Model Selection to Find a Sufficient Model Fitting to Thermal Performance of Metabolic Traits*

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Abstract

Determining thermal dependence of biological traits provides understanding in distribution patterns of species and is helpful in assessing the impact of climate change on biological systems. Here, I fitted four plausibe models to observed data of metabolic traits under different temperatures to calculate thermal performance curves. Model selection by either AIC or BIC were conducted to find one most sufficient model fitting to empirical data of each curve. In most curves, AIC and BIC give support to the same model and Ratkowsky model has the highest frequency of being selected. However, for some thermal performance curves in the dataset, the selected model fails in describing thermal dependence of metabolic traits, indicating that the four plausible models are not suitable and more models need to be involved. Overall, the results show that Ratkowsky model is sufficient for most thermal performance curves involved in this study.

1 Introduction

Temperature is an important abiotic factor that influences the functioning of organisms, especially for ectotherms whose body temperatures reflect that of their environments to different extent. It affects the rates of biochemical reactions and consequently has profound influence on different biological activities like metabolism, growth, development and reproduction [1]. And this can lead to further consequences in abundance and distribution of organisms [2]. Besides, interactions among species are also affected by thermal environment [3].

Thermal performance curve describes the dependence of performance (usually, the rate of a physiological activities or fitness) on temperature quantitatively [1]. Generally, organisms response to temperature fluctuation in a similar manner. The value of performance peaks at some temperature point and decreases when temperature deviates from the maximum point, while extremely high or low temperatures are lethal [1, 4]. The mathematical modelling of thermal performance curve provides a framework for the estimation of physiological characters like the optimum temperature at which performance peaks, upper and lower thermal limits of performance, and thermal tolerance range [4]. Besides, it is also helpful in predicting performance of organisms when temperature fluctuates. Thus, thermal performance curve is helpful in better understanding distribution patterns of species. There is evidence that the thermal tolerance range of a species is often corresponded to the temperature fluctuation of its habitat, indicating the importance of temperature as a selective force in shaping distribution pattern [5, 6]. There is also evidence showing that thermal sensitivity plays a role in the dynamics of biodiversity [7]. Furthermore, investigations in thermal performance curve help better predict the impact of current climate change on biological process [4, 8].

Currently, there are numerous mathematical models with different properties that are used to illustrate thermal performance curves of different clades [4, 9]. Which model, or models are sufficient in describing thermal dependence of performance is the main concern of this study. Using a dataset of observed data from 841 thermal performance curves of different metabolic traits, I calculated these curves by fitting four plausible models to them. Then I conducted model selection to find one model that is most sufficient to describe the observed data. Akaike information criterion (AIC) or Bayesian information criterion (BIC) was used as model selection criterion [10]. Besides, whether metabolic trait or habitat type is corresponded to models that get most support from empirical data was assessed.

2 Materials and Methods

2.1 Original Data

The original dataset used here is named as ThermRespData.csv and its field names are defined in another file called BiotraitsTemplateDescription.pdf. Both files are accessible in https://github.com/mhasoba/TheMulQuaBio/tree/master/content/data. The main fields of interest are OriginalTraitValue (trait values) and ConTemp (temperatures in Celsius scale). Each thermal performance curve is corresponded to a unique ID from 1 to 903. Among them 62 curves contain negative trait values and were removed. So a total of 841 thermal performance curves was used in following analysis.

2.2 Plausible Models

Denote by B the trait value and T the temperature. The function that describes the relationship between temperature and trait value is

$$B = B(T) \tag{1}$$

Plausible models are: (1) quadratic polynomial model with constants B_0, B_1 and B_2:

$$B(T) = B_0 + B_1 T + B_2 T^2 \tag{2}$$

(2) cubic polynomial model with constants B_0, B_1, B_2 and B_3:

$$B(T) = B_0 + B_1 T + B_2 T^2 + B_3 T^3 \tag{3}$$

(3) Briere model with constants B_0, T_0 and T_m [11]:

$$B(T) = B_0 T(T - T_0)\sqrt{T_m - T} \tag{4}$$

T_0 and T_m are lower and upper thermal limits of performance.

(4) Ratkowsky model with constants T_0, T_m, a and b [12]:

$$B(T) = \{a(T - T_0)(1 - e^{b(T - T_m)})\}^2 \tag{5}$$

T_0 and T_m are lower and higher thermal limits of performance.

