TaxonBodyMassML: Taxonomy-informed prediction of body mass using gradient-boosted trees

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Abstract

1. Body mass is a key ecological trait governing metabolic rates, life-history characteristics, interaction strengths, and community structure and dynamics. Despite its centrality to ecology and ecological modelling, direct body mass measurements exist for only a small fraction of all scientifically described species.
2. We present `TaxonBodyMassML`, a machine-learning tool to predict the body mass of heterotrophic taxa from their Linnaean taxonomy alone. Trained on 36,573 species-level body mass records compiled from 345 primary sources and databases, the underlying model combines learned entity embeddings of the kingdom-to-genus ranks with a gradient-boosted tree regressor to achieve $R^2 = 0.91$, RMSE = 0.56 $\log_{10}$ units, and MAE = 0.32 $\log_{10}$ units on a held-out test set of 3,657 species spanning approximately 22 orders of magnitude in body mass. Conformal prediction intervals, calibrated separately for each level of taxonomic resolution, provide user-selectable coverage without model retraining.
3. The tool accepts scientific names at any taxonomic level with tolerance for misspellings via fuzzy matching, optionally returns the measured mass for species in its database or a point estimate in grams with optional prediction intervals for these and all taxa, and requires no phylogenetic tree or correlated trait data.
4. `TaxonBodyMassML` is available as an R package, a Python package, and an open web interface (https://taxonbodymassml.github.io).

Keywords: body size; machine learning; entity embeddings; XGBoost; conformal prediction; trait prediction; taxonomy; metabolic scaling; allometric ecological networks.

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Introduction

Body mass is a fundamental ecological axis, scaling with individual metabolic rates across organisms spanning the tree of life to link an individual's physiology to its resource requirements, home range size, dispersal distance, reproductive output, lifespan and more (Blueweiss et al., 1978; Brown et al., 2004; Schmidt-Nielsen, 1984). Body mass also determines the architecture and interaction strengths of ecological networks because larger species consistently consume or dominate smaller ones to generate size-structured trophic and competitive hierarchies (Brose et al., 2006; Werner and Gilliam, 1984). Body mass thereby also links individual physiology to the dynamics of entire food webs, communities, and ecosystems (Woodward et al., 2005). It therefore serves ecologists as the basis for building and parameterizing many forms of applied and theoretical models, including bioenergetic consumer–resource and allometric trophic network models (e.g., Williams et al., 2007; Yodzis and Innes, 1992).

Despite this pervasive importance, direct body mass measurements are available for only a small fraction of described species. Data gaps exist even in the best-studied vertebrate groups (González-Suárez et al., 2012; Etard et al., 2020, but see Jones et al. 2009, Wilman et al. 2014, and Faurby et al. 2018), and are much larger still for invertebrates, microorganisms, and many other poorly sampled taxonomic groups. Analyses that require body mass for every species in a dataset therefore face either data exclusion, imputation, or ad hoc guessing.

Established imputation methods carry non-trivial prerequisites. Phylogenetic comparative approaches (Goolsby et al., 2017; Thorson and van der Bijl, 2023; Sanchez-Martinez et al., 2024) require a calibrated, ultrametric phylogenetic tree and observed trait values for relatives, and in some cases also environmental covariates (Sanchez-Martinez et al., 2024). These prerequisites are often unavailable for many taxonomic groups within a given community or ecosystem. Hierarchical Bayesian trait gap-filling (Schrodt et al., 2015) requires a matrix of partially observed trait values across species, and random-forest imputation (Stekhoven and Bühlmann, 2012) requires the co-occurrence of multiple traits for the same species. Several other machine learning approaches have also shown good performance for trait prediction when taxonomy or phylogenetically derived features are used as inputs — for both categorical (e.g., Gendre et al., 2024) and continuous (e.g., Moura et al., 2024) traits — but generally still require ancillary data beyond a species name alone. Moreover, comparative evaluations show that no single imputation method performs ideally across missing-data scenarios (Johnson et al., 2021; Penone et al., 2014).

Linnaean taxonomy ranks are the one predictor that should be universally available for every scientifically described organism: they are used to record all known life on Earth and are accessible from continually-updated global databases. Body mass, in turn, exhibits particularly strong phylogenetic signal (Blomberg et al., 2003), meaning that closely related taxa are consistently similar in mass. The Linnaean hierarchy directly reflects this evolutionary relatedness and thus serves as an informative predictor even without an explicit tree. Recent work has shown that phylogenetic model-based methods retain an advantage for single-trait prediction when a resolved phylogeny is available (Richard-Bollans and Silvestro, 2026). However, when it is not, taxonomy provides the most broadly accessible proxy for evolutionary relatedness.

Here we present `TaxonBodyMassML`, a tool to predict the body mass of heterotrophic taxa using their Linnaean taxonomy ranks kingdom through genus. Its model combines learned entity embeddings of each rank (Guo and Berkhahn, 2016) with a gradient-boosted tree regressor (Chen and Guestrin, 2016). The mass of species recorded in the compiled database on which the model is trained (36,573 species) can optionally be returned directly. For taxa whose mass is predicted, the tool provides conformal prediction intervals at any user-specified coverage level, calibrated separately for each level of taxonomic resolution. `TaxonBodyMassML` tolerates misspelled taxon names via fuzzy matching and is delivered through three open interfaces: a web application, an R package, and a Python package.

