`Matilda v1.0`: An R package for probabilistic climate projections using a reduced complexity climate model

`Matilda`: An R framework for probabilistic climate analysis

Joseph K Brown*, Leeya Pressburger, Abigail Snyder, Kalyn Dorheim, Steven J Smith, Claudia Tebaldi, and Ben Bond-Lamberty

Joint Global Change Research Institute, Pacific Northwest National Laboratory, 5825 University Research Ct. #3500, College Park, MD 20740 USA

*Corresponding author
Email: joseph.brown@pnnl.gov

Abstract

A primary advantage to using reduced complexity climate models (RCMs) has been their ability to quickly conduct probabilistic climate projections, a key component of uncertainty quantification in many impact studies and multisector systems. Providing frameworks for such analyses has been a target of several RCMs used in studies of the future co-evolution of the human and Earth systems. In this paper, we present `Matilda`, an open-science `R` software package that facilitates probabilistic climate projection analysis, implemented here using the Hector simple climate model in a seamless and easily applied framework. The primary goal of `Matilda` is to provide the user with a turn-key method to build parameter sets from literature-based prior distributions, run Hector iteratively to produce perturbed parameter ensembles (PPEs), weight ensembles for realism against observed historical climate data, and compute probabilistic projections for different climate variables. This workflow gives the user the ability to explore viable parameter space and propagate uncertainty to model ensembles with just a few lines of code. The package provides significant freedom to select different scoring criteria and algorithms to weight ensemble members, as well as the flexibility to implement custom criteria. Additionally, the architecture of the package simplifies the process of building and analyzing PPEs without requiring significant programming expertise, to accommodate diverse use cases. We present a case study that provides illustrative results of a probabilistic analysis of mean global surface temperature as an example of the software application.

1 Introduction

The human-Earth system is fundamentally integrated with impacts and feedbacks tightly interconnecting outcomes across human decisions and the broader environment. Human decisions regarding land use, water use, and energy consumption affect the broader Earth system, which can subsequently drive future human decisions [1,2]. Multisectoral models are those that include representations of energy, water, land, socioeconomic, and climate sectors in an integrated framework. The Global Change Analysis Model (GCAM), and similar multisectoral models can be used to explore future scenarios with different water, energy, land use, and socioeconomic outcomes that interact with the Earth system. Representative Concentration Pathways (RCPs), for example, provide scenarios that reach varying magnitudes of radiative forcing by the end of the century based on changing GHG emissions and land use [1–3]. Shared Socio-economic Pathways (SSPs) provide scenarios driven by plausible changes in global developments including population and economic growth, fossil fuel dependency, and costs of environmental degradation [3,4]. The development of an SSP-RCP framework (hereafter, SSPs) combines the climate and societal futures of SSPs and RCPs [3,5]. These scenarios can be used in Earth system models (ESMs) to explore future climate outcomes given different possible emissions scenarios. However, the breadth at which ESMs can investigate the climate system comes at a significant computational expense.

Reduced complexity climate models (RCMs) play a significant role in quickly assessing how key climate variables may look in the future by applying probabilistic projections, which are made possible because of their simplified computational complexity [6–11]. By representing only the most critical Earth system processes with reduced resolution in temporal and spatial dimensions, RCMs are a useful alternative to more powerful but much slower ESMs in many cases [9,12]. The computational efficiency of RCMs makes them an ideal tool for constructing perturbed parameter ensemble (PPE) simulations, which are RCM ensembles built by running the model iteratively with different parameter sets [7,13,14]. This ability enables effective sampling of the parameter space, propagation of parameter uncertainty to RCM ensembles, and provides a framework for probabilistic projection quantification [7–9,15,16].

The capacity for RCMs to conduct probabilistic projections with PPEs is critical, but few RCMs have an easy-to-use and open-source workflow for this capability. In Phase 2 of the Reduced Complexity Model Intercomparison Project (RCMIP), Nicholls et al. [17] highlight the use of extant RCMs to perform probabilistic analyses to inform Earth system knowledge by creating PPEs. Among the RCMIP models investigated; MAGICC, FaIR, and Hector are some of the most relevant, with MAGICC and FaIR used in previous reports by the Intergovernmental Panel on Climate Change (IPCC) [12]. While both models are extensive and widely used for probabilistic projections [18–20], they have some drawbacks. For example, while FaIR demonstrates skillful outputs in RCMIP evaluations [17], it lacks a turnkey mechanism for computing probabilistic distributions of climate variables [7,14]. This places a significant programming responsibility on the user. Hector has similarly lacked a seamless method for probabilistic projections. MAGICC is also one of the best-performing RCMs in RCMIP and takes advantage of a rigorous statistical approach [10,21]. However, while it aims to shift to open-source, it is currently a closed-source model. To use MAGICC to the fullest capability of the model, users must contact model developers for access to the software package and probabilistic distribution.

We address some of these drawbacks in our development of the R package `Matilda`. `Matilda` is an open-science framework that provides a simplified method for conducting probabilistic climate projections without imposing a significant programming burden on the user. Our method generates parameter sets from Monte Carlo estimation of prior distributions from the literature. It then builds PPEs, weights them for realism against observed data, and computes probabilistic climate projections. While `Matilda` is flexible enough to operate with many RCMs, it was designed explicitly for seamless integration with Hector.

Hector is an open-source, object-oriented simple climate carbon-cycle model capable of emulating more complex ESMs and is executed in C++ [6,9,11]. It takes advantage of the computational benefits described above by operating on a global spatial scale and annual time step. The model functions by converting user-specified emissions to atmospheric concentrations which are used to calculate radiative forcing [6,9]. Hector then uses total radiative forcing to derive global temperature change and other climate variables [9,11]. Despite its reduced complexity, Hector provides a good representation of CMIP6 outputs for major climate variables across SSP scenarios [22]. In addition to operating as a stand-alone

carbon-climate model, Hector is also used as the default climate module for GCAM [6]. Hector can also be run as an R package and through a web-accessible interface, making it accommodating to a larger user base [22–24]. Hector's design and performance make it an excellent candidate for developing a user-friendly probabilistic climate projection tool in R. Pressburger et al. [13] show the benefits of applying such a framework to account for uncertainty of model parameters when assessing near- and long-term sources of atmospheric CO_2. With `Matilda`, users will be able to easily use Hector to conduct probabilistic climate projection analyses without the burden of complex coding requirements. `Matilda` thus provides seamless integration with the Hector reduced complexity climate model.

The objectives of this paper are twofold: 1) we introduce the `Matilda R` package that provides a simple framework for conducting probabilistic climate projection analyses using the Hector simple climate model and 2) we showcase the package functionality with a case study that provides illustrative results but is not meant to be a comprehensive probabilistic analysis. We conclude with a list of future developments that can improve the long-term utility of `Matilda`.

2 Software Description

Here we introduce the software functions and basic workflow of the package (Fig. 1). We use applied examples to show package functionality by assessing climate change projections from the SSP 2-4.5 emissions scenario (i.e., middle of the road SSP with the year 2100 radiative forcing level of 4.5 W/m^2), providing step-by-step code and explaining the significance of each function.

Fig 1. Matilda workflow. Diagram detailing the `Matilda` workflow to compute probabilistic projections. Dotted lines indicate opportunities for the user to define their own program specification. The dashed line in step 3 indicates the ability of the user to evaluate ensemble members repeatedly with different scoring criterion.

2.1 Installing the Software

The `Matilda` software is available on `GitHub`. To install from our `GitHub` repository:

1)

```
library(remotes)
install_github("jgcri/matilda")
```

Once installed, the package is loaded as with any other `R` package:

2)

```
library(matilda)
```

Matilda functions are fully integrated with Hector's R interface, and therefore when Matilda is installed and loaded, the hector package (https://jgcri.github.io/hector/) is also loaded. Matilda requires the use of Hector V3 or newer [22].

2.2 Software Documentation

Full descriptions of package functions can be accessed in the package's help documentation. Furthermore, detailed documentation and vignettes are available from our GitHub repository (github.com/jgcri/matilda).