2.3 Model Fitting

To conduct model fitting, least square method was used, and non-linear models were fitted using Levenberg-Marquardt algorithm [13, 14]. Maximum iteration number was 200.

For fitting of Briere model, start values of T_0 and T_m were the lowest and highest sampled temperatures of each curve and they are denoted by T_{0st} and T_{mst} respectively. From Eq. (4),

$$B_0 = \frac{B(T)}{T(T - T_0)\sqrt{T_m - T}} \tag{6}$$

For each curve, remove samples with lowest and highest temperatures and denote the rest as $\{(T_i, B_i), i = 1, 2, \cdots, n - 2\}$, where n is sample size. So from Eq. (6), a rough estimation of B_0, denoted by B_{0est} can be given by

$$B_{0est} = \frac{\sum_{i=1}^{n-2} \frac{B_i}{T_i(T_i - T_{0st})\sqrt{T_{mst} - T_i}}}{n - 2} \tag{7}$$

The start values of B_0 was taken from a uniform distribution between 0 and $2B_{0est}$. Each curve was fitted 100 times with different start values of B_0. As for fitting of Ratkowsky model, start values of T_0 and T_m were the lowest and highest sampled temperatures of each curve. Start values of a and b were taken from set $\{10^i : i = -5, -4, -3, -2, -1, 0, 1, 2, 3, 4\}$ iteratively. So for each curve, there are ten start values of a and b, and 100 combinations of them. Hence, each curve was fitted 100 times with different start values.

2.4 Model Selection

After model fitting, AIC and BIC of all models were calculated using following equations [10]:

$$AIC = -2L + 2k \tag{8}$$

$$BIC = -2L + klnn \tag{9}$$

where n is sample size, k is number of parameters in the model, and L is maximized log-likelihood value of the model. L is given by the following equation [10]:

$$L = -\frac{n}{2} ln \frac{RSS}{n} \tag{10}$$

where RSS is residual sum of squares of the model.

2.5 Model Averaging

In non-linear model fitting, dataset for each thermal performance curve was fitted 100 times and multiple solutions with similar AIC or BIC could be obtained. To find one most sufficient model supported by observed data, I conducted model averaging. Among all solutions obtained through dataset of one thermal performance curve, those with lowest AIC or BIC values were selected and averaged. For one thermal performance curve, denote by l the number of optimal solutions with lowest AIC or BIC among all solutions obtained by non-linear model fitting, and θ_i the ith solution, then the parameters of averaged model, denoted by θ, is given by following equation [10, 15]:

$$\theta = \sum_{i=1}^{l} \omega_i \theta_i \tag{11}$$

The weight ω_i is given by smoothed AIC or BIC method [15]:

$$\omega_i = \frac{e^{-xIC_i/2}}{\sum_{i=1}^{l} e^{-xIC_i/2}} \tag{12}$$

where xIC_i is the AIC or BIC of ith solution. Here, model averaging was conducted to solutions with equal AIC or BIC values, so

$$\omega_i = \frac{1}{l} \tag{13}$$

Then I calculated AIC and BIC of the averaged model and conducted model selection among linear and non-linear models.

2.6 Computating Tools

Most scripts are written in R 4.0.3, taking advantage of its powerful packages in model fitting and visualization, and of in-built functions for form processing. R package minpack.lm was used for model fitting, while visualization was conducted by R packages ggplot2, gridExtra and cowplot. The report was written using LaTeX because it is efficient in typesetting. A bash script was used to compile LaTeX source code. Finally, a python3 script was written to run all scripts using os module.

3 Results

3.1 Model Fitting and Selection

For each curve, models with lowest AIC or BIC were selected and they are either quadratic, cubic, of Briere or of Ratkowsky. No curve has multiple models equally supported by AIC or BIC. Among 841 thermal performance curves, 639 (76.0%) of them can be fitted by Briere model, and 649 (77.2%) of them can be fitted by Ratkowsky model. After model fitting, Briere or Ratkowsky models with lowest AIC or BIC values among all solutions were selected and averaged before further model selection. Figure. 1 provides examples of models that were used in selection among linear and non-linear models, and Figure 2 illustrates the distributions of AIC and BIC for each curve.

