Model Selection using Multi-Objective Optimization

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Abstract

Choices in scientific research and management require balancing multiple, often competing objectives. *Multiple-objective optimization* (MOO) provides a unifying framework for solving multiple objective problems. Model selection is a critical component to scientific inference and prediction and concerns balancing the competing objectives of model fit and model complexity. The tradeoff between model fit and model complexity provides a basis for describing the model-selection problem within the MOO framework. We discuss MOO and two strategies for solving the MOO problem; modeling preferences pre-optimization and post-optimization. Most model selection methods are consistent with solving MOO problems *via* specification of preferences pre-optimization. We reconcile these methods within the MOO framework. We also consider model selection using post-optimization specification of preferences. That is, by first identifying Pareto optimal solutions, and then selecting among them. We demonstrate concepts with an ecological application of model selection using avian species richness data in the continental United States.

Keywords: competing models, decision theory, model selection, multiple objectives, Pareto frontier, optimal solution

1 INTRODUCTION

The goal of modeling scientific processes varies from identifying the important factors driving a system, to robust prediction into the future or across space. Multiple competing models are considered in most cases, each model based on hypotheses of spatial or temporal structure in parameters, heterogeneity among individuals within a population, or candidates for covariates influencing the process of interest. Ultimately, one model from the candidate models, or a composition of candidate models, is selected for inference or prediction. Model selection is one of the most common problems in scientific research, and numerous model-selection methods are available (e.g., Akaike, 1973; Mallows, 1973; Schwarz et al., 1978; Gelfand and Ghosh, 1998; Burnham and Anderson, 2002; Hooten and Hobbs, 2015). Each model-selection method represents an approach to balancing the bias due to missing important factors (model fit) with imprecision due to overfitting the data (model complexity). Each method represents a different *a priori* weighting of the relative importance of model fit and model complexity. While guidelines exist, there is no consensus among statisticians on best methods for this model selection process (Hooten and Hobbs, 2015).

Multi-objective optimization (MOO) is a formal decision-theoretic framework for optimizing problems with more than one objective (Marler and Arora, 2004; Williams, 2016; Williams and Kendall, 2017). MOO is commonly used in engineering, economics, and other fields for which decisions must balance trade-offs between ≥ 2 competing objectives (Marler and Arora, 2004). When a decision maker has competing objectives, a solution that is optimal for one objective might not be optimal for the other objective and a single solution that optimizes multiple objectives does not exist. With competing objectives there exists many (possibly infinite) solutions that might be considered "optimal" (i.e., Pareto optimal; Williams and Kendall, 2017). However, in most decision contexts, a decision maker can only make one choice (e.g., which model to use to predict into the future?). To choose among solutions, a decision maker must include their preferences among objectives to identify a final solution. MOO provides a mathematical framework for quantifying preferences for examining multi-objective problems.

The MOO framework is described generally as

$$\boldsymbol{f}(\boldsymbol{\theta}^*) = \text{optimum}_\theta \boldsymbol{f}(\boldsymbol{\theta}), \tag{1}$$

where $\boldsymbol{f}(\boldsymbol{\theta}) = (f_1(\boldsymbol{\theta}), ..., f_k(\boldsymbol{\theta}))$, such that $g_j(\boldsymbol{\theta}) \leq c_j,\ j = 1, 2, ..., J,$ and $h_l(\boldsymbol{\theta}) = d_l,\ \ l = 1, 2, ..., L,$ $f_i(\boldsymbol{\theta})$ represent the k different, potentially competing, objective functions, $\boldsymbol{f}(\boldsymbol{\theta})$ is a vector of the different objective functions, g_j and h_l represent J inequality constraints and L equality constraints, respectively, and $\boldsymbol{\theta}$ is a vector of design variables (Marler and Arora, 2004; Cohon, 2013).