Methods

Training data

The database we assembled (`TaxonBodyMass_DB` v6.0.0) comprised body mass records for 42,304 distinct taxon names aggregated from 393 primary sources and databases (of which 345 contributed records that survived the filtering steps described below), including the `FracFeed` database (Novak et al., 2026) which motivated its compilation. The top sources uniquely contributing the most species-level records (i.e., species found in no other contributing source) were Feldman et al. (2016) (n = 2,561), Cai et al. (2025) (n = 1,782), Brose (2018) (n = 1,768), and FishBase (n = 1,473; Froese et al., 2014). We implemented manual and AI-assisted audits (using Anthropic's Claude Sonnet 4.6) of all species names to identify misspellings, formatting errors, and records with non-scientific names (e.g., functional or family-level groupings). We similarly identified potentially erroneous body mass values, either replacing these values through manual searches of the literature, excluding them entirely when no attributable value was found, or excludeing them when multiple sources disagreed about a taxon's mass by more than an order of magnitude. When life-stage information was provided in a database, we restricted records to adult (including "male" or "female") or life-stage unspecified values. When multiple records existed for the same species within a source, we computed and used the geometric mean of those records. When records existed for the same species across multiple sources, we computed and used the arithmetic mean of those records. (This latter step differs from the published v.5 of the `FracFeed` database for which we ranked the sources and used the value from only the top-ranked source.) Citations for all contributing sources can be found in Supplementary Section S6, in the GitHub repository `https://github.com/TaxonBodyMassML/TaxonBodyMass_DB`, and through the function `create_bib()` which we describe below.

We attempted to resolve all provided species names to the full seven-rank Linnaean taxonomy using seven sequential API lookups. Higher-rank classification fields were pre-seeded into each record prior to any API query when the contributing body mass dataset supplied them. First, the GBIF Backbone Taxonomy (GBIF Secretariat, 2023) was queried via its fuzzy-match batch API to return a canonical name and kingdom-through-species classification, plus a per-record match confidence score. Species assignments with a confidence score below 75 were discarded, though higher-rank fields from those matches were retained. GBIF matches with a confidence score of 90 or above were permitted to override source-provided higher ranks. We then attempted to resolve remaining unmatched records by querying the National Center for Biotechnology Information Taxonomy API (NCBI, Sayers et al., 2022), which requires exact name matching, followed by the World Register of Marine Species (WoRMS, Ahyong et al., 2026), accepting exact, phonetic, and near-1-character matches. Records still unresolved after these steps were processed through three additional sequential fallbacks: the Catalogue of Life Checklist-Bank (COL, Bánki et al., 2026), the Integrated Taxonomic Information System (ITIS, Integrated Taxonomic Information System, 2026), and the Wikidata SPARQL endpoint (Vrandečić and Krötzsch, 2014). Finally, for species still lacking complete higher-rank classification, a second GBIF query using the usageKey classification endpoint was used to fill missing ranks. Records with no accepted species match in any lookup and those that we could not correct manually were excluded.

Of the 42,304 records in the full dataset, 41,917 were resolved to an accepted species. We then removed autotrophs (649 names): the kingdoms Plantae, Viridiplantae and Fungi; the predominantly photosynthetic phyla (diatoms and other ochrophytes, haptophytes, cryptophytes, green, red and glaucophyte algae, charophytes, streptophytes, euglenophytes, and cyanobacteria); and a curated list of photosynthetic or mixotrophic dinoflagellate and euglenid genera. We retained heterotrophic protists such as ciliates, foraminifera, apicomplexans, kinetoplastids and heterotrophic dinoflagellates. Collapsing synonyms to one record per accepted species left 37,689 species; removing the 1,116 taxa whose sources disagreed by more than an order of magnitude (above) left 36,573 species, all with a complete kingdom-to-genus classification, which were used for modelling. Body mass of these records spanned ~ 22 orders of magnitude, from *Francisella tularensis* (1.0×10^{-14} g) to *Balaena mysticetus* (8.75×10^{7} g). The dataset was heavily dominated by Animalia (36,273 species, 99.2%), with its four most represented classes being Aves, Reptilia, Mammalia, and Actinopterygii (Tables 1 and 2).

Table 1: Data coverage by kingdom (one record per species; mass range in $\log_{10}$ g).

		Mass range ($\log_{10}$ g)	
Kingdom	Species	min	max
Animalia	36,273	−10.8	7.9
Chromista	135	−11.3	−1.9
Bacteria	125	−14.0	−10.4
Protozoa	39	−12.5	−4.0
Archaea	1	−12.0	−12.0

Model training

Body mass (in grams) was $\log_{10}$-transformed prior to modelling. The ~ 22 orders of magnitude span of values in the data motivated this transformation and ensured that large-bodied taxa did not dominate the loss function. All performance metrics (RMSE, MAE) reported throughout are therefore in $\log_{10}$ body-mass units.