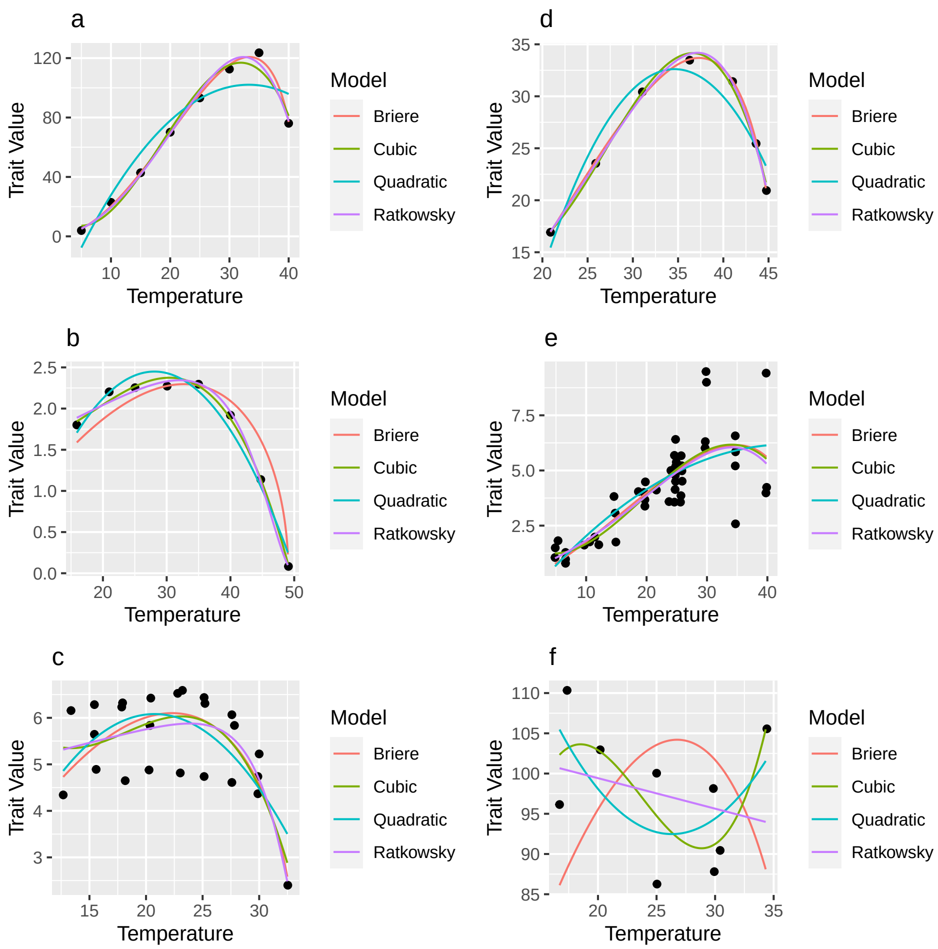

Figure 1: Examples of models used for model selection. Criterion of selection within non-linear models is AIC for subfigure **a**, **b** and **c**; and BIC for subfigure **d**, **e** and **f**. The IDs of thermal performance curves are: 148 (**a**), 204 (**b**), 322 (**c**), 138 (**d**), 237 (**e**), 519 (**f**).