2.3 Configuring a Model Core

An analysis in Matilda begins by setting up a Hector model instance, termed a "core". A Hector core is an object that contains information about model inputs, current state, and outputs for a specific Hector run. The information contained in an initiated core comes from an INI file holding metadata, emissions scenarios, and model parameters needed to run Hector.

We call newcore() (a hector function) to initiate a core containing information to conduct model runs using the SSP 2-4.5 emission scenario:

3)

```
ini_file <- system.file("input/hector_ssp245.ini", package = "hector")

core_ssp245 <- newcore(ini_file, name = "SSP_245")
```

2.4 Parameter Estimation and Establishing Parameter Sets

The basis of running Hector in a probabilistic setup relies on establishing a set of parameter configurations that are used to run the model iteratively. Matilda uses parameter information gathered from the literature to inform prior distributions (Table 1). To build parameter sets, we draw parameter values from their prior distributions using Monte Carlo sampling. Each parameter is sampled independently from its marginal prior distributions defined using mean and standard deviation estimates as in:

$$\theta_i \sim N(\mu, \sigma) \qquad (1)$$

where θ_i is a given Hector parameter and $N(\mu, \sigma)$ is the normal distribution of parameter θ_i using hyperparameters μ (mean) and σ (standard deviation). Some parameters have marginal distributions best represented using lognormal distribution, in such cases, $N(\mu, \sigma)$ is substituted by $logN(\mu, \sigma)$ (Table 1). Using informed prior marginal distributions from the literature as a starting point for building perturbed parameter sets enables the exploration of a range of possible parameter values from viable parameter space built on existing knowledge [13,25]. Parameter draws are combined into parameter sets for Hector using a uniform multivariate

distribution. This parameter estimation process ultimately establishes parameter sets that account for parameter uncertainty and can be used to build an ensemble of model runs. In other words, we use prior information about individual parameters to build parameter sets, but we do not know which sets will result in the most skilled model results before considering observed data.

Table 1. Hector parameters used in Matilda. Hector parameters used to generate parameter sets in this work. The distributions are indicated as mean ± standard deviation. References from where distributions are derived are included.

Parameter	Description	Units	Distribution	Reference of uncertainty
α	Aerosol forcing scaling factor	Unitless	1.0 ± 0.23 (Normal)	Smith et al (2020) (25)
β	CO_2 fertilization factor	Unitless	0.55 ± 0.10 (Normal)	Jones et al (2013) (26)
ECS	Equilibrium Climate Sensitivity	℃	3.0 ± 0.65 (Lognormal)	Sherwood et al (2020) (27)
K_{eff}	Ocean heat diffusivity	$cm^2\ s^{-1}$	1.16 ± 0.118 (Normal)	Vega-Westhoff et al (2019) (28)
NPP_0	Pre-industrial net primary productivity	Pg C yr^{-1}	56.2 ± 14.3 (Normal)	Ito (2011) (29)
Q_{10}	Temperature sensitivity of heterotrophic respiration	Unitless	2.2 ± 1.0 (Lognormal)	Davidson and Janssens (2006) (30)

In `Matilda`, we build parameter sets by calling `generate_params()`. Parameter distributions are independent of the SSP scenario, however to run this function the user must still provide an established Hector core. Additionally, the user must specify the number of parameter sets desired (`draws`). Using `generate_params()` will produce randomized draws each time it is run. Therefore, the user should either save the resulting data frame or use `set.seed()` if replication of parameter sets is critical to the analysis. In this example we use our previously established core to produce a set of 25 parameter configurations and display a subset of samples from the result:

4)

```
param_sets <- generate_params(core = core_ssp245, draws = 25)

print(param_sets)
```

```
##      BETA    Q10_RH NPP_FLUX0 AERO_SCALE DIFFUSIVITY      ECS
## 1 0.5429609 1.7033771  50.47088  1.2697224    1.070107 2.410262
## 2 0.5234430 1.4867288  51.41584  0.6596398    1.209486 3.092423
## 3 0.4225671 1.3724196  75.76174  0.9010108    1.037287 2.335147
## 4 0.4857051 1.9163999  86.77007  0.7581231    1.243966 2.712076
```

Parameters can be easily added or omitted from the new parameter set data frame. For example, to run the model with a subset of parameters, undesired columns can be omitted from the data frame. This will result in a data frame that only contains parameter distributions that the user wishes to perturb. Similarly, the user can characterize additional parameter distributions and add them as new columns to the data frame, as long as the parameter is described in Hector.

Once established, the parameter sets are used as inputs for independent Hector model runs. Thus, each model run represents a multivariate parameter combination as follows:

$$m_i = \left(\theta_{1_i}, \theta_{2_i}, \theta_{3_i}, \ldots, \theta_{n_i}\right) \quad (2)$$

where m_i is an individual ensemble member and $\theta_{\{1-n\}_i}$, are parameters sampled to build an independent configuration. Using different parameter sets to run Hector allows us to build PPEs and determine how different parameter combinations from a viable parameter space interact to affect climate variable projections. This method effectively propagates parameter uncertainty to model ensemble uncertainty, a process described as forward uncertainty propagation [32].

2.5 Forward Uncertainty Propagation and Running the Model

We run Hector for each of the parameter sets by calling `iterate_model()`, which runs the model for each parameter set and combines the results into a data frame object representing the new PPE. To run `iterate_model()`, the same core object is used as in previous steps and we also must supply the object where parameter sets are stored:

5)

```
results <- iterate_model(core = core_ssp245, params = param_sets)

print(results)
```

```
##              scenario year          variable    value    units run_number
## 1 Unnamed Hector core 1745 CO2_concentration 277.1500 ppmv CO2          1
## 2 Unnamed Hector core 1746 CO2_concentration 277.1886 ppmv CO2          1
## 3 Unnamed Hector core 1747 CO2_concentration 277.2234 ppmv CO2          1
## 4 Unnamed Hector core 1748 CO2_concentration 277.2558 ppmv CO2          1
```

The resulting data frame returns 25 separate runs, as indicated by the `run_number` column; in this case, the total number of rows is 55600 (25 runs × 4 output variables × 556 years). Each run includes values for the major climate variables of a Hector default output (CO_2 concentration, total radiative forcing, CO_2 forcing, and global mean air temperature) for the years 1745-2300 (the time range defined by the SSP INI file we chose above).

While a core object and a data frame of parameter sets are the only required arguments to run `iterate_model()`, additional arguments can be supplied to reduce the variables and year range returned for each run using `save_vars` and `save_years`, respectively. This reduces the size of the data stored in memory, which may be important when running the model to build large ensembles (e.g., 15,000 as in [13]). Any output variable from Hector can be returned using `save_vars()` for any year range subset from 1745-2300. In the following example, we supply these arguments to return values only for CO_2 concentration and global mean air temperature for the year range 1745-2100:

6)

```
results <- iterate_model(core = core_ssp245, params = param_sets, save_vars
= c("CO2_concentration", "global_tas"), save_years = 1745:2100)
```

The resulting data frame has only 17800 rows, a 68% savings over the full example above.

2.6 Model Evaluation Approach and Scoring Model Runs

Evaluating ensemble members is important in climate model assessment because it allows for a more accurate representation of the true underlying system by accounting for uncertainties propagated from parameter sets. The concept of weighting ensemble members is intuitive; members that are skilled and agree well with the historical record should receive a higher weight than members that do not largely replicate what we know to be a realistic climatic projection [8]. By assigning weights to ensemble members, based on their performance against observed data, more reliable projections can be made for future climate scenarios as parameter uncertainty is propagated to model forecasts. Ensemble members closely aligned with historical climate data will contribute more information to our probabilistic projections than members with outputs deviating significantly from the historical record. In parallel, we can use forward uncertainty propagation to better understand what parameter sets interact with Hector in a way that yields the most realistic result. This can then be used to update prior parameter distributions (although we do not do so here).

Scoring PPE members in `Matilda` is conducted using `score_runs()` which requires (1) a results data frame, (2) a scoring criterion, and (3) a scoring function/algorithm. The results data frame typically comes from calling `iterate_model()`, as above.

