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

by

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ABSTRACT

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Under the Supervision of Professor John Williams

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# Introduction

Human-induced global environmental change, including climate warming, anthropogenic land use, and the spread of invasive species, threatens to severely alter biodiversity patterns worldwide in the coming century (Lowe et al., 2011; Root & MacMynowski, 2005; Thuiller, 2007; Thuiller et al., 2008a). Habitat degradation and fragmentation and a loss of climatically suitable areas are expected to result in large-scale biotic reorganizations, including the extinction of over one-quarter of all species (Thomas, 2010). Climate exerts significant control over species distributions, particularly over those of vascular plants (Salisbury, 1926; Woodward, 1987), implying that warming associated with anthropogenic perturbations to atmospheric CO2 concentrations can have a significant impact on species ranges (Lowe et al., 2011). Statistical methods that quantify species responses to climatic gradients, known as species distribution models (SDMs), can be used to forecast future biotic assemblages under different warming scenarios (Clark et al., 2014; Guisan & Thuiller, 2005a; Guisan & Zimmerman, 2000; Guisan et al., 2013; Maguire et al., 2015; Wilfried Thuiller et al., 2008a). A growing volume of ecological data, both contemporary and fossil, is available to inform these models, commonly housed in community-specific, structure databases. 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). However, though growing collections of modern and historical 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 provision and use configurable and on-demand computer resources (Mell & Grance, 2012). The present study develops a method for identifying the optimal computer hardware on which to run SDMs, describing a flexible and skillful framework that can be used to inform provisioning strategies as well as 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 processes 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., 2014), as well as private industry (Mosco, 2014), have adopted techniques to cope with large datasets. As the volume of ecological data increases and the need for high resolution, accurate projections of biotic distributions become more pressing and reducing project scope (e.g., Bolker et al., 2009) can no longer be considered a valid option. However, 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). With the rapid commercialization of cloud computing and the widespread availability of public cloud providers like Amazon Web Services (AWS) and the Google Cloud Compute Engine (GCE), scientists now have a seemingly unlimited supply of computing resources at their disposal.

There are few guiding principles on when, if ever, the benefits in reduced computing time outweigh the financial costs of a 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; 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., 2011).

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 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 more take explicit advantage of parallelism and distributed computing frameworks.

# Background and Previous Work

## Big Data in Ecology

With the contemporary influx of massive geonomic sequences, long term monitoring projects, phylogenetic histories, and biodiversity occurrence data, robust, expressive and quantitative methods are essential to the future of the biological sciences, and require the development of new 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 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 are records of presence, absence, or abundance of individuals of a species, clade or higher taxonomic grouping that are fundamental to biodiversity analyses, ecological hypothesis testing, and global change research. These data are increasingly being stored in large, dedicated 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. 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’ (Soberon & Peterson, 2004), ‘Ecoinformatics’ (Michener & Jones, 2012), and ‘Paleoecoinformatics’ (Brewer et al., 2012) have been developed and 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 (Soberon & 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 (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, like cloud-based computing services, that facilitate Big Data analysis. For example, Apache Hadoop, a popular distributed computing framework, 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 in a particular field, and the kinds of software tools that are commonly used in that industry (Manyika et al., 2015). While Big Data most often drescribes datasets between several terabytes and several petabytes (240 to 250 bytes), ecology’s traditional lack of experience with massive datasets and limited analysis software in the discipline, suggests that ecological occurrence data may be characterized as Big Data.

The 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. While the datasets are not particularly large in storage volume, they are composed of millions of heterogenous records with complex linkages to one another. Further developments, like application programming interfaces (APIs) and language specific bindings (e.g., R packages or python modules), supplement the tasks of accessing, filtering and working with large occurrence datasets (Goring et al., 2015; Hernández & Sgarbi, 2016). While occurrence data does not require the disk space of popular commercial applications, it has recently demonstrated a need for new, custom-built tools to store, analyze, visualize, and use.