Pareto optimality is a concept of optimality used for eq. 1 when no value of $\boldsymbol{\theta}$ simultaneously optimizes all functions f_i. A Pareto optimal solution for a minimization problem is a solution $\boldsymbol{\theta}^* \in \boldsymbol{\Theta}$ for which there is no other solution $\boldsymbol{\theta} \in \boldsymbol{\Theta}$ such that both $f(\boldsymbol{\theta}) \leq f(\boldsymbol{\theta}^*)$, and $f_i(\boldsymbol{\theta}) < f_i(\boldsymbol{\theta}^*)$ for at least one function i (Deb, 2001; Marler and Arora, 2004). For decision problems with competing objectives, there are many (potentially infinite), Pareto optimal solutions. The set of solutions that are Pareto optimal are known as the Pareto set (or Pareto frontier or efficiency frontier). Each solution in a Pareto set has an implied set of preferences for the objective functions f_i (Deb, 2001; Williams and Hooten, 2016). Thus, choosing among a set of Pareto optimal solutions requires assuming (either implicitly or explicitly) preferences for the objective functions f_i. Preferences among objective functions can be specified pre- or post-optimization, representing two separate strategies to solving eq. 1 (Williams and Kendall, 2017). When specifying preferences pre-optimization, decision makers explicitly describe preferences of objective functions and select the Pareto optimal solution associated with their choice of preferences. When specifying preferences post-optimization, decision makers first examine the set of Pareto optimal solutions. Then the decision maker chooses the final Pareto optimal solution based on the trade-offs observed among the set. The choice implies decision-maker preferences.

One of the most common methods for incorporating preferences for f_i into a decision problem pre-optimization, is the weighted-sum method (Athan and Papalambros, 1996; Das and Dennis, 1997; Cohon, 2013; Williams and Kendall, 2017). The weighted-sum method is described by

$$f(\boldsymbol{\theta}) = \sum_{i=1}^{k} w_i f_i(\boldsymbol{\theta}), \tag{2}$$

for which the optimal solution is

$$f(\boldsymbol{\theta}^*) = \text{optimize}_{\boldsymbol{\theta}} \sum_{i=1}^{k} w_i f_i(\boldsymbol{\theta}). \tag{3}$$

The weights w_i are chosen by the decision maker to reflect the importance of each objective function f_i. The weighted-sum method is a composition that results in a single objective function over which to optimize. When optimizing one objective function, an unequivocal optimal choice can be made.

We examine model selection within the MOO framework and demonstrate that several methods commonly used for model selection in scientific research are specific cases of the MOO problem solved using the weighted-sum method with *a priori* specification of preferences. We examine concepts of the MOO framework, specifically Pareto optimality, as it relates to several common model selection methods. Finally, we examine the second strategy of MOO, post-specification of preferences, and its application to the model selection problem in scientific research. We demonstrate the concepts presented using an example from the field of ecology involving variable selection in a generalized linear regression model for avian species richness data.

2 MODEL SELECTION AS A MOO PROBLEM

Methods for model selection typically consist of minimizing a weighted sum of two functions, often described heuristically as a function for model fit and a function for model complexity (e.g., Burnham and Anderson, 2002, p. 87). That is, from eq. 2 we obtain

$$f(\boldsymbol{\theta}^*) = \min_{\boldsymbol{\theta}} \sum_{i=1}^{2} w_i f_i(\boldsymbol{\theta}), \tag{4}$$

where $\boldsymbol{\theta}^*$ represents the optimal solutions from the set of design variables $\boldsymbol{\theta}$ (i.e., model parameters), describing fit and complexity of any model, w_i are weights for the importance of the objectives associated with model fit and complexity, and f_i are functions that quantify the value of model fit and complexity. Clearly, eq. 4 is a specific form of the MOO problem defined in eq. 3. Theoretical justification exists for choices of objective functions $f_i(\boldsymbol{\theta})$ and their corresponding weights w_i (Akaike, 1973; Mallows, 1973; Schwarz et al., 1978; Gelfand and Ghosh, 1998; Burnham and Anderson, 2002; Link and Barker, 2006; Hooten and Hobbs, 2015). Although there is no consensus among statisticians on specific model selection methods, most of the theoretical development related to model selection can be described by two general functions for f_i. Differences in model selection criteria are often the result of different choices in weights. The most common objective function for model fit is the negative log-likelihood of the data, given parameters (i.e., the deviance). That is, if f_1 is the objective function associated with model fit, it is described as

$$f_1(\boldsymbol{\theta}) = -\log(L(\boldsymbol{\theta}|\boldsymbol{y})). \tag{5}$$