Scoring criteria define information used to compare ensemble members against observational data. A scoring criterion can be built by the user by calling `new_criterion()` and simply requires the climate variable to be used in the comparison, the years of comparison, and observed data values for the years specified. For example, a new criterion can be created based on global mean air temperature from a dataset containing observed warming values from 1990-2023:

7)

```
temp_data <- read.csv("example_temperature_data.csv")

head(temp_data)
```

```
##   year anomaly_C
## 1 1990 0.3605625
## 2 1991 0.3388965
## 3 1992 0.1248968
## 4 1993 0.1656585
## 5 1994 0.2335498
## 6 1995 0.3768662
```

```
user_temp_criterion <- new_criterion(var = "gmst", years = temp_data$year,
obs_values = temp_data$anomaly_C)

print(user_temp_criterion)
```

```
## Criterion for screening Hector:  gmst 1990  to  2023
```

This defines a custom criterion: a time series of 34 (1990-2023) values that will be compared against Hector's "gmst" (global mean surface temperature anomaly) output variable.

The `Matilda` package has internally available scoring criteria for easy use, including `criterion_co2_obs()` and `criterion_gmst_obs()`. Data contained in `criterion_co2_obs()` is pulled from the Mauna Loa record of observed annual mean atmospheric CO_2 concentration (32), while `criterion_gmst_obs()` uses observed annual mean global surface temperature anomaly data retrieved from the HadCRUT5 data set (33).

Scoring functions in `Matilda` apply different mathematical algorithms to compute model weights based on the results and scoring criterion. We provide multiple mechanisms to weight model outputs against observations, and users can define their own custom functions as well. There are currently two internally available scoring functions called `score_bayesian()` and `score_ramp()`, that differ in functionality and computational complexity.

2.6.1 Scoring Function: `score_bayesian()`

Bayesian probability theory provides a rigorous framework combining prior information, observational data, and model simulations to achieve analytical goals related to parameter estimation, model evaluation, and uncertainty quantification [35,36]. Here, we use Bayesian inference to assess PPE members and assign weights according to the probability of ensemble member m_i conditional upon observed data **Y**. This is described as the posterior probability and, consistent with Bayes' theorem, is proportional to the product of a chosen likelihood function of m_i given observed data and prior information of m_i(prior probability) [37]. We can express this in equation form as:

$$P(m_i|Y) \propto L(m_i|Y) \times P(m_i) \qquad (3)$$

where $P(mi|\mathbf{Y})$ is the posterior probability of m_i conditional upon observed data **Y**, $L(m_i|\mathbf{Y})$ is the chosen likelihood function, and $P(m_i)$ is the prior information of ensemble member m_i.

As demonstrated in Eq. 3, posterior probabilities (i.e., model weights) are dependent on prior knowledge about ensemble member m_i and a likelihood function that quantifies the agreement between ensemble member m_i and observed data **Y**. Here, we base our likelihood function on root-mean-square error (RMSE) which is commonly used as a statistical evaluation of model performance in climate research and is optimal under the assumption that errors are normally distributed [38,39]. For a given time series of observed data $\mathbf{Y}_{(t)}$ (i.e., scoring criteria) and a corresponding time series of each ensemble member $m_{i(t)}$, RMSE is a quantification of the averaged difference between the observed and modeled data and is calculated using the following formula:

$$RMSE_i = \sqrt{\frac{1}{N}\sum_{i=1}^{N}\left(\mathbf{Y}_t - m_{i(t)}\right)} \qquad (4)$$

where RMSE_i is an independent RMSE value representing how well PPE member i agrees with observations and N represents the total number of data points in the time series. We further use these RMSE_i values in our chosen likelihood function. Assuming a normal distribution, our proportional likelihood can be calculated as:

$$L(m_i|Y) = e^{-\frac{(RMSE_i)^2}{2\sigma^2}} \qquad (5)$$

In this equation, a decay relationship exists between RMSE_i and $L(m_i|\mathbf{Y})$, indicating a gradual decrease in $L(m_i|\mathbf{Y})$ as RMSE_i increases. In other words, the likelihood of an ensemble member decreases as the disagreement with observations increases. The value of σ in Eq. 5 plays a crucial role in controlling the rate of likelihood decay by defining the unit of acceptable variance in the data. The relationship is explained in detail below and can be visualized in Fig 2.

As described in Section 2.4, we enforce an equally distributed prior $P(m_i)$ across all ensemble members because although we use prior information about individual parameters of Hector to build parameter sets, we do not know which sets will result in the most skilled model results before considering observed data. Taking all this information together, weights are estimated in `score_runs()` as normalized posterior probabilities of each ensemble member, taking into account both agreement with observed data and prior beliefs about ensemble members using the following formula:

$$\omega_i = \frac{L(m_i|Y) \times P(m_i)}{\sum_{i=1}^{N}\left(L(m_i|Y) \times P(m_i)\right)} \qquad (6)$$

where ω_i is a weight assigned to each ensemble member.

We provide an example of using `score_bayesian()` as the scoring function when calling `score_runs()`. For this example, we use the result produced in code block 5, and assess the agreement between ensemble members and observed data with the `criterion_co2_obs()` scoring criterion:

8)

```
scored_hector_runs <- score_runs(results, criterion_co2_obs(),
score_bayesian, sigma = 2)

print(scored_hector_runs)
```

```
##     weights    run_number
## 1 0.093578592          1
## 2 0.005328194          2
## 3 0.138975159          3
## 4 0.008768552          4
## 5 0.040364027          5
```

The resulting data frame returns 25 weights assigned for each Hector run (indicated by `run_number`). Weights for each ensemble member will be nonzero positive values that sum to 1. Weights closer to 1 represent ensemble members in strong agreement with observed data and weights closer to 0 correspond to members that are not in strong agreement with observed data. It is important to note that weights are asymptotic and thus no one ensemble member can score exactly 1 or reach a value of exactly 0 due to the normalization process.

The `sigma` value in code block 8 is a parameter that sets the decay rate determining how quickly the likelihood values decrease as RMSE values increase. Because `sigma` represents the unit of acceptable deviation, a lower `sigma` value leads to a faster decay rate, meaning that the likelihood decreases more rapidly with increasing RMSE values. Conversely, a higher `sigma` reduces the decay rate, and ensemble member likelihood decreases more slowly with respect to increasing RMSE values. This results in more weight being assigned to ensemble members

that have a lower likelihood. In Figure 2, we show how different `sigma` values lead to different decay rates, meaning that weights are distributed differently depending on `sigma`. In effect, this determines how severely an ensemble member is penalized as it departs from a criterion.

Fig 2. Decay rates from varying sigma values. Root mean square error (RMSE) plotted against likelihood, conditional upon observed data. Different colors indicate decay rates for different sigma values in `score_bayesian()`. Setting higher values to `sigma` decreases the deviation penalty applied to ensemble members.

This parameter thus gives users the ability to govern the sensitivity of the likelihood decay as RMSE values increase. By adjusting the `sigma` value, the user has control over the weight assigned to different ensemble members based on their RMSE values. Setting a lower `sigma` value will result in more weight placed on ensemble members with low RMSE values. In comparison, a higher `sigma` value will give relatively more weight to ensemble members with higher RMSE values. We use the standard deviation of the observed data as the default quantification of `sigma`, which results in a relatively gradual tapering of the likelihood as RMSE increases. We provide options in `score_bayesian()` to set a value to `sigma` directly or to weight ensemble members within easily defined units of acceptable deviation from observed data.

We note that users should make adjustments to `sigma` that are in line with the context and evaluation purpose specific to their analytical goals. The case study at the end of this paper provides an example of assessing ensemble member weights for different acceptable deviation limits.

2.6.2 Scoring Function: `score_ramp()`

The `score_ramp()` function is a simpler and more transparent scoring algorithm that computes the absolute difference between ensemble members $m_i(t)$ and observed data $\mathbf{Y}(t)$ at each time step:

$$D(t) = |Y(t) - m_i(t)| \qquad (7)$$

Scores are then computed based on how far absolute differences $D(t)$ are from arbitrarily selected minimum (w_1) and maximum (w_2) divergence values. For example, $D(t) \leq w_1$ indicates small differences between modeled and observed data at time t and will result in a score of 1, whereas $D(t) \geq w_2$ indicates significant divergence of modeled data from observed data and will result in a score of 0 (Fig 3). In cases where $D(t)$ falls between w_1 and w_2, scores are computed using a linear function that decreases as $D(t)$ values get closer to w_2 and further from w_1 (Fig 3).