A second important 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. Under this framework, a dataset is described by its Volume, Variety, Veracity, and Velocity. Yang & Huang (2013) describe this framework, noting 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 over 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 macrofossil extraction efforts -- data gathering 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 occurrences described 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 highly diverse with many complicated interrelationships. As shown in Figure 2a, Neotoma’s holdings feature 23 dataset categories, including X-ray fluorescence (XRF) and isotopic measurements, macro fossils of both vertebrates and plants, modern and fossil pollen records, and freshwater diatom and water chemistry series. Similarly, GBIF stores 9 distinct record types, 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 data that is a discrete representation of a continuous physical feature, correlations between parameters, space, time, and processes at different scales (Yang et al., 2011), making storage and management difficult. Finally, occurrence data represents the work of many dispersed individual researchers and research teams. Controlled vocabularies and data structures of aggregating databases helps to efficiently assimilate large numbers of records, however, 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 and dating uncertainty in Neotoma are high as well. Out of a sample of 32,341 age controls (e.g., radiocarbon dates) 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 paleoecological data (Dawson et al., 2016). Moreover, contextual information is undoubtedly lost in the aggregation process in the dataset. Though some procedural information accompanies the data records to the database, process details are difficult to coerce into metadata fields and important details are often lost.

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, 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 to researchers to immediately analyze new biodiversity 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 significant variety, and should therefore be considered Big Data. Traditional statistical analysis techniques incorporating occurrence data may begin to suffer because they were not designed to handle Big Data. To fully and accurately derive value from new data being added to these databases, novel techniques for modeling and analyzing this data are required.

## 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 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 -- utility computing 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 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, 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). 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, 2015; Schnase et al., 2014).

Cloud services have also been used in the geosciences, and in ecological modeling problems specifically. Yang et al. (2011) 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., 2011). In practice, cloud-optimized implementations of numerical models, such as real-time dust storm forecasting, have improved model performance significantly (Yang et al., 2011). 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 workflows, suggesting that an integrated 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, 2009a), using 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 increased the uptake of these techniques substantially in recent years (Franklin, 2010; Svenning et al., 2011). Citations for SDMs outpaced the field average (National Science Board, 2016) by 3.8% per year between 204 and 2014, according to a Web of Science search (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 in the models, 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 provided in the training set. 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 to assess 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 an anthropogenic climate change context, 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) 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 grouping modeling algorithms into data-driven and model-driven algorithms. The data-driven/model-driven dichotomy is introduced in Hastie et al. (2009) and is often employed when differentiating between ‘statistical’ (model-driven) and ‘machine learning’ (data-driven) algorithms. I add 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., 2008a; Veloz et al., 2012).

Supervised learning techniques use a set of training examples, , where both *x* and *y* are known, to approximate the real relationship between the two, with a function, . The learned approximation 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, , . Models can either make *a priori* assumptions about the form of the input-output relationship (model-driven) or adapt to fit any given matrix of training examples (data-driven).

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 linear and logistic regression (Franklin, 2010).

An increase in available computing power has spurred the development and application of non-parametric, data-driven learning algorithms. While not reliant on stringent assumptions about the form of the predictor-response 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). SDM literature analysis suggest 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 MaxEnt, 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 develop the relationship between environmental predictors and species presence. 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, 2009b). 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 models 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 SDM users employ data-driven models. Of 100 randomly sampled papers from recent publications in Web of Science that met the query “*(Species Distribution Model) OR (Ecological Niche Model) OR (Habitat Suitability Model)*”, the overwhelming majority utilized 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 experiments). Models in the model-driven category included generalized linear models (15), logistic regression (5) and multiple linear regression (2). Data-driven models 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.

### 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 (Elith et al., 2006). 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., 2009b). 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. (2008a) cautions “limits to the broad application of this approach may be posed … by the computational challenges encountered in the statistical fitting of complex models.” While modern computing infrastructure may alleviate some of this problem, the computation intensity of SDMs can cause challenges that are difficult to resolve without reducing model complexity.