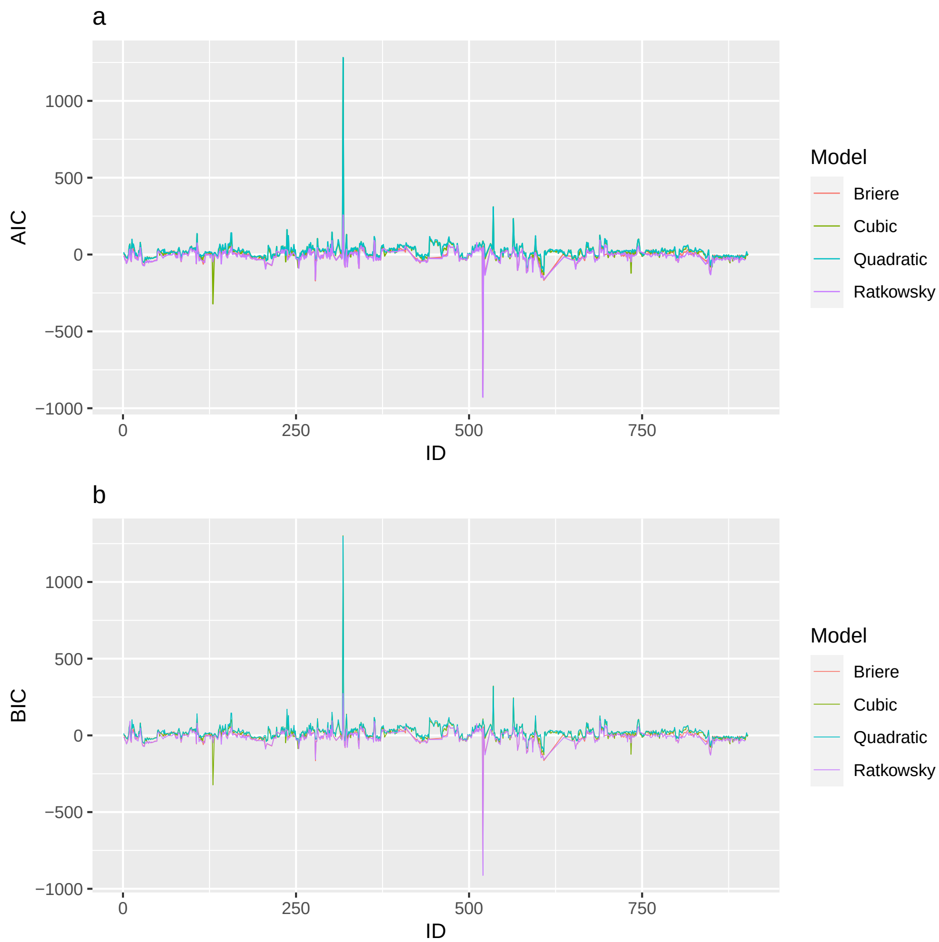

Figure 2: The distribution of AIC and BIC. The lateral axis represents the IDs of curves, and the vertical axis represents values of AIC (**a**) or BIC (**b**). The colours of lines represent different plausible models.

When AIC is used as criterion for model selection, 57 (6.78%) curves are fitted by quadratic polynomial function and 160 (19.02%) curves for cubic polynomial function. As for non-linear models, 190 (22.59%) curves are fitted by Briere model, and the rest 434 (51.61%) curves are fitted by Ratkowsky model. When BIC is used for model selection, 218 (25.92%)

curves are fitted by linear models (55 quadratic polynomial model and 163 cubic polynomial model). 191 (22.71%) curves are fitted by Briere model, while the rest 432 (51.37%) curves are fitted by Ratkowsky model. 18 curves are sufficiently fitted by different models under different criteria for model selection as shown in Table 1.

Table 1: Curves That AIC and BIC Support Different Models

ID	AIC-supported	BIC-supported
99	Briere	Ratkowsky
105	Ratkowsky	cubic
232	Ratkowsky	Briere
318	Ratkowsky	Briere
330	Briere	Ratkowsky
351	Briere	Ratkowsky
426	Ratkowsky	Briere
496	Briere	Ratkowsky
569	Ratkowsky	Briere
635	quadratic	cubic
644	quadratic	cubic
669	Ratkowsky	Briere
681	Ratkowsky	Briere
737	Briere	Ratkowsky
745	Ratkowsky	Briere
765	Briere	Ratkowsky
827	Ratkowsky	Briere
879	Briere	Ratkowsky

3.2 Selected Models for Curves of Different Metabolic or Habitat Types

To assess preferred models for thermal performance curves of differnet metabolic traits or species living in different habitat types, 18 curves were removed because AIC and BIC supported different models. So a total of 823 curves were involved.

In the original dataset, the metabolic trait of each curve is defined in the field of StandardisedTraitName (trait name for comparison), which contains three categories: gross photosynthesis rate, net photosynthesis rate and respiration rate. Another field relevant to trait name is OriginalTraitName (trait name as it found in source). It should be noted there are four curves have no StandardisedTraitName, while their OriginalTraitName are oxygen evolution rate in thylakoid membranes (IDs: 698, 699) and cell specific photosynthesis rate (IDs: 441, 442). They were not involved in assessing which model is suitable for different metabolic traits. As for habit type of each curve, it is defined in another field (Habitat), which is composed of four types: aquatic, freshwater, freshwater/terrestrial, marine and terrestrial. Here I assessed which model is suitable for determining thermal performance of species living in terrestrial or non-terrestrial (aquatic, freshwater, freshwater/terrestrial and marine) habitats.