Fig 3. Decay rate for score_ramp(). Example of decay method for `score_ramp()` where $w_1 = 5$ and $w_2 = 10$. Ensemble members with an average deviation from observation < 5 will score 1 and ensemble members with an average deviation > 10 will score 0. Scores of ensemble

members with average deviation between w_1 and w_2 will decrease from 1 linearly as average deviation approaches w_2.

We can express this linear decay with the following formula:

$$S(t) = \frac{(w_2 - D(t))}{(w_2 - w_1)} \qquad (8)$$

where $S(t)$ is the score at time t. Once computed, scores are averaged across the entire time series, resulting in a single score for each ensemble member. Scores for ensemble members are normalized in `score_runs()` to assign a weight between 0-1 to skilled versus unskilled members, where more skilled ensemble members will be weighted closer to 1 while less skilled ensemble members will receive weights closer to 0. Similar to the normalization step above, weights are estimated using the following formula:

$$\omega_i = \frac{S_{i(t)}}{\sum_{i=1}^{N}(S_{i(t)})} \qquad (9)$$

where ω_i is a weight assigned to each ensemble member from the normalized mean score of each member $S_{i(t)}$.

Below we provide a code example using `score_ramp()` as the scoring function in a `score_runs()` call. As in code block 8, we use the results produced in code block 5 and assess the agreement between ensemble members and observed data with the `criterion_co2_obs()` scoring criterion:

9)

```
scores <- score_runs(result, criterion_co2_obs(), score_ramp, w1=0, w2=10)

print(scores)
```

```
##     weights     run_number
## 1 1.044760e-02          1
## 2 7.575543e-10          2
## 3 6.271913e-02          3
## 4 8.717546e-21          4
## 5 6.774904e-13          5
```

Similar to scoring ensemble members with `score_bayesian()`, the resulting data frame returns 25 weights assigned to each ensemble member (indicated by `run_number`).

Weighted ensemble members can be used to visualize a cone of uncertainty to help understand error produced from known parameter combinations and/or parameter sampling distributions. In Figure 4, we show all ensemble members weighted using our two scoring algorithms. The

ensemble shading visually demonstrates how `score_bayesian()`, with a default `sigma`, distributes weights more evenly across likely ensemble members, whereas `score_ramp()` assigns higher weights to ensemble members falling closer to the minimum divergence range of w_1 (when w_1 = 0 and w_2 = 10 ppm).

Fig 4. Weighted ensemble members using different scoring algorithms. Perturbed parameter ensemble (PPE) projections plotted for atmospheric CO_2 concentration from 1960-2100 weighted using the A) `score_ramp()` and B) `score_bayesian()` algorithms. Ensemble member weights are indicated by color shading with the solid red line representing observed atmospheric CO_2 concentrations from 1959-2021.

A time test on an analysis weighting 1000 ensemble members shows that the difference in computation time between the two scoring algorithms is negligible, with both functions computing weights for N = 1000 runs in a fraction of a second. Despite the similarities between the two scoring algorithms, the differences in approach and customization options can lead to variations in the behavior and performance of each method (Fig 4). It is therefore important to consider the specific goals of an analysis and characteristics of the data when selecting which scoring algorithm to use. Ultimately, differences in weights produced by the different scoring algorithms will impact the probabilistic projections of resulting variables.

2.7 Defining and Calculating Metrics and Probabilities

Once the ensemble members are scored we can use them to compute informative metrics from model projections. Calculating metrics from the final weighted PPE requires (1) a results data frame and (2) a metric object, which must first be defined by the user.

Metric objects determine what data the user is most interested in extracting and summarizing from the results data frame. For example, a metric object can identify information needed to estimate global mean air temperature (`global_tas`) for the 20-year average used by the IPCC to represent long-term temperature change (2081-2100). We complete this by calling the function `new_metric()`:

10)

```
metric_lt <- new_metric(var = "global_tas", years = 2081:2100, op = mean)

print(metric_lt)
```

```
## Probabilistic Hector Metric:  mean global_tas 2081  to  2100
```

This defines a new custom metric object: obtain the mean global air temperature (global_tas) for the years 2081-2100. The argument op in code block 10 describes an operation that can be performed on the model data to compute a descriptive statistic for each member of the ensemble. While we define a 20-year mean global_tas metric in this example, the user can also

easily compute the median, min, max, standard deviation, etc. for each ensemble member. Additionally, users can specify a single year rather than quantifying statistics over a range of years (e.g., 2100 vs. 2081-2100).

Once this metric is defined, we call `metric_calc()` to compute metric values for each ensemble member using the results data frame:

11)

```
values_metric_lt <- metric_calc(results, metric_lt)

print(values_metric_lt)
```

```
##     run_number metric_result
## 1            1      2.315857
## 2            2      3.083498
## 3            3      2.232456
## 4            4      2.474680
## 5            5      1.975036
```

The resulting data frame returns 25 separate metric values (indicated by the `metric_result` column) representing the 2081-2100 mean warming of global air temperature.

When metrics of interest are calculated and weights are assigned to PPE members based on agreement with historical record, we have the necessary information to address questions such as, "*What is the probability that long-term mean temperature change will remain between 2.0-3.5 ℃ relative to pre-industrial reference?*"

We approach such a question by calling `prob_calc()`, a function that sums PPE weights as they are binned into metric ranges identified by the user. Running `prob_calc()` requires (1) a data frame where metric values can be identified, (2) bins defined by the user, and (3) a data frame where PPE weights can be identified. Here, we provide an example of `prob_calc()` usage:

12)

```
# Establishing metric ranges
temp_range <- c(1.5, 2.0, 2.5, 3.0, 3.5, 4.0, Inf)

# Producing probabilities
prob_calc(metrics = values_metric_lt$metric_result,
          bins = temp_range,
          scores = scored_hector_runs$weights)
```

```
##     bins       scores  probability
## 1 (1.5,2] 4.897565e-02 4.897565e-02
## 2 (2,2.5] 3.802494e-01 3.802494e-01
```

```
## 3 (2.5,3] 5.707749e-01 5.707749e-01
## 4 (3,3.5] 9.643701e-10 9.643701e-10
## 5 (3.5,4] 1.122272e-08 1.122272e-08
```

In this example we use PPE weights computed using the `score_bayesian()` algorithm. The `prob_calc()` result shows the total probability that long-term projections of mean warming will fall within each of the temperature ranges defined by our bins (1.5-2 ℃, 2-2.5 ℃, 2.5-3 ℃, 3-3.5 ℃, 3.5-4 ℃, and >4 ℃) for the SSP scenario represented in our core object (SSP 2-4.5). With the result above, for example, we can conclude that there is a 95% probability that the long-term average global warming will remain between 2.0-3.0 ℃ relative to pre-industrial reference.

3 Case Study: Probabilistic Temperature Projections Across Four SSP Scenarios

Here, we present a case study to demonstrate the core utility of Matilda. We note that this case study is meant only to show the utility of the package and is an illustrative example. It is not meant to be presented as a full probabilistic analysis of temperature change from SSP scenarios. In this case study we will use Hector with four SSP scenarios from CMIP6 (SSP1-1.9, SSP1-2.6, SSP2-4.5, SSP3-7.0) [5] to compute mean temperature change over the long-term 20-year average presented in IPCC AR6 [40]. We interpret our results similar to the IPCC, using scaled likelihoods: very likely (90-100%), likely (66-100%), about as likely as not (33-66%), unlikely (0-33%), and very unlikely (0-10%) [40]. This case study examines the probabilities of long-term (2081-2100) global mean surface temperature change relative to a pre-industrial reference in each of the four SSP scenarios.