## 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). The theoretical complexity of an algorithm is most often considered when considering an algorithm’s scalability (Goldsmith et al., 2007), 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. These studies use observations of algorithm runtime under different parameterizations and inputs to build models that predict the run time of future model runs, seeking a method “with the generality of a big-O bound by measuring and statistically modelling [sic] the performance … across many workloads” (Goldsmith et al., 2007). Brewer & 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., 2014a). Algorithms for solving very difficult (-Hard/-Complete) combinatorial problems, can exhibit high runtime variance between different problem instances. Empirical runtime modeling can be used to select the model that will most efficiently reach a solution (Hutter et al., 2014a; Leyton-Brown et al., 2003). Hutter et al. (2014a) 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., 2014a). 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., 2014a; Hutter et al., 2014b).

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 are a result of 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. 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

To conceptualize the optimal configuration for an SDM modeling workflow, it is useful to conceptualize the modeling process using the following framework. Here, the workflow is presented as a series of steps that advance a user towards her goal of obtaining scientific insight from an SDM model. As a rational consumer (Simon, 1986), the modeler will wish to minimize her costs, in both time and money, while maintaining the maximum accuracy under given budgetary constraints.

1. Consider a pool of computing resources, , that is characterized by its hardware capabilities, such as memory and CPUs.
2. Consumers of computing services are part of a market driven by supply and demand, and face costs set by computing providers that are proportional to the computing power provided: Figure 5 demonstrates an instance of a Google Cloud Computing Engine’s cost surface as a function of memory and CPUs.
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 a given model, a finite set of use cases for that model 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 by the modeler.
4. Assume the time to compute a given algorithm with a given set of inputs is proportional to , the effective computing power. In addition to computing the model, however, 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

In this formulation, 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. 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. Elith et al., 2006 notes the potential impact of user experience on the modeling time and results. represents time to transfer the output from the computation to the user, which may be non-trivial if the model is run on a set of remote resources and the 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 optimal 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. Moreover, 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 and Research Questions

# Methods

## Data Collection

### SDM Data Preparation

I systematically collected data on the execution time and accuracy of 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). All of the SDMs were executed using the R statistical environment (R Core Team, 2016) using implementations in the standard packages for SDM. GBM-BRT tree 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 (Hastie, 2016), and random forests with the randomForest package (Liaw & Wiener, 2002).

Each SDM was fit using fossil pollen 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 using the neotoma R package (Goring et al., 2015), and filtered to only include those dated 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.

Climatic covariates were obtained from downscaled and debiased Community Climate System Version 3 (CCSM3) model simulations for North America (Lorenz et al., 2016a). The 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 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, O’brien, 2007). The variables retained were BV2 (mean diurnal temperature range), BV7 (annual temperature range), BV8 (mean temperature of westtest quarter), BV15 (precipitation of warmest quarter), BV17 (precipitation of warmest quarter), and BV18 (precipitation of driest quarter).

Future climate layers for AD2100 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

The Google Cloud Compute Enginge (GCE) infrastructure was 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 adhear to user-defined specifications. 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 an arbitrary hardware configuration. Debian Linux virtual machines 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.

### SDM Model Protocol

For a virtual machine of a given hardware configuration, data parameters (number of covariates and number of training examples) were communicated to the computing node via a configuration file. Pre-processed occurrence points were partitioned into a testing set (20%) and a training set (80%) of the number of rows (training examples) and columns (covariates). The SDM model was fit using the training data, projected onto the modeled future climate, and assessed for accuracy. SDM accuracy was evaluated using the testing set and quantified using the AUC statistic. Learning (hyper)parameters were initially evaluated as a potential predictor, but were discarded as uninformative. Timing was done within R using the proc.time function. No database I/O was done inside of the timing script, so network connection speed is not expected in influence the results.