Table 2 illustrates the sufficient models for thermal performance curves of different metabolic traits. A total of 819 thermal performance curves of three metabolic traits are involved. For models of each metabolic trait, non-linear model occupies a larger proportion (75.0% in gross photosynthesis rate, 78.8% in net photosynthesis rate, and 66.2% in respiration rate) than linear models. Besides, Ratkowsky model takes a bigger amount than Briere model in all metabolic traits except gross photosynthesis rate.

Then I classified thermal performance curves according to whether the species studied is specific in terrestrial habitats (Table 3). Non-linear model takes the biggest amount of sufficient models for both two kinds of habitat type (82.1% for terrestrial habitat and 55.2% of non-terrestrial habitat), and Ratkowsky model occupies biggest proportion among four plausible models.

Table 2: Selected Models for Thermal Performance Curves of Different Metabolic Traits

Model	Gross photosynthesis rate	Net photosynthesis rate	Respiration rate	Total
Quadratic	0	19	36	55
Cubic	9	80	71	160
Briere	16	73	94	183
Ratkowsky	11	294	116	421
Total	36	466	317	819

Table 3: Selected Models for Thermal Performance Curves from Species in Different Habitat Types

Model	Terrestrial	Non-terrestrial	Total
Quadratic	21	34	55
Cubic	81	79	160
Briere	134	49	183
Ratkowsky	335	90	425
Total	571	252	823

3.3 Preferred Models May not Describe the Observed Data Sufficiently

Through model selection, I selected one model for each curve and it is the most sufficient one in terms of describing the thermal performance curve among four plausible models. However, the preferred models of some curves still fail in describing thermal performance throughout the temperature range between lower and upper thermal limits of performance. As the growth of temperature in this range, performance is supposed to increases, peaks at some point, and then drops [1, 4]. The preferred models of some curves are not bell-shaped (Figure. 3). Furthermore, ecologically unrealistic estimations of thermal limits of performance are also given by some selected models (Figure 4).