After initiating cores for each of the four scenarios, we generate 1000 parameter sets using `generate_params()`. For consistency, these 1000 parameter sets remain the same for each scenario. We call `iterate_model()` to run Hector across all scenario cores using parameter sets to propagate parameter uncertainty to PPE members. When running the models, we extract the global mean surface temperature (`global_gmst`) for the years 1960-2100. Running the model with 1000 parameter sets across four SSP scenarios takes ~100 minutes to run serially on a single processor. Our resulting ensemble members are weighted by calling `score_runs()`. We weighted ensemble members using observed mean annual global surface temperature as a scoring criterion (`criterion_gmst_obs()`) with the Bayesian scoring algorithm (`score_bayesian`).

Assessing different `sigma` values informs acceptable RMSE ranges for ensemble members and weights them accordingly. For example, we show how weighting ensemble members using `score_bayesian()` within one unit of the standard deviation of observed global mean surface temperature (default `sigma`) places a higher likelihood on ensemble members with lower RMSE values, while increasing the acceptable deviation limit to two units of the standard deviation of

the observed data decreases the penalty of ensemble members with relatively higher RMSE values (Fig 5).

Fig 5. Likelihood of ensemble members given different sigma values. Likelihood of perturbed parameter ensemble (PPE) members for an example emissions scenario based on root mean square error (RMSE) using the `score_bayesian()` algorithm. Blue line shows the use of default `sigma` value: The algorithm penalizes ensemble members as RMSE values deviate from observed data by one unit of standard deviation. Red line shows the use of a customized sigma value: Setting `sigma` to two units of standard deviation of observed values and thus assigns weight to ensemble members falling within this acceptable deviation range. Black dots represent individual ensemble members.

In this example analysis, we maintain `sigma` at its default value and then visualize PPE members for each SSP scenario analyzed (Fig 6a). This provides some evidence of the range of possible global mean surface temperature futures under each scenario. The most likely outcomes are those that most accurately reflect historical global mean surface temperature patterns (Fig 6a). To summarize the modeled data using our metric of interest (20-year mean of global surface temperature for the years 2081-2100), we first establish our metric definition using `new_metric()` and then call `metric_calc()` to compute metrics from our evaluated PPE. For each SSP scenario, we compute probabilistic projections of long-term mean warming using `prob_calc()` for 0.5 ℃ temperature bins for each SSP scenario (Fig 6b).

Fig 6. Global mean surface temperature projections and warming probabilities across four emissions scenarios. A) 1000-member perturbed parameter ensemble (PPE) projecting global mean surface temperature from 1950-2100 for each SSP scenario. Darker blue ensemble members represent those members that best reflect historical temperature observations. B) Stacked bars blocked by the probability of different temperature ranges for each SSP scenario. Lower emissions scenarios (SSP1-1.9 and SSP1-2.6) have a higher probability of temperature remaining below 2.0 ℃ than higher emissions scenarios (SSP2-4.5 and SSP3-7.0).

From this example, we can infer that when averaged over 2081-2100, the probability of remaining below 2.0 ℃ warming decreases steadily as we transition from the low emissions scenario (SSP1-1.9) to the higher emissions scenario (SSP3-7.0) (Fig. 6b). We can compute approximate probabilities for different temperature ranges for the SSP scenarios by summing probabilities in desired ranges. For example, in the low emission scenario SSP1-1.9, the probability that warming will remain below 2.0 ℃ in our long-term warming projection is ~96%. Alternatively, we can achieve precise probabilities by altering `bin` widths supplied to `prob_calc()` to ranges that can be compared with IPCC results [40]. For example, in IPCC AR6 the SSP1-1.9 scenario is *very likely* (90-100%) to be warmer by 1.0 ℃-1.8 ℃ relative to pre-industrial reference, while the SSP3-7.0 scenario is *very likely* to be warmer by 2.8 ℃-4.6 ℃ [40]. We find similar results here, where SSP1-1.9 is *very likely* (97%) to be warmer by 1.0 ℃-2.0 ℃ and SSP3-7.0 is *very likely* (92%) to be warmer by 2.4 ℃-4.8 ℃ relative to the pre-industrial reference. For scenarios SSP1-2.6 and SSP2-4.5, the corresponding *very likely* ranges in IPCC AR6 are 1.3-2.4 ℃ and 2.1-3.5 ℃, respectively [40]. For these scenarios, we again find

very likely temperature ranges similar to what IPCC AR6 indicates, where SSP1-2.6 is *very likely* (94%) to be warmer by 1.1 ℃-2.6 ℃ and SSP2-4.5 is *very likely* (92%) to be warmer by 1.7 ℃-3.8 ℃ relative to the pre-industrial reference.

The results from this example case study assume that models can be accurately evaluated using a single scoring criterion (such as observed global mean surface temperature). However, it is widely recognized that evaluating climate models often involves considering multiple lines of evidence. For example, comprehensive model evaluation should involve assessing performance across various observed climate variables (e.g., temperature and CO_2 concentrations and the interactions that exist among those variables), as well as more complex models (i.e., ESMs). The form of the scoring function is also non-univocal in most applications and motivates the flexibility of `Matilda` in allowing different choices.

4 Conclusion

Using RCMs for probabilistic climate projections is critical for exploring uncertainty in the future integrated human-Earth system [13,17–19]. The use of RCMs presents a viable approach to tackle this challenge, as they possess the capability to simulate perturbed parameter ensembles (PPEs) rapidly and can emulate the behavior of more complex ESMs [17] for some key large-scale observable quantities. However, despite their proficiency, some challenges arise when employing several RCMs for probabilistic climate projection analysis. These challenges include closed-source designs and placing heavy programming responsibility on the user [7,10,14,21], which can make both analysis and interpretation difficult.

`Matilda` is an open-source, turn-key, flexible framework that provides tools to complete probabilistic climate projections using the Hector model. We show how this tool streamlines probabilistic projection analysis and makes such analytical approaches more accessible to the large community of `R` users, with seamless integration with Hector. By expanding the ways Hector can be used, `Matilda` can help address questions of climate uncertainty under different emissions scenarios and pursue other probabilistic analyses. We hope that `Matilda` can be particularly valuable when coupled with GCAM and similar models to understand the propagation of uncertainty in the human-Earth system [6,19,20,41].

We aim to continue the development of `Matilda` in a number of ways. First, we aim to develop enhanced parameter sampling options to enable more robust sampling without relying heavily on *a priori* assumptions about the parametric form of prior distributions. Improving this process can be addressed by implementing more Bayesian approaches into parameter sampling (e.g., Markov Chain Monte Carlo sampling) [42]. Future versions of the package will also automate the process of adding more parameters to a parameter set. Second, providing more methods for model evaluation will improve the robustness of an analysis. While our case study assumes that models can be accurately evaluated using a single scoring criterion like observed global mean surface temperature, it is widely recognized that climate model evaluation is often improved by considering multiple lines of evidence. Comprehensive model evaluation should

involve assessing performance across various observed climate variables (e.g., temperature and CO_2 concentrations and the interactions among those variables) and/or existing ESMs. Finally, we intend to develop further `Matilda`'s ability to be integrated with additional RCMs. This integration would provide a unified approach for conducting probabilistic projection analysis across different models. By doing so, we can effectively address questions that focus on clarifying uncertainties arising from structural differences among models within the RCM community.

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Author Contributions

Conceptualization: Joseph K. Brown, Ben Bond-Lamberty.
Data curation: Joseph K. Brown, Ben Bond-Lamberty.
Methodology: Joseph K. Brown, Ben Bond-Lamberty, Leeya Pressburger, Kalyn Dorheim, Abigail Snyder, Claudia Tebaldi, Steven J. Smith.
Software: Joseph K. Brown, Ben Bond-Lamberty, Leeya Pressburger, Abigail Snyder, Claudia Tebaldi.
Writing – Original Draft Preparation: Joseph K. Brown.
Visualization: Joseph K. Brown
Writing – Review & Editing: Ben Bond-Lamberty, Leeya Pressburger, Kalyn Dorheim, Abigail Snyder, Claudia Tebaldi, Steven J. Smith.
Project Administration: Ben Bond-Lamberty.
Supervision: Ben Bond-Lamberty.