Configurations were composed of five experimental variables: number of gridcells in the prediction, number of training examples in the training set, number of covariates in the training set, gigabytes of memory on the VM, and CPU cores on the VM. Each configuration. In total, 26,730 runs were made. 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 (Bleich & Kapelner, 2016). By employing a Bayesian modeling approach, the response at each leaf node is a probability distribution, rather than a single maximum likelihood estimate. For more details about the model and its implementation, see Bleich & Kapelner (2016). Runtime and accuracy were modeled separately for each SDM. Both models were fit using default priors on the parameters and hyperparameters, suggested by the authors. Runtime was modeled on a log scale, which has been shown to improve prediction on high-variance datasets {Hutter:2014ci}. The response data 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 of 50 trees. The first 250 iterations were discarded as burn-in, leaving 1000 posterior samples to analyze and evaluate.

## Model Evaluation

The predictive skill of the 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 distribution. 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 in turn left out of a model, 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 corresponding accuracy model was used to predict the accuracy of a finite number of regularly spaced training example-covariate configurations. This set of predictions included every 100 training exmples between 1 and 10,000 and every number of covariates between one and five. Hardware configuration was included, as hardware should not affect SDM accuracy. 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, thus, 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 the data input for the performance model. This model was used to predict the runtime of an experiment with the given number of training examples and covariates on a set of 287 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 a distribution of 1000 posterior samples. 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 cut into clusters using the silhouette rule for maximizing within-cluster homogeneity while maximizing out-of-cluster variance {Rousseeuw:1987gv}.

Finally, the clusters were plotted in time-cost-uncertainty space. The 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. A data constrained optimization would allow such small datasets to be considered. In this 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, yielding an estimate of the highest-accuracy configuration that would fall below the user-defined threshold on runtime.

# Limitations and Assumptions

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. Furthermore, limit my analysis to include only two hardware components, CPU cores and memory, to keep the project to a manageable scope, effectively eliminating Tinterp and Toutput. 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 the predictive models described here.

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 instances, I am limited to only the CPUs provided by Google, which may be updated or changed as they wish. At the current time, GCE provides only one processor type, a 2.6 GHz Intel Xeon E5 processor. Fortunately, my results will not be biased by using machines with different 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:2012fw}), 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 methodological limitation was computational cost. In order to gather enough data to develop a robust predictive model, I limited the number of models running longer than several hours. 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. 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 becomes mainstream. The optimization framework, however, is robust to both changing hardware capabilities and costs. To incorporate new or better 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 clustering would need to be re-run using the new costs.

# Results

## Model Performance

Predictive models of performance and accuracy were skillful when compared to a holdout testing set. While results varied across SDM classes, all models 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, both demonstrating values of approximately 0.96, and an MSEs of approximately 0.05 log-seconds2. The estimates from all models were tightly constrained, as indicated by low standard deviation of the mean posterior distribution of prediction. The posterior SD for GAM, GBM-BRT, and MARS were all between 0.01 and 0.035 log-seconds -- small when compared to the mean of the distribution, suggesting low uncertainty. The full results are presented as Table 1 and shown in Figure 7.

Both GAM and RF models were less explanatory than the other two SDMs, both demonstrating lower values than the other two models. It is likely that several factors contribute to this lack of predictive skill. The GAM runs tended to converge within several seconds (maximum 10.3s), potentially exposing it to a stronger influence by low-level system processes not explicit in the model, resulting in a higher variance dataset, and therefore lower model explanatory power. In contrast, the other three SDM types typically take minutes to hours to terminate (maximum in training: GBM-BRT 5,285.0 s). Another possible reason for the poorer model performance is a smaller training datasets. 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 low predictive skill. While the parameter space appears to be relatively well coverage 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). The RF model was the best performing model, with an of of 0.98 and a MSE of less than 3.5x10-5 AUC. Moreover, all of the models indicate low uncertainty and well-constrained posterior estimates on their predictions. GAM results have higher than average uncertainty associated with them, again perhaps due to small training set size. Full results of the accuracy assessment are presented in Table 2 and Figure 8.