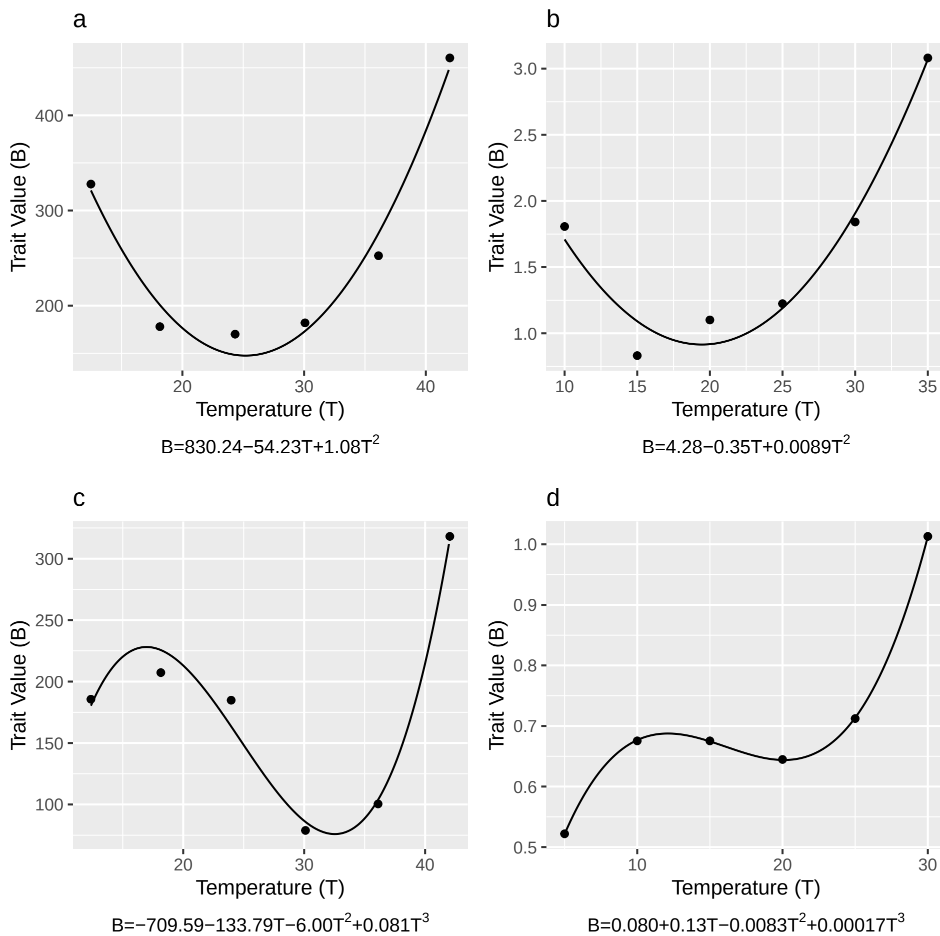

Figure 3: Examples of preferred models that are not bell-shaped curves. IDs of thermal performance curves are: 456 (**a**), 841 (**b**), 455 (**c**), 600 (**d**). Mathematical expression of each model is given at the bottom of each subfigure. For these datasets, AIC and BIC support the same models with equal parameters.

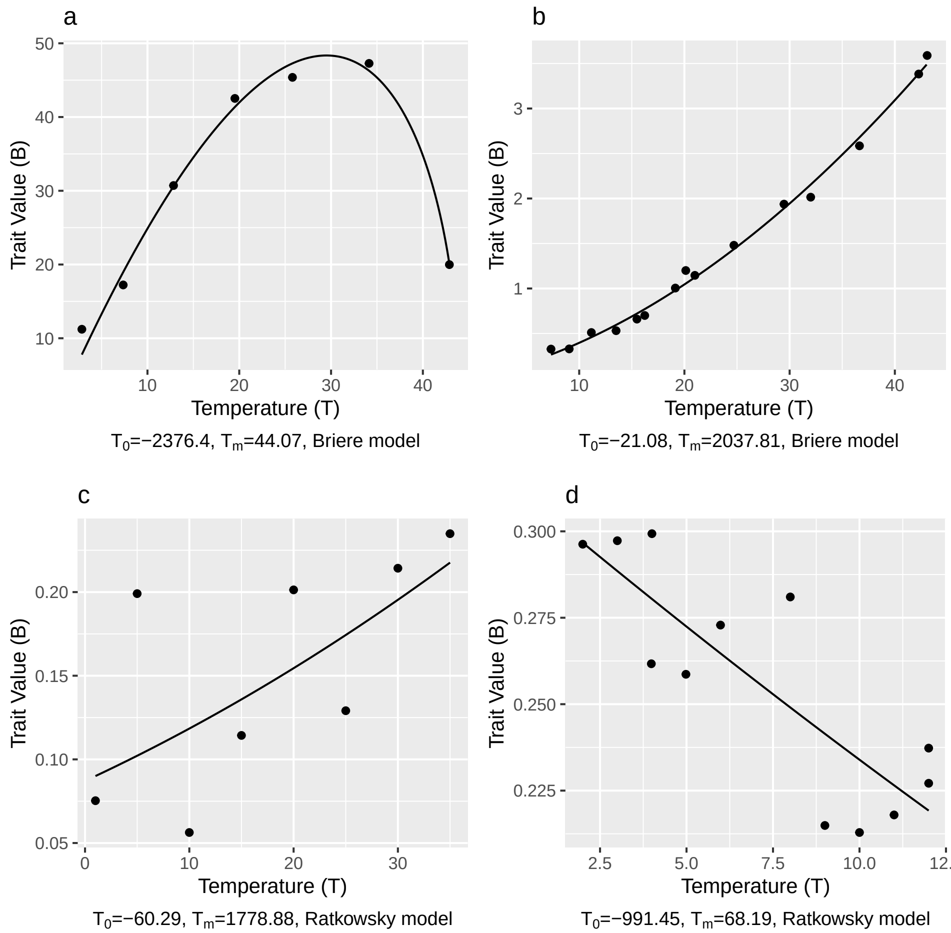

Figure 4: Examples of preferred models that give unrealistic estimations of thermal limits of performance. IDs of thermal performance curves are: 81 (**a**), 215 (**b**), 46 (**c**), 254 (**d**). Criterion of model selection is AIC, and estimations of lower and upper thermal limits of performance, denoted as T_0 and T_m, are given at the bottom of each subfigure.