Although the deviance is the most common objective function for model fit, others have been used. For example in Mallows' C_p, $f_1(\boldsymbol{\theta}) = \frac{\sum_{i=1}^{n}(y_i - \hat{\mu}_{\text{sub}})^2}{\sum_{i=1}^{n}(y_i - \hat{\mu}_{\text{full}})^2} - n$, where $\hat{\mu}_{\text{sub}}$ equals the estimated mean of a sub-model in consideration, $\hat{\mu}_{full}$ equals the estimated mean of the full model in consideration, and n equals the sample size (Mallows, 1973).

Hooten and Hobbs (2015) summarize several objective functions for model complexity using a function proportional to

$$f_2(\boldsymbol{\theta}) = \sum_{j=1}^{p} |\theta_j - \mu_j|^{\gamma}, \tag{6}$$

known as the *regulator*, *regularizer*, or *penalty*. In eq. 6, p represents the number of parameters in the model, γ is the degree of the norm; a user-defined parameter that controls the relative penalty of the distance between θ_j and μ_j, θ_j are parameter estimates for centered and scaled covariates, and μ_j is a location parameter, often set to 0. Substituting the choices of $f_1(\boldsymbol{\theta})$ and $f_2(\boldsymbol{\theta})$ from eqs. 5 and 6 into eq. 4, we obtain the following multi-objective optimization problem

$$\begin{aligned} f(\boldsymbol{\theta}) &= w_1 f_1(\boldsymbol{\theta}) + w_2 f_2(\boldsymbol{\theta}), \\ &= w_1(-\log(L(\boldsymbol{\theta}; \mathbf{y}))) + w_2 \sum_{j=1}^{p} |\theta_j - \mu_j|^{\gamma}, \end{aligned} \tag{7}$$

with the objective of $\min_{\boldsymbol{\theta}}(f(\boldsymbol{\theta}))$. Equation 7 is the general function used in many model selection methods including Akaike's information criterion (AIC), AIC for small samples (AIC$_c$), quasi-AIC (QAIC), QAIC for small samples (QAIC$_c$), Schwartz's information criterion (BIC), ridge regression, LASSO (least absolute shrinkage and selection operator), natural Bayesian shrinkage, and some forms of posterior predictive loss (Table 1; Gelfand and Ghosh, 1998; Hooten and Hobbs, 2015). Each of the listed model selection methods result from specific choices of $\boldsymbol{w}$ and γ, which we report in Table 1. For example, let the weights be: $w_1 = 2$, $w_2 = 2$, and set γ to zero. With these weights, eq. 7 simplifies to $-2\log(L(\boldsymbol{\theta}|\boldsymbol{y})) + 2p$, or AIC (Table 1).

Expressing model selection methods in terms of eq. 3 has an important result that links model selection to Pareto optimality. For positive weights $\boldsymbol{w}$, any solution to eq. 3 is a Pareto optimal solution (Marler and Arora, 2010). Thus, any model selection method that can be expressed in terms of eq. 7 (i.e., the methods in Table 1) results in a solution that is Pareto optimal with respect to the objectives of maximizing model fit and minimizing model complexity.

3 MODEL SELECTION USING POST-OPTIMIZATION SELECTION OF WEIGHTS

Solving a MOO problem with competing objectives using post-optimization specification of weights requires first identifying as many Pareto optimal solutions as possible, then choosing among the Pareto optimal solutions (Williams and Kendall, 2017). Pareto optimal solutions for the objective functions in eqs. 5 and 6 are models for which increasing the value of eq. 5 requires a decrease in the values in eq. 6, and *vice versa*. One method for identifying Pareto optimal solutions with two objective functions, each depending on $\boldsymbol{\theta}$, is to plot the values of eqs. 5 and 6 for each candidate model on opposing axes to identify the Pareto frontier (e.g., Fig. 1). After the Pareto frontier is identified, the decision maker can select the model based on the trade-offs observed in the Pareto frontier. This is analogous to *best subset selection*, an active area of statistical research (e.g., Hastie et al., 2009). Thus, the selection of the final model is made without explicitly choosing weights $\boldsymbol{w}$ associated with the model selection criteria listed in Table 1. However, if a choice from the Pareto frontier is also optimal with respect to specific model-selection criterion, the weights of that selection criterion are implied.