## Model Drivers

Factors that control runtime of SDM vary between algorithms. One of the most important contributors for several SDMs is the number of training examples with which the SDM is fit. The influence of this term on GBM-BRT, GAM, and RF runtime is similar (>36% reduction in ). As data-driven algorithms, these SDMs rely heavily on creating structure from the given input dataset, and their runtime should be strongly tied, asymptotically, to the number of training examples {Hastie:2009et}. However, surprisingly, the number of environmental covariates does not appear 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, this evaluation, under real workloads, does not suggest that the number of covariates has a strong influence. 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.

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, show a slight dependence on CPU cores (~5.55%), as their computations can be spread across multiple processing units. However, the overall trend of low dependence on hardware capabilities is surprising, indicating that, without additional optimization, SDMs should run at roughly the same speed on all computers.

MARS shows a surprising and dependence on memory. Upon further investigation, it appears that an error in sampling design that incorrectly weighted some portions of the parameter space 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 clearly seen in the results 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 the case of, RF and GBM-BRT, data volume accounts for nearly 80% of the model’s total predictive skill. As seen in the runtime model, GAM appears different than the other three SDMs, and is only strongly controlled by the number of covariates in the training set. Theory suggests that hardware and cells should have no influence on the accuracy of the SDM. Indeed, when evaluated, these terms are very close to zero.

## 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. In all the models, the accuracy-maximizing point lies at the right-hand size of the training example-covariate space. Most points lie close to the top right of the space, using all available data, expected from theory and empirical analysis of model drivers. The space was limited due to experimental design constraints, so supplying additional data may further increase SDM accuracy. However, given a review of the SDM literature, 10,000 training examples and five covariates fall within typical SDM workflows. Interestingly, the MARS achieves its highest accuracy with only 1000 training examples, rather than >9000 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 (98). In all cases, additional covariates continued to increase accuracy up to the five covariates included in this analysis.

### Hardware Configuration

The optimal configuration of hardware for each SDM was calculated using the unconstrained optimization routine. Figure 10 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 CPU cores. As suggested by moderate dependence on CPU cores in the runtime model, random forests are best suited to between four and seven CPU cores, demonstrating their ability to be parallelized across multiple cores. MARS require anywhere between 1 and 25 cores, however, due to the sampling issues described above, this results should be interpreted carefully.

Memory requirements are generally low for all SDMs except for MARS. RF and GBM-BRT are both optimized at only one GB of memory. GAM optimization suggests they 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 a higher performance VM with 25 GB of memory. This is further confirmed when looked at the runtime drivers, where virtually no structure in the data is explained by instance memory. Therefore, this SDM can be interpreted as requiring only one GB of memory. Finally, MARS is optimized at 16 GB of RAM. Again, these results should be discarded or interpreted carefully. 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, suggesting biased model training data.

# Discussion

## Establishing 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 factors that contribute to SDM accuracy. Theory might suggest that additional covariates and training examples would uniformly enhance model prediction and ability to characterize future examples. However, the empirical dataset suggests that this is not the case. 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 data configurations, suggesting an accuracy substitution rate (ASR) inputs that characterizes the amount of one input that can be substituted to get to the accuracy obtained by an increase in the other input. The rate clearly changes between models and at different points in the data configuration space.

All SDMs show a rapid increase in accuracy with the addition of the first 1000 training examples, after which the number of covariates is the more important term in increase accuracy. GAM, GBM-BRT, and MARS all show nearly vertical contours of accuracy after approximately 2500 training examples, indicating that additional occurrence observations are unlikely to significantly affect model accuracy. Instead, more covariates are needed 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 accuracy contours indicates that the ASR decreases, so that many thousands of training examples are needed to substantially increase accuracy. Moreover, adding more covariates is unlikely to significantly affect accuracy.

