ecological inference made from these models and the computational optimization of modeling algorithms will facilitate inference from much more data.

# Conclusion

My results suggest fairly short runtimes and very low costs, for all models. The longest observations of runtime are only several hours, far short of the several weeks suggested by Elith et al. (2006). However, as data volumes grow and modeling approaches become more common, even these short runtimes become formidable. Many studies now model hundred 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 is not feasible. Therefore, while the individual results presented here may seem small, they add up quickly for all but the smallest modeling activities typical in contemporary SDM literature.

In this thesis, I presented a framework for approaching the tradeoff between accuracy, time, and money when considering the provision of computing resources for species distribution models. A theoretical model for determining the time for a user to reach her modeling goal was developed and empirical observations collected for over 30,000 simulations of four SDMs. Predictive models of SDM runtime and accuracy were built using Bayesian regression trees and used to evaluate the controls on SDM accuracy and execution time. The data-hardware configuration that maximized accuracy while jointly minimizing execution time and cost was identified and appraised for each SDM.

The predictive models and optimization framework show considerable skill, and can be used to improve researchers allocation of time and money, as well as inform model developers on future priorities. My findings suggest that contemporary models are unable to effectively leverage high performance computing resources (Figure 12), and are likely to struggle to find insight from massive global biodiversity databases. Future model development should be directed towards enabling state-of-the-art SDM algorithms to support very large datasets.

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# Figures

## Figure 1: Growth of Community Biodiversity Databases Through Time

Figure 1: Growth of Community Biodiversity Databases Through Time. Tracks the growth of the Global Biodiversity Information Facility (A, left) and the Neotoma Paleoecological Database (B, right).

## Figure 2: Biodiversity Database Record Heterogeneity

Figure 2: Biodiversity Database Record Heterogeneity. Describes the relative heterogeneity of record types in the Global Biodiversity Information Facility (A, left) and the Neotoma Paleoecological Database (B, right). Note that vertical axis in panel A describes millions of occurrence records, while the axis in panel B describes dataset types, due to the respective data models of the two databases.

## Figure 3: SDM Citations, 1997-2015

Figure 3: SDM Citations, 1997-2015. Tracks the number of published literature 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 in the 2016 Science and Engineering Indicators (NSB-2016-2, National Science Board (U.S.), 2016) (black).

## Figure 4: Classification of Selected Studies

Figure 4: Classification of Selected Studies. 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 of Knowledge on (“Species Distribution Model\*” OR “Ecological Niche Model\*” OR Habitat Suitability Model\*”), from which a subset of 100 studies was used for scoring. Scoring was based on Hastie et al. (2009), Franklin (2009) and Elith et al. (2006). Studies that used unsupervised clustering routines were classified separately, since they cannot be used in model-prediction tasks.

## Figure 5: Google Cloud Engine Custom Infrastructure Pricing Scheme

Figure 5: Google Cloud Engine Custom Instance Pricing Scheme. Presents the supply and demand driven market price surface faced by consumers of computing utilities in dollars per hour as a function of the computer hardware provided.

## Figure 6: Flowchart of Unconstrained Optimization Procedure

Figure 6: Flowchart of Unconstrained Optimization Procedure. Illustrates the four-step process of optimizing the data-hardware configuration for an SDM.

## Figure 7: Performance Model Evaluation

Figure 7: Performance Model Evaluation. Plots observed SDM runtime against the predicted SDM runtime for configurations in the holdout testing set. Black line shows the y=x line expected from a perfectly-predictive model. Note the logarithmic axes, and the highly variable scale of prediction between SDMs.

## Figure 8: Accuracy Model Evaluation

Figure 8: Accuracy Model Evaluation. Plots the expected SDM accuracy, measured by the AUC statistic, against the predicted accuracy. The black line shows the x=y line, expected by a perfectly-predictive model.

## Figure 9: Results of SDM Hardware Optimization

Figure 9: Results of SDM Hardware Optimization. Shows the optimal hardware configuration for the accuracy-maximizing experiment for each SDM type. Given the potentially biased results, interpret the MARS optimal configuration with care, as its dependence on high levels of memory may be spurious.