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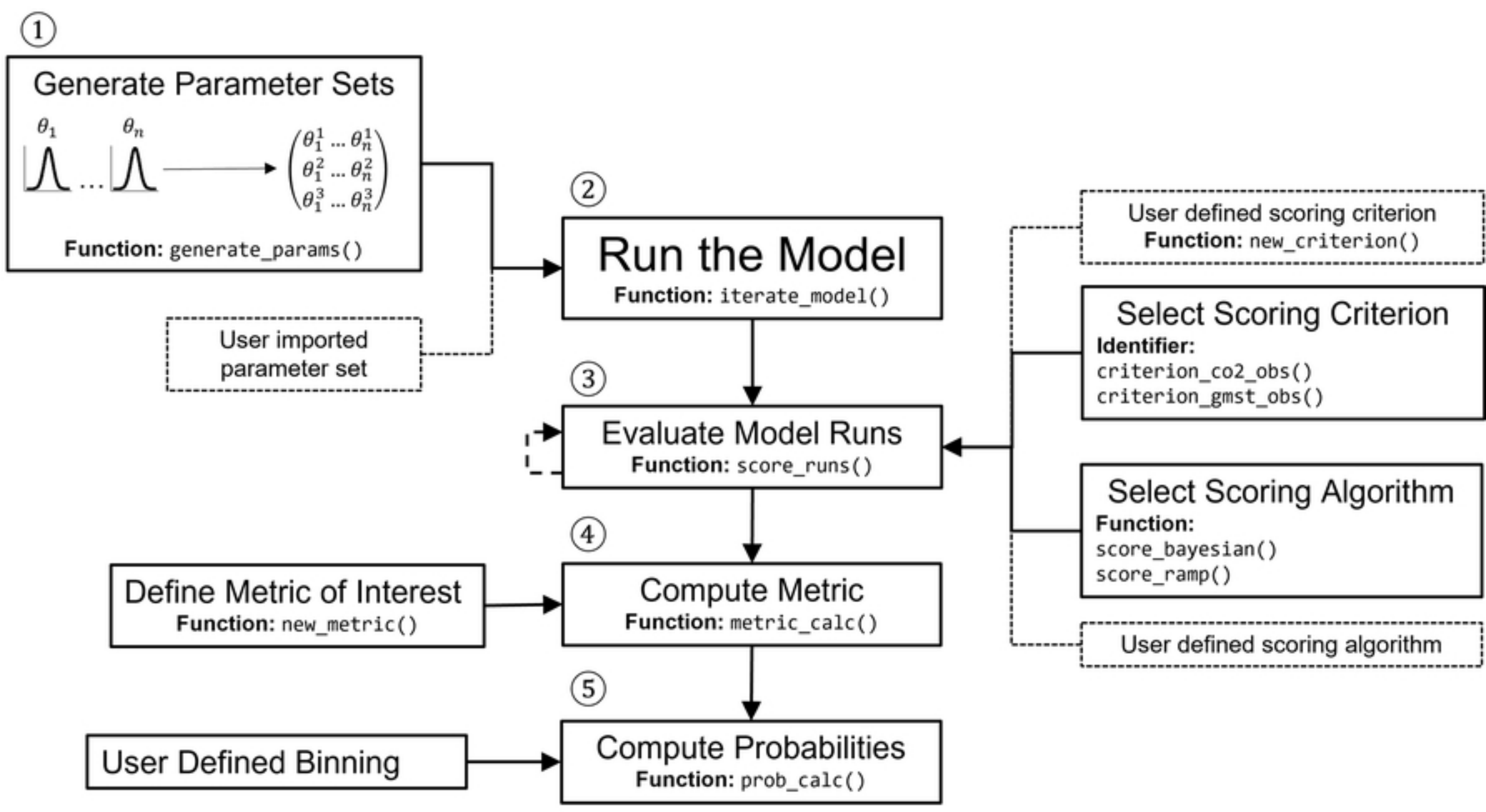
①
Generate Parameter Sets
θ_1 θ_n
$\begin{pmatrix} \theta_1^1 \dots \theta_n^1 \\ \theta_1^2 \dots \theta_n^2 \\ \theta_1^3 \dots \theta_n^3 \end{pmatrix}$
Function: generate_params()
User imported parameter set
②
Run the Model
Function: iterate_model()
③
Evaluate Model Runs
Function: score_runs()
④
Define Metric of Interest
Function: new_metric()
Compute Metric
Function: metric_calc()
⑤
User Defined Binning
Compute Probabilities
Function: prob_calc()
User defined scoring criterion
Function: new_criterion()
Select Scoring Criterion
Identifier:
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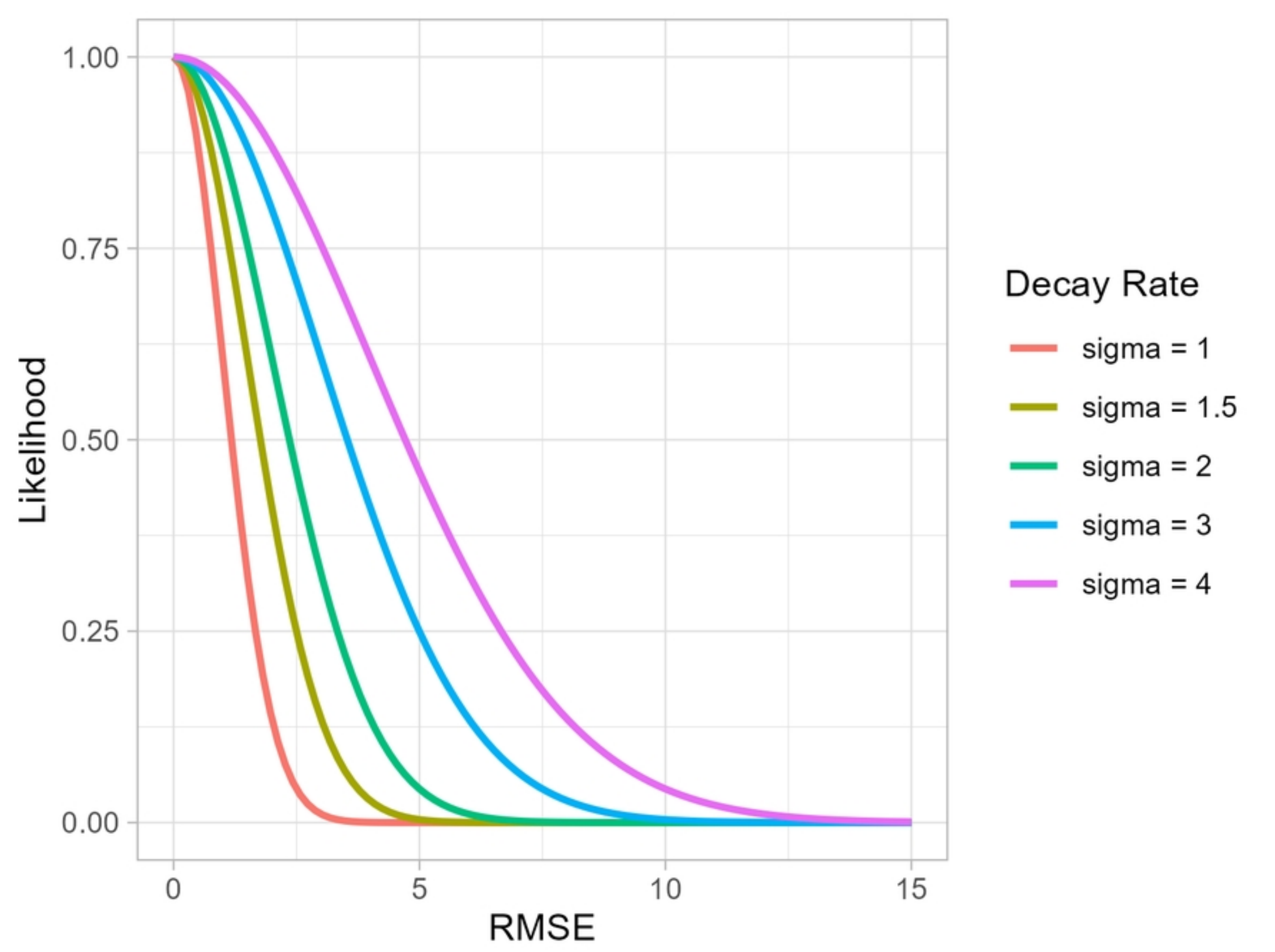
criterion_gmst_obs()
Select Scoring Algorithm
Function:
score_bayesian()
score_ramp()
User defined scoring algorithm