The ASR is important to evaluate for three reasons. First, it provides the model user with guidance on how to achieve the maximum accuracy with the given data. While SDM 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 particularly rare species, a researcher can estimate the relative return in accuracy of identifying additional occurrence points and weight that against the effort needed to find 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 adding additional training examples. The time and effort going to collecting these training examples could be better spent identifying additional covariates than additional training examples. Third, the execution time models respond differently to increased numbers of training examples than to numbers of covariates, and knowing the ASR enhances the execution time of the SDM. Assume, for example, a model where the same accuracy can be be achieved using many covariates and few training examples, or few covariates and many training examples. If the data is available, it makes more sense in the optimization framework to run the model with fewer training examples, since SDMs are strongly influenced by the number of training examples. The ASR effectively describes the tradeoffs between the two parameters so that this choice can be modeled.

## Sequential Model Hardware Responses

The most R implementations of GAM, GBM-BRT[[5]](#footnote-5), and MARS are all fit sequentially, one instruction after another. The algorithms underlying these R functions are not easy to parallelize, as the model building process involves loops over the entire dataset, a procedure that cannot easily be 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 optimals at a low number of CPU cores. In both cases, there is no demonstrated advantage of a more parallel configuration.

Moreover, 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 optimal at 16GB of RAM, though there is no theoretical reason for greater memory requirements than the other sequential algorithms. Anecdotal evidence suggests that SDMs may fail under very large dataset sizes. Although not tested rigorously, datasets exceeding 100MB, or several hundred thousand rows, 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 tested configurations costing more than $5. While more expensive, GBM-BRT may result in an increase in AUC of nearly 0.15. This increase in accuracy is 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.

Prediction uncertainty varies between SDMs. GAM predictions have a mean posterior standard deviation of about 0.5 -- approximately 10% of their total runtime, indicating relative certainty in these predictions. Both MARS and GBM-BRT, have larger percent uncertainties – sometimes approaching 50% of the prediction mean. There is less overall variance in GAM runtime, while MARS and GBM-BRTs have much larger variance overall in the experimental dataset, so the corresponding models place less confidence in each prediction. It is important to remember, however, that the clustering step in the optimization takes both posterior spread and execution time into account when determining the optimal configurations. Therefore, optimal configurations have both a low mean time and cost and a high certainty.

## Random Forest Model Hardware Responses

The RF algorithm can be easily split across into small subtaks, 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 core. The maximum expected accuracy is approximately that of GBM-BRT, but can be achieved in a fraction of the time. Both SDMs achieve maximize accuracy with 10,000 training examples and 5 covariates. However, when optimized, random forests can be fit in between 10% and 30% of the time to fit a GBM-BRT model. Given the approximately equal expected accuracy, the economically rational researcher would therefore be best served by running the RF model, run in parallel across many cores, rather than waiting for the GBM-BRT to converge.

The RF optimal cluster 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. In total, these two considerations balance out -- illustrating the tension between hardware costs and time costs 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 (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 as parallel efficiency, the difference between parallel (*TN*) and serial (*T*1) runtimes of the algorithm, divided by the number of cores (*N*) the parallel implementation was run on, given as:

Figure 12 demonstrates diminishing marginal returns achieved by the RF algorithm when run on on multiple processors and on different sized training datasets. The difference between a model run sequentially and one run in parallel but with just two cores is large, while the marginal benefit of adding the 16th or 24th core is comparatively small. An infinitely parallel algorithm would have an efficiency of 1, incurring no diminishing marginal 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 more training examples, are better suited to parallelization and show higher efficiency than small modeling problems with few training examples. SDM runs with over 10,000 training examples experience a much slower decline in efficiency than runs with 1,000 training examples. The derivative of the efficiency curves associated with the larger datasets are still non-zero, indicating that the addition of more cores is still contributing to faster runtimes. However, the near-zero slope associated with smaller datasets suggests that no performance is gained by provisioning additional processors for these runs. Biodiversity database size trends suggests that much more data will be available to research to fit SDMs over the next decade. Therefore, SDMs, when fit with parallel methods, are likely to see increased benefits of running in a cloud-based environment. As more data becomes available with which to fit SDMs and large training sets are used, parallel efficiency will remain high, suggesting researchers will see performance returns when fitting models on highly parallel configurations.