4 Discussion

Investigations in how organisms response to temperature fulctuation are helpful in better understanding the impact of recent and future climate change on biological systems [16, 17]. In assessment of thermal performance, it is important to choose an appropriate mathematical model that is best supported by empirical data and is able to provide relatively precise estimations of dependent variable using given values of independent variable. Currently, there are plenty of mathematical models used in fitting thermal performance curves, and model selection criteria can be used to explicate how sufficient a model is in describing thermal performance curves [4, 9, 10]. In order to find which model is best supported by observed data of thermal performance, I fitted four plausible models to a dataset composed of 841 thermal performance curves and conducted model averaging and selection using either AIC or BIC as criterion. In most cases, AIC and BIC prefer the same model. The results also showed that under both selection criteria, Ratkowsky model is sufficient in quantifying thermal performance for about 51% of curves in the dataset.

In model selection, a set of plausible models are ranked by some criterion and the most appropriate one is selected. AIC and BIC are two criterion for model selection. They take both fit and model complexity into consideration to balance under- and over-fitting to observed data [10, 18]. Although AIC and BIC are quite similar in forms, they are divergent in theoretical motivations. BIC is based on Bayesian statistical analysis and is an approximation reflecting the probability that the plausible model is the true model that generated the empirical data [19]. Minimized BIC is corresponded to maximized posterior probability among all plausibilities and can be thought as a criterion for model selection [20]. However, whether there is such a "true model" is controversial [21], and the theoretical basis of BIC is disputed [19]. As for AIC, it measures the predictive performance of each candidate model by estimating Kullback-Leible information loss [19, 22, 23], and is thus well-founded in information theory. Here, I conducted model selection using AIC and BIC as criterion respectively. In most cases, they prefer the same model. However, I tend to use AIC as model selection criterion because of its solid theoretical foundation.

In non-linear model fitting, an iterative algorithm is employed to gain a numerical local optimal solution, which is sensitive to start values [13, 14]. Here, I fitted each non-linear model 100 times with different start values before model selection, attempting to find the global optimal solution. For one thermal performance dataset, multiple solutions can be obtained by different start values while they have equal and lowest AIC or BIC. This is because of limited accuracy in numerical calculation of AIC and BIC by R scripts. To deal with this, I conducted model averaging using smoothed AIC or BIC method. When multiple plausible models get nearly equivalent support from observed data (*e.g.* similar AIC or BIC values), model averaging is a good method to give estimations of model parameters or predict values of response variables [10].

Generally, thermal performance curve is supposed to be a bell-shaped curve with ecologically realistic lower and upper thermal limits of performance [1, 4]. However, some models supported by AIC or BIC are not bell-shaped curves, as exemplified in Figure 3. Others may give estimations of thermal limits of performance that are too low or too high to be realistic, as exemplified in Figure 4. Such models may fit to the observed data well (*e.g.* Figure 3d and Figure 4a), but fail in describing the whole thermal performance curve. A possible reason is that there are not enough sampes from a wide enough temperature range to allow the models to capture the change of performance over temperature in different ranges. For example, curve 215 only contains samples of relatively low temperature (*i.e.* temperatures of all samples are no greater than the optimum temperature where performance peaks) as it is shown in Figure 4b. An alternative explanation is that none of the four plausible models are suitable for describing the observed data. AIC and BIC can only explicate the relative goodness of each model in a given set of models [10, 15, 18] and it is possible that no model in the given set can fit to the observed data sufficiently. Under these circumstances, more models are needed to be used in fitting and selection.

Overall, I conducted model fitting, averaging and selection using observed data of 841 thermal performance curves. Plausible models include quadratic polynomial model, cubic polynomial model, Briere model and Ratkowsky model. AIC and BIC were used as model selection criterion. For most curves, AIC and BIC give support to the same model. The results shows that for more than a half of thermal performance curves involved here, Ratkowsky model is the most sufficient one among four plausibilities. When curves are classified according to metabolic trait or habitat type of species, Ratkowsky model is most sufficient one for a majority of curves in most categories. However, some selected models cannot describe the whole thermal performance curves or contain unrealistic parameters, indicating that none of the four models is suitable for fitting to the observed data.

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