figure_01


1.00
0.75
0.50
0.25
0.00
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10
15
RMSE
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sigma = 1.5
sigma = 2
sigma = 3
sigma = 4

figure_02

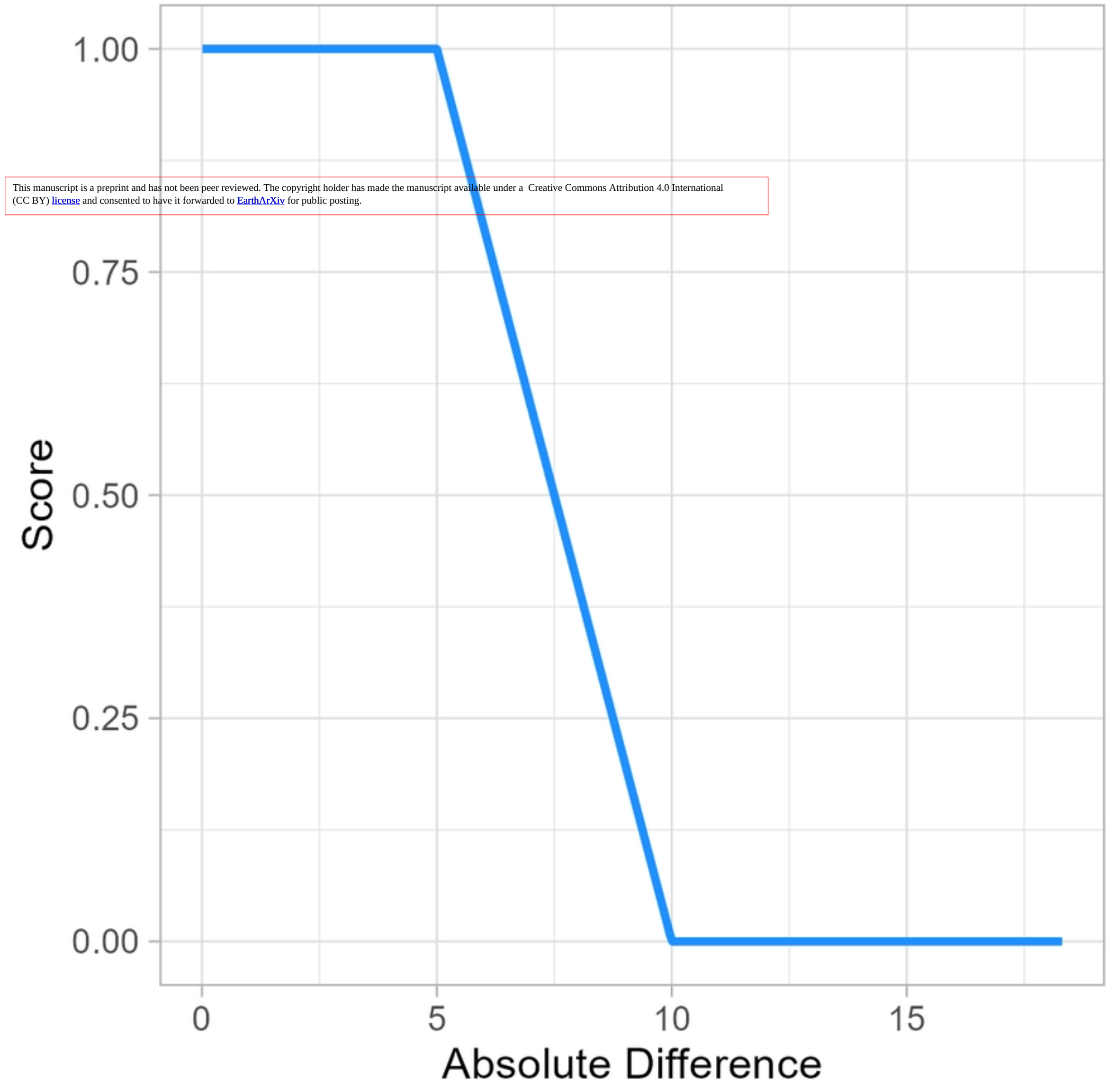
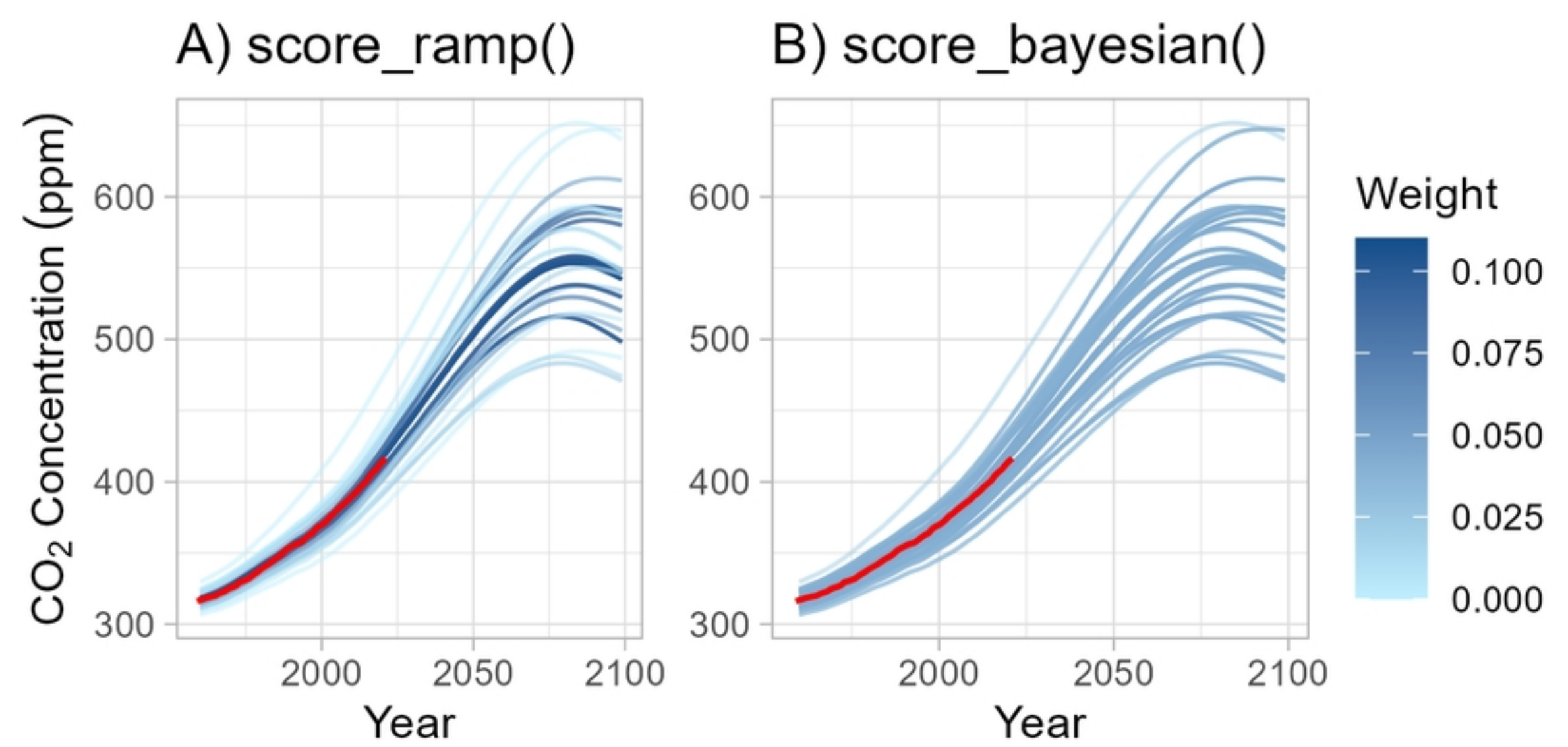