## 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 to provide guidance to researchers when infinite resources are not available. For example, a constraint on the number of training examples or covariates available to the research seems probable, as a review of SDM literature shows that a significant portion of recent studies had less than 100 training examples (Appendix 1). The low-friction availability of biodiversity records in databases like Neotoma and GBIF suggests that these studies were fit with such small datasets due to lack of available data. Similarly, many studies also use fewer than five environmental covariates.

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 computed SDMs for arbitrary datasets on a server and returned the results to a 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 too long to respond (Roth, 2013). If a maximum-accuracy experiment for GBM-BRT is requested, the wait over 1 hour for a response, 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 server manager can provision the cheapest resources, return results of high accuracy, and continue to keep their audience engaged.

Another potential extension of this work was weighted optimization to preferentially weight one or two of the three components included in the determination of the optimal clusters. With unconstrained 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, then about prediction certainty, and finally about the time it takes to complete the modeling. Weighting each axis would allow the user to determine the most important components of the optimization.

## 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 so they can be easily scaled to high-performance VMs. 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.

To achieve performance gains in a cloud-based system, a significant amount of technical skill would be required to simultaneously provision multiple, isolated VM instances. Each node could then run independently, fitting own SDM experiment. To make this work automatically, efficiently, and without error would be difficult. Particularly the centralization of results into a cohesive database would be a challenging task.

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, they are 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. Public cloud providers make such scalability easily, by allowing users to put all necessary modeling code and programs onto a virtual hard disk, and then automatically scaling the underlying hardware configuration up or down depending on the problem size.

Of course, 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. When only a few modeling experiments are being run, it is likely that this step would far outweigh any benefit obtained by efficient hardware scaling. 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 service (e.g, de Souza Muñoz et al., 2009) as a service (e.g., Granell, 2013), cost and time optimization will be helpful.

## Framework Extensibility

Though these results are specific to the specific 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. Modeling and optimization could be completed as described above, albeit with additional terms constituting each model. Even models with many parameters could be incorporated, by treating algorithm parameters as additional components (Hutter, 2014).

Furthermore, I hypothesize that 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.

## 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 larger training datasets that are expected as biodiversity database size increases. Austin (2007) argues that a solid foundation of ecological theory is most essential to the correct prediction and interpretation of SDMs. He claims that the ecological underpinnings of the statistics may be even more important the statistical method itself. Elith & Leathwick (2009a) suggest that additional improvements in species distribution modeling will come not from novel learning techniques, but from the incorporation of more ecologically relevant information into the statistical modeling process. Indeed, “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, 2009a).

Due to rapidly increasing occurrence databases, 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 advanced computing infrastructure, including multiple cores and effective memory management. 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). While incorporation of additional ecological relevant information will help to strengthen the ecological inference made from these models, the incorporation of Big Data 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. Empirical observations of the run time and accuracy of over 30,000 simulations for four SDM classes were collected under systematically varied inputs, yielding a robust experimental dataset. 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 optimal data-hardware configuration that maximized accuracy while jointly minimizing execution time and cost was identified 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, and are likely to struggle to incorporate insight from the massive influx of data into global biodiversity databases. Future model development should be directed towards enabling state-of-the-art SDM algorithms to support very large datasets.

# References

# Figures

# Tables

# Appendices

## Appendix A: Literature Meta-Analysis

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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)