## Figure 10: SDM Accuracy Substitution Curves

Figure 10: SDM Accuracy Substitution Curves. Shows the accuracy substitution rate as a function of training dataset volume for each SDM algorithm. Contour interval is 0.01 AUC and labels are every 0.05 AUC.

## Figure 11: Parallel Efficiency of Random Forests

Figure 11: Parallel Efficiency of Random Forests. 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 may be interpreted as the marginal return gained by provisioning additional cores for running the algorithm. The perfect efficiency line is shown, though according to Amdahl (1967), this is impossible to achieve under real circumstances.

## Figure 12: Mean Configuration Distance from Optimal

Figure 12: Mean Configuration Distance from Optimal. Shows the mean distance of each hardware configuration from the origin over all SDMs when each configuration’s distance to the origin was averaged over each SDM. Green indicated closer to the optimal for all SDMs, while orange suggests further from optimal. MARS was omitted from the figure, due to its potentially misleading sampling and dependence on memory. The large green area between two and four cores is likely strongly controlled by GAMs lack of dependence on memory. Note the large portion of the space far from the origin. Remember that uncertainty is considered in the analysis.

# Tables

## Table 1: Performance Model Evaluation Statistics

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| SDM | Training | Testing | MSE |  | Posterior SD |
| 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 1:* Performance model evaluation statistics. Training denotes the number of data points used to fit the model with. Testing represents the number of data points that were used in evaluation, held out from model fitting, approximately equal to 20% of the total dataset. MSE is the mean squared prediction error, measured in log-seconds2. 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.

## Table 2: Accuracy Model Evaluation Statistics

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| SDM | Training | Testing | MSE |  | Posterior SD |
| 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 2:* Accuracy Model Evaluation Statistics. Fields are as in Table 1.

## Table 3: Controls on SDM Performance and Accuracy

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Performance Model** | RF | MARS | GBM-BRT | GAM |
| Number of Covariates | -0.03% | 0.02% | -1.67% | 0.25% |
| CPU Cores | -5.55% | -0.37% | -0.04% | -0.63% |
| GB Memory | -0.65% | -4.20% | -0.12% | 0.08% |
| Number of Training Examples | -38.36% | -36.92% | -71.74% | -1.22% |
| Cells | 0.01% | -5.01% | -5.69% | -33.67% |
|  |  |  |  |  |
| **Accuracy Model** | RF | MARS | GBM-BRT | GAM |
| Number of Covariates | -34.39% | -29.29% | -16.40% | -50.45% |
| CPU Cores | -0.09% | 0.08% | -0.07% | 0.01% |
| GB Memory | -0.02% | -0.53% | -0.30% | 0.00% |
| Number of Training Examples | -45.72% | -26.67% | -67.84% | -0.34% |
| Cells | 0.00% | 0.07% | -0.03% | 0.01% |

*Table 3:* Controls on SDM performance and accuracy. Table presents the reduction in explanatory power (, converted to percent) when a model fit will all terms except one is compared to the full model, for the execution time model (top) and accuracy model (bottom). Results were rounded to two decimal places.

## Table 4: Accuracy-Maximizing Data Configurations

|  |  |  |  |
| --- | --- | --- | --- |
| 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 |

*Table 4:* Accuracy-Maximizing Points for each SDM. Fixed accuracy is the estimated accuracy given the corresponding number of training examples and covariates. Training examples represents the number of training examples that optimize SDM accuracy, during the unconstrained optimization procedure. Covariates represent the optimized number of covariates with which to fit the model.

# 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](http://dx.doi.org/10.5061/dryad.3cp3t" \t "_blank) | 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 |
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| 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 |
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## Appendix B: Data Collection Protocol

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

## Appendix C: Bayesian Model Priors

1. As of November, 2016. [↑](#footnote-ref-1)
2. http://www.nsf.gov/pubs/2013/nsf13602/nsf13602.htm [↑](#footnote-ref-2)
3. https://aws.amazon.com/government-education/research-and-technical-computing/. Accessed 18 September, 2016. [↑](#footnote-ref-3)
4. https://cloud.google.com/compute/pricing#custommachinetypepricing [↑](#footnote-ref-4)
5. 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 be done on multiple processing cores, but model fitting is done sequentially. [↑](#footnote-ref-5)