figure_03


A) score_ramp()
B) score_bayesian()
CO_2 Concentration (ppm)
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300
2000
2050
2100
Year
Weight
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0.075
0.050
0.025
0.000

figure_04

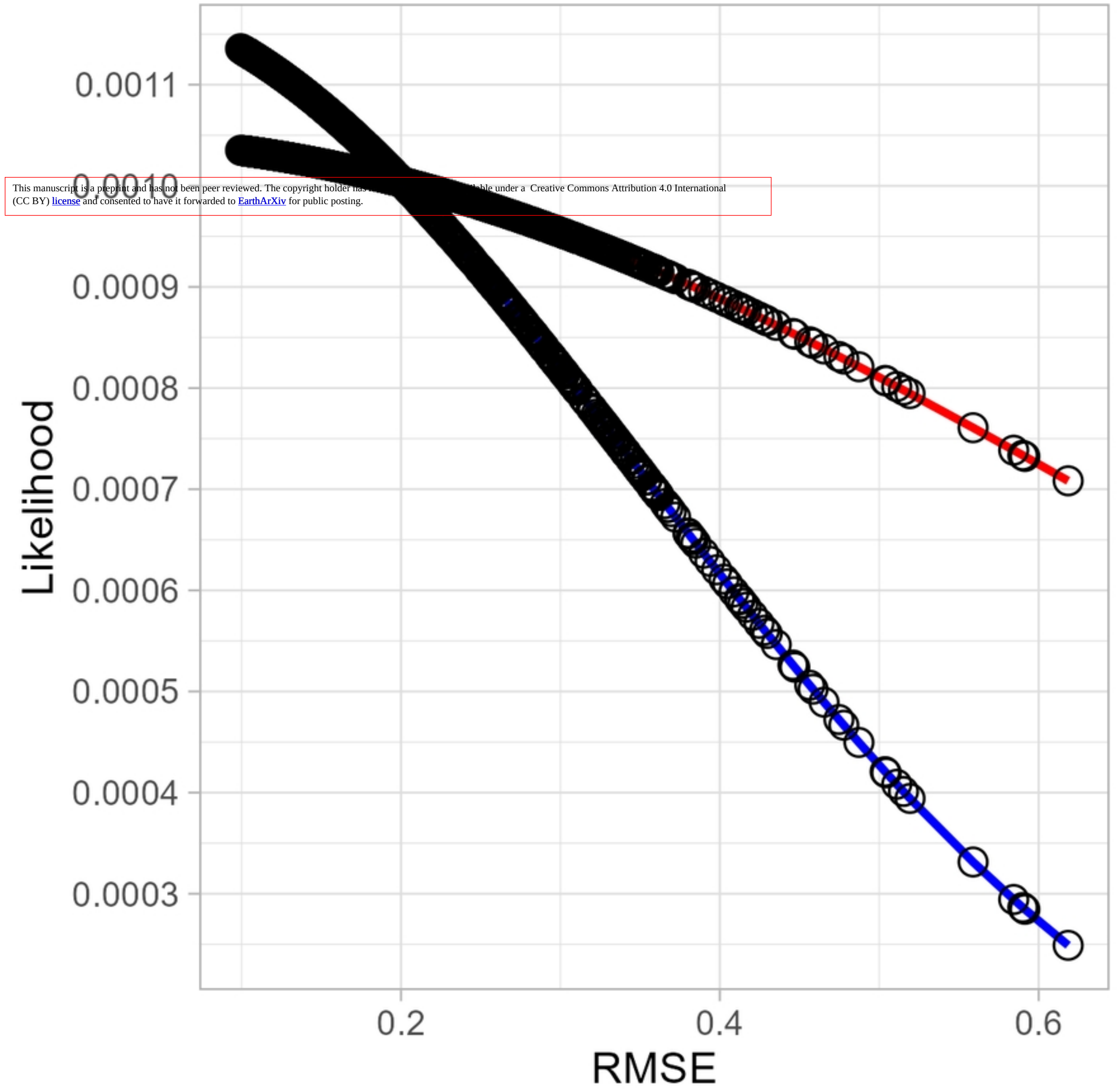

figure_05

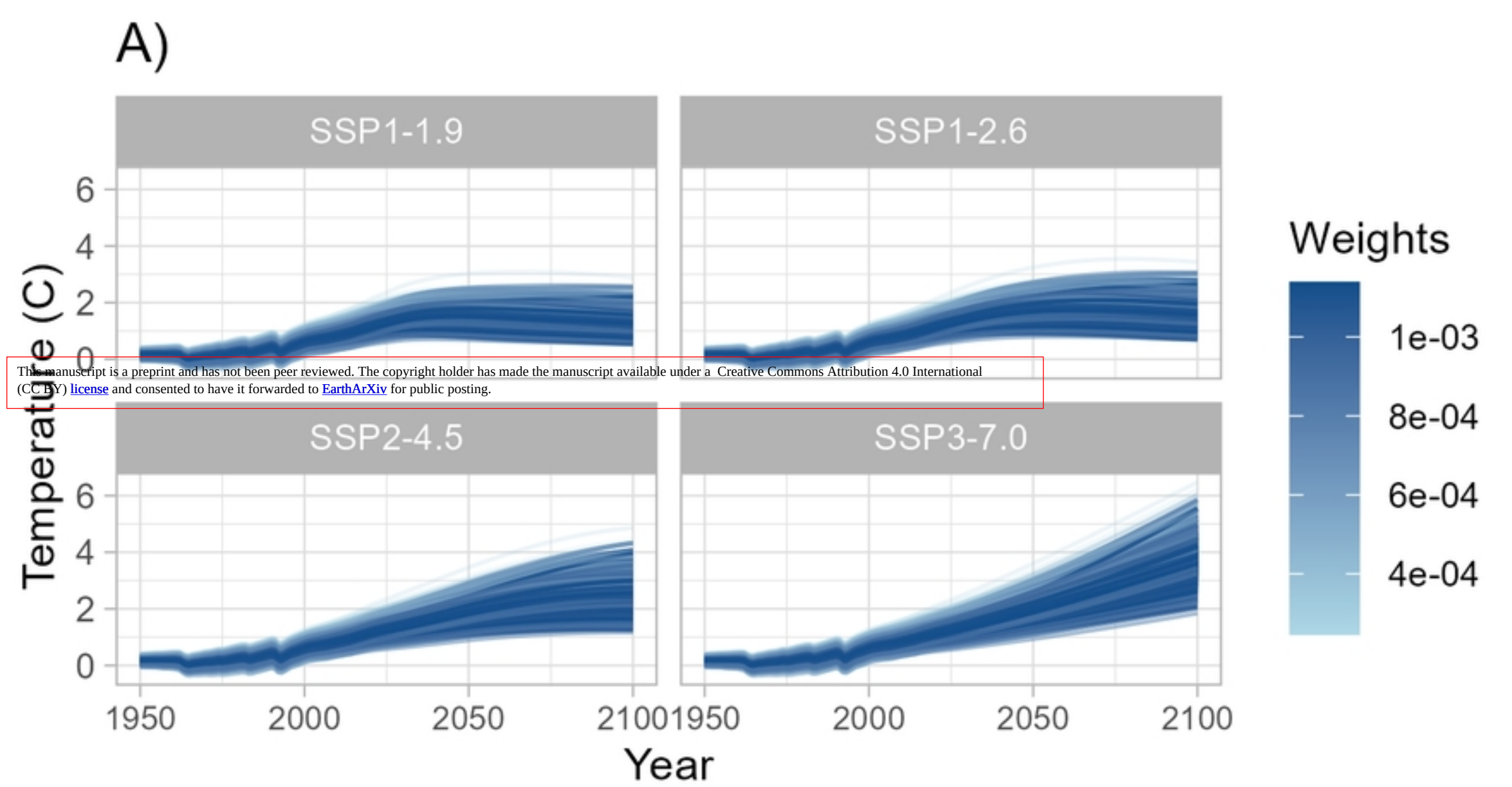

figure_06