Model selection method	w_1	w_2	γ	Note
AIC	2	2	0	
AIC$_c$	2	$2(\frac{n}{n-p-1})$	0	
QAIC	$\frac{2}{\hat{c}}$	2	0	$\hat{c} = \chi^2/df$
QAIC$_c$	$\frac{2}{\hat{c}}$	$2(\frac{n}{n-p-1})$	0	$\hat{c} = \chi^2/df$
BIC	2	log(n)	0	
*Ridge regression	1	User defined or estimated	2	Larger values of w_2 shrink $\boldsymbol{\beta}$ to 0.
*LASSO	1	User defined or estimated	1	Larger values of w_2 shrink $\boldsymbol{\beta}$ to 0.

Table 1: Values of weights (w_i) and γ for the multi-objective optimization problem of model selection described in eq. 7 for various model selection methods. The objective function for model fit is -log($L(\boldsymbol{\theta}|\boldsymbol{y})$), where $\boldsymbol{\theta} \equiv \boldsymbol{\beta}$; the objective function for model complexity is $\sum_{j=1}^{p} |\beta_j - \mu_j|^\gamma, j = 1, ..., p$. AIC = Akaike's information criterion; AIC$_c$ = Second-order information criterion; QAIC = quasi-AIC; BIC = Schwartz information criterion; n = sample size; p = no. parameters in model. (*) indicates objective function for model fit defined by: $\sum_{i=1}^{n}(y_i - \beta_0 - \boldsymbol{x}'\boldsymbol{\beta})^2$. See Burnham and Anderson (2002) and Hooten and Hobbs (2015) for additional details.

4 EXAMPLE: AVIAN SPECIES RICHNESS IN THE U.S.

Model selection is regularly used in the field of ecology to select variables to include in linear and generalized linear regression models. We examine the variable selection problem within a MOO framework by considering avian species richness in the contiguous U.S. as a function of state-level covariates. These data were originally used to demonstrate model selection techniques in Hooten and Cooch (In Press). As in Hooten and Cooch (In Press), we seek to model the number of avian species y_i ($i = 1, \ldots, 49$) counted in each of the contiguous states in the U.S. and Washington D.C., based on covariate information $\mathbf{x}_i$ collected in each state. The covariate information includes the area of the state, the average temperature, and the average precipitation. We modeled count data using a Poisson distribution

$$y_i \sim \text{Poisson}(\lambda_i),$$

where λ_i represents the mean species richness in each state. We linked mean species richness to the covariate data using the log link function

$$\log(\lambda_i) = \beta_0 + \beta_1 x_{1,i} + \ldots + \beta_p x_{p,i}. \tag{8}$$

We considered a total of 24 different models, representing different linear and quadratic combinations of eq. 8; each of the 24 candidate models are provided in Table 2. We used the `glm` function in R statistical software version 3.3.2 (R Core Team, 2013) to fit the models to the data. Code to fit the models and plot Fig. 1 is provided in the Appendix.

4.1 Model selection using AIC

To conduct model selection for the avian species richness data, we used the objective function in eq. 7 with values of $\boldsymbol{w} \equiv 2$, and $\gamma = 0$ (i.e., AIC). That is, for a Poisson likelihood, the weighted objective function was

$$f(\boldsymbol{\beta}_m) = 2\Bigg(\sum_{i=1}^{n}(\lambda_{i,m} - y_i \log(\lambda_{i,m}) + \log(y_i!))\Bigg) + 2\sum_{j=1}^{p_m}|\beta_{j,m}|^0, \tag{9}$$

where $\boldsymbol{\beta}_m$ is the subset of parameters for model $m = 1, ..., 24$, n is the sample size, and the term $\log(y_i!)$ can be omitted because it is independent of $\boldsymbol{\beta_m}$, and therefore, constant among models, provided the likelihood is not changed.

The model from Table 2 that minimized eq. 9 (i.e., the AIC top model) included the intercept a linear area effect, and a quadratic precipitation and temperature effect. All other model fitting results are shown in Table 2.

Table 2: Model selection results from avian species richness data. AIC is Akaike's information criterion, ΔAIC $=$ is the difference in AIC compared to the top model. Asterisks (*) indicate Pareto optimal models, $f_1(\boldsymbol{\beta})$ and $f_2(\boldsymbol{\beta})$ are described in eq. 5 and eq. 6, respectively.

$\log(\lambda_i) =$	$f(\boldsymbol{\beta})$ (i.e., AIC)	ΔAIC	$f_1(\boldsymbol{\beta})$	$f_2(\boldsymbol{\beta})$
β_0	741.1	229.8	369.6	1*
$\beta_0 + \beta_1 x_{\text{area},i}$	571.2	59.9	283.6	2*
$\beta_0 + \beta_1 x_{\text{temp},i}$	669.2	157.9	332.6	2
$\beta_0 + \beta_1 x_{\text{precip},i}$	706.1	194.8	351.0	2
$\beta_0 + \beta_1 x_{\text{area},i} + \beta_2 x_{\text{temp},i}$	526.7	15.4	260.3	3*
$\beta_0 + \beta_1 x_{\text{area},i} + \beta_2 x_{\text{precip},i}$	567.7	56.4	280.9	3
$\beta_0 + \beta_1 x_{\text{temp},i} + \beta_2 x_{\text{precip},i}$	536.7	25.5	265.4	3
$\beta_0 + \beta_1 x_{\text{area},i} + \beta_2 x^2_{\text{area},i}$	572.8	61.5	283.4	3
$\beta_0 + \beta_1 x_{\text{temp},i} + \beta_2 x^2_{\text{temp},i}$	668.0	156.7	331.0	3
$\beta_0 + \beta_1 x_{\text{precip},i} + \beta_2 x^2_{\text{precip},i}$	704.9	193.6	349.4	3
$\beta_0 + \beta_1 x_{\text{area},i} + \beta_2 x_{\text{temp},i} + \beta_3 x_{\text{precip},i}$	515.3	4.0	253.7	4*
$\beta_0 + \beta_1 x_{\text{area},i} + \beta_2 x^2_{\text{area},i} + \beta_3 x_{\text{temp},i}$	524.3	13.0	258.1	4
$\beta_0 + \beta_1 x_{\text{area},i} + \beta_2 x^2_{\text{area},i} + \beta_3 x_{\text{precip},i}$	565.6	54.3	278.8	4
$\beta_0 + \beta_1 x_{\text{temp},i} + \beta_2 x^2_{\text{temp},i} + \beta_3 x_{\text{area},i}$	528.2	16.9	260.1	4
$\beta_0 + \beta_1 x_{\text{temp},i} + \beta_2 x^2_{\text{temp},i} + \beta_3 x_{\text{precip},i}$	535.5	24.2	263.8	4
$\beta_0 + \beta_1 x_{\text{precip},i} + \beta_2 x^2_{\text{precip},i} + \beta_3 x_{\text{area},i}$	568.1	56.8	280.0	4
$\beta_0 + \beta_1 x_{\text{precip},i} + \beta_2 x^2_{\text{precip},i} + \beta_3 x_{\text{temp},i}$	524.2	12.9	258.1	4
$\beta_0 + \beta_1 x_{\text{area},i} + \beta_2 x^2_{\text{area},i} + \beta_3 x_{\text{temp},i} + \beta_4 x^2_{\text{temp},i}$	525.7	14.4	257.8	5

$\beta_0 + \beta_1 x_{\text{area},i} + \beta_2 x^2_{\text{area},i} + \beta_3 x_{\text{precip},i} + \beta_4 x^2_{\text{precip},i}$	567.1	55.8	278.6	5
$\beta_0 + \beta_1 x_{\text{temp},i} + \beta_2 x^2_{\text{temp},i} + \beta_3 x_{\text{precip},i} + \beta_4 x^2_{\text{precip},i}$	518.0	6.7	254.0	5
$\beta_0 + \beta_1 x_{\text{area},i} + \beta_2 x^2_{\text{area},i} + \beta_3 x_{\text{precip},i} + \beta_4 x^2_{\text{precip},i} + \beta_5 x_{\text{temp},i}$	512.2	0.9	250.1	6
$\beta_0 + \beta_1 x_{\text{area},i} + \beta_2 x^2_{\text{area},i} + \beta_3 x_{\text{precip},i} + \beta_5 x_{\text{temp},i} + \beta_6 x^2_{\text{temp},i}$	519.2	7.9	253.6	6
$\beta_0 + \beta_1 x_{\text{area},i} + \beta_2 x_{\text{precip},i} + \beta_3 x^2_{\text{precip},i} + \beta_4 x_{\text{temp},i} + \beta_5 x^2_{\text{temp},i}$	511.3	0	249.6	6*
$\beta_0 + \beta_1 x_{\text{area},i} + \beta_2 x^2_{\text{area},i} + \beta_3 x_{\text{precip},i} + \beta_4 x^2_{\text{precip},i} + \beta_5 x_{\text{temp},i} + \beta_6 x^2_{\text{temp},i}$	512.8	1.5	249.4	7*

Finally, a common practice for pre-specification of weights in MOO problems in other applications includes examining the sensitivity of the optimal choice relative to the selected weights (Barron and Schmidt, 1988; Insua, 1990). An analogous procedure in the model selection framework is to examine the optimal solutions relative to different information criteria because different criteria represent different objective weights (Table 1). The AIC, AIC$_c$, and BIC criteria all resulted in the same top model suggesting the optimal solution for these data was robust to several different choices of weights.

4.2 Model selection by examining Pareto optimal solutions

Using avian species richness data, we examined model selection *via* specification of preferences post-optimization (Fig. 1). That is, we identified Pareto optimal solutions among the 24 models, and then considered potential methods for selecting a model. To identify Pareto optimal solutions, we used a graphical approach and plotted the values f_1 and f_2 described in eq. 9 for each model on opposing axes to identify solutions along the Pareto frontier (Fig. 1). Identifying Pareto optimal solutions does not require specifying w_1 or w_2, and therefore does not require adhering to an information criterion. The Pareto optimal set included 6 models; one model for each number of parameters $1, \ldots, 7$, except $p = 5$, where both model fit and complexity could be simultaneously improved by using the top model containing four parameters. Each Pareto solution represented the model that minimized eq. 9 among all models with the same number of parameters. There were 17 dominated models (i.e., models that were not Pareto optimal; Fig. 1). The AIC top model was a Pareto optimal solution; this was expected because AIC (and other information criteria) is a specific formulation of the weighted-sum method and is therefore *sufficient* for Pareto optimality (Marler and Arora, 2010). Each of the Pareto solutions correspond to a specific set of weights in eq. 7.

Given the information on Pareto optimal solutions in Fig. 1, selecting a final model for inference can proceed in many ways, depending on the application and the nature of the parameters under consideration. A decision maker can use the information on Pareto optimal solutions to view trade-offs of fit gained by adding (or subtracting) additional parameters from the model,

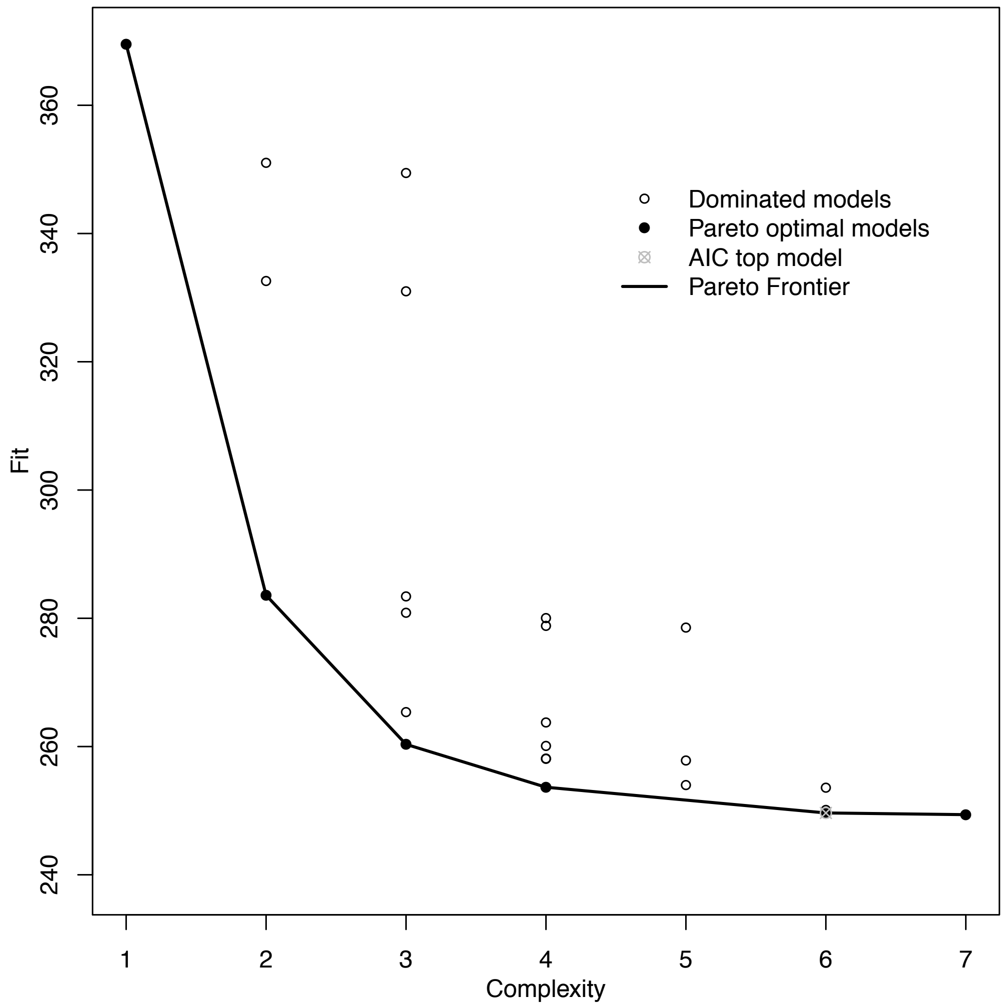

Figure 1: Model fit ($f_1(\boldsymbol{\theta}) = -\log(L(\boldsymbol{\theta}|\boldsymbol{y}))$ vs. model complexity ($f_2(\boldsymbol{\theta})$ = no. parameters) for each candidate model fit to avian species richness data. Optimal solutions minimize fit (moving towards bottom of figure) and complexity (moving to the left of figure). The top model using $f(\boldsymbol{\theta})$ = AIC was a Pareto optimal solution. Two *candidate models* (i.e., ΔAIC < 2) were not Pareto optimal (i.e., they were dominated by another model).

and choose a Pareto optimal solution with trade-offs acceptable to the decision maker. Some parameters might be associated with covariates for which annual data are difficult, expensive, or impossible to collect. The trade-offs in terms of model fit can be assessed relative to the expense of collecting additional data for these parameters. If the increase in model fit from the Pareto optimal solution that requires the additional (expensive) covariate data does not justify the additional expense, another Pareto optimal solution may be preferred.

Another approach is to examine the curvature of the Pareto frontier. An elbow shape (e.g, Fig. 1: $p = 3$) can be identified, where increasing the number of parameters has diminishing marginal returns in terms of f_1, and decreasing the parameter size has a large affect on f_1. In the avian species richness data, the largest improvement in model fit, per parameter added, was adding area to the null model (an 86 unit improvement to fit; Fig. 1). Subsequent parameter additions showed diminishing marginal returns in model fit; the second biggest improvement in model fit was adding precipitation to the area model (23 units), followed by adding temperature to the area + precipitation model (7 units). No models with five parameters occurred on the Pareto frontier.

Another approach is to compare the trade-offs to biological significance of the parameters involved and the need to make inference on those parameters. For example, if a parameter is required to inform a management decision, such as survival rates for harvest decisions, a decision maker would prefer to choose a Pareto optimal solution that included survival rates. Another approach might be to choose a Pareto optimal solution such that the maximum number of parameters is constrained by the amount of data. For example, if an investigator wishes to constrain the number of parameters in the model such that $p < \frac{n}{15}$, the investigator could select the Pareto optimal solution that maximized model fit within the constrained set. In the avian species richness data, with $n = 49$, this would suggest choosing the Pareto optimal model with three parameters (with log linear predictor $\beta_0 + \beta_1 x_{area,t} + \beta_2 x_{temp,t}$; Table 2).

Finally, models that are optimal in terms of model selection criteria could be highlighted as reference points on the Pareto frontier to guide decisions on the final model choice. Ultimately, the use of the Pareto frontier is that it provides visual information on the trade-offs of the objectives of the decision maker; in this case, maximizing model fit and minimizing complexity.

5 DISCUSSION

The explicit application of multi-objective optimization to model selection using the objective functions defined in eqs. 5 and 6 ties several important properties of MOO to common methods used in scientific research to select a model. First, many different model selection methods are special cases of the weighted-sum method; each method representing different objective weights. This provides a unifying framework to quantitatively and visually compare model-selection methods based on different theoretical foundations. Practitioners of multi-objective optimization in operations research or other decision-theoretic fields usually recommend sensitivity analyses of the resulting decisions given the choice of objective weights (Keeney and Raiffa, 1976; Williams and Kendall, 2017). A sensitivity analysis for the model selection problem consists of evaluating multiple model selection criteria (representing different objective weights) to examine the robustness of the solution to the choice of criterion. Many practitioners argue against this approach, suggesting that a criterion should be selected based on its theoretical motivation (e.g., AIC is asymptotically efficient; BIC is consistent, Aho et al., 2014). Others view a specific information criterion as one line of evidence to assist in a decision and report different criteria side-by-side (e.g., Araújo and Luoto, 2007; Parviainen et al., 2008). The former appears to be the dominant paradigm in ecological research, whereas the latter is common in other fields. Second, many model selection methods result in Pareto optimal solutions because they are specific formulations of eq. 2, which is sufficient for Pareto optimality. Thus, there is a decision-theoretic basis for model selection methods that can be expressed in the form of eq. 7 in terms of optimality criteria.

Although we described the model selection problem heuristically in terms of maximizing model fit and minimizing model complexity, we could have replaced model fit with predictive ability as the objective of interest. Predictive ability is the most commonly sought model characteristic for model selection, and many information criteria and other model selection methods were developed to optimize predictive ability (Akaike, 1973; Stone, 1977; Gelfand and Ghosh, 1998; Hoeting et al., 1999; Burnham and Anderson, 2002; Hooten and Hobbs, 2015). Many information criteria have weights and penalties that serve as bias corrections for optimization in terms of predictive ability (Konishi and Kitagawa, 1996). That is, many information criteria are based on bias-corrected log likelihoods, for which the model complexity is a correction factor to remove asymptotic bias of the log likelihood of a fitted model (Konishi and Kitagawa, 1996). The MOO problem in terms of maximizing predictive ability and accounting for model bias is similar in spirit to the MOO problem of maximizing model fit while minimizing model complexity.

Model selection by examining trade-offs of fit and complexity post-optimization has been used in several other applications. Users of Mallows' C_p often conduct similar investigations (Mallows, 1973). Freitas (2004) examined Pareto optimality in the related question comparing prediction and simplicity for data mining. Viewing each model's trade-offs, in terms of objectives, provides a visual assessment of the model selection problem, a potentially useful tool for ultimately choosing a model for inference or prediction. As is the case with any multi-objective optimization problem, the additional flexibility in model choice based on post-optimization specification of preferences could be viewed as either a positive or negative trait, depending on how an investigator values the order for which preferences are specified. Specifying preferences pre-optimization for the model selection problem benefits from being objective in the sense that a decision maker chooses how to weigh their specific objective functions without being influenced by how weights will alter the outcome of optimization. Specifying preferences post-optimization has the added flexibility of choosing a Pareto optimal solution that provides the best trade-offs for context dependent decision problems.

SUPPLEMENTARY MATERIAL

Appendix: R statistical software script to fit models described in Table 2 to avian species richness data, and calculate and plot values for eqs. 5 and 6 shown in Fig. 1.

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