Features. The six Linnaean taxonomy ranks `kingdom`, `phylum`, `class`, `order`, `family` and `genus` were the sole provided features. No morphological, environmental, or phylogenetic covariates were used. Species identity was deliberately not a feature: because the data contain one record per species, a species feature would only memorise individual records (which can optionally be returned directly; see *Distribution and usage* below). Each rank was encoded against the vocabulary of values present in the training split 5 kingdoms, 39 phyla, 115 classes, 458 orders, 2,148 families and 9,431 genera). Values

Table 2: Data coverage by class (the 20 classes with the most species; one record per species; mass range in $\log_{10}$ g).

		Mass range ($\log_{10}$ g)	
Class	Species	min	max
Aves	10,403	0.3	5.0
Reptilia	9,955	−0.9	5.3
Mammalia	5,764	0.2	7.9
Actinopterygii	4,942	−2.0	6.3
Insecta	1,002	−6.4	1.2
Amphibia	924	−1.3	4.4
Malacostraca	620	−4.5	4.2
Arachnida	489	−8.4	1.5
Gastropoda	267	−10.8	4.2
Testudines	226	1.2	5.3
Elasmobranchii	193	0.3	6.9
Copepoda	186	−5.9	−1.2
Bivalvia	137	−4.5	5.5
Cephalopoda	108	−1.0	4.5
Polychaeta	105	−4.7	2.3
Collembola	86	−5.9	−3.0
Clitellata	75	−5.4	0.8
Asteroidea	65	−1.9	3.0
Gammaproteobacteria	63	−14.0	−10.4
Branchiopoda	56	−5.7	1.9

absent from that vocabulary, including any rank left unresolved for a query, map to a reserved `UNK` token.

Entity-embedding model. The model for the default `method` of `TaxonBodyMassML` has two stages. Stage 1 is a small neural network, implemented in PyTorch (v2.14.0; Paszke et al., 2019), that learns an entity embedding (Guo and Berkhahn, 2016) for every value of every rank: dense vectors of 4, 8, 8, 16, 16 and 32 dimensions for kingdom through genus, concatenated into an 84-dimensional input to a multilayer perceptron (84 → 64 → 32 → 1, ReLU activations) trained for 100 epochs with an L1 (mean absolute error) loss so that taxa with similar body masses come to lie close together in embedding space. The `UNK` vector of each rank is the mean of that rank's learned embeddings.

Stage 2 discards the perceptron and fits an XGBoost gradient-boosted tree regressor (Chen and Guestrin, 2016) (Python `xgboost` v3.3.0) to the 84 embedding features, minimising the mean absolute error in $\log_{10}$ body mass. The MAE objective is more robust than squared error to the heavy-tailed distribution of body-mass residuals across taxonomic groups and means that the point prediction targets the median body mass of taxa sharing a given taxonomy.

`TaxonBodyMassML` also provides a single-stage XGBoost model fitted directly to the six categorical ranks as an alternative prediction `method` (see *Distribution and usage* below). Its motivation, hyperparameters and a side-by-side comparison with the embedding model are given in Supplementary Section S5.

Training, test and calibration splits. The 36,573 species were split randomly into a 32,916-species training set and a 3,657-species held-out test set without stratification. For conformal calibration (below) the training set was further split 80/20 into a 26,332-species fitting partition and a 6,584-species calibration partition. The distributed models were then refit on the full training set.

Hyperparameters. The Stage-2 hyperparameters were optimised with `Optuna` (v4.9.0; Akiba et al., 2019) using the Tree-structured Parzen Estimator sampler, 100 trials and 5-fold cross-validation within the training set (best cross-validated MAE 0.335 $\log_{10}$ units). The Stage-1 network was refit within each cross-validation fold, on that fold's training rows and vocabulary, so that the cross-validated MAE carries no information from the validation folds. Final values and the search ranges are given in Supplementary Section S1.

Conformal prediction intervals. Split-conformal prediction intervals were constructed following the standard approach (Shafer and Vovk, 2008; Lei et al., 2018). Absolute residuals $|y_{\text{true}} - y_{\text{pred}}|$ of the model fitted to the fitting partition were computed for the 6,584 calibration species and stored with the model. Users can specify an arbitrary coverage level $1-\alpha \in (0,1)$, where α is the miscoverage rate, when making inferences for taxa with unknown body mass. The empirical $(1-\alpha)$-quantile q is computed on-the-fly from the stored residuals and the prediction interval $[\,10^{\log_{10}\hat{y}-q},\ 10^{\log_{10}\hat{y}+q}\,]$ is returned (symmetric in $\log_{10}$ space). Because the distributed model is refit on all training data, these intervals are slightly conservative.

Two interval methods are available via the `interval_method` argument. The `"pooled"` method computes a single q from all calibration residuals pooled together, yielding the standard marginal conformal guarantee for queries resolved to genus. The default `"stratified"` method provides approximate rank-conditional coverage. For this method, calibration residuals were computed separately for each taxonomic rank by masking all finer-rank columns to `UNK` before re-predicting on the calibration partition, and these rank-specific residual sets were stored with the model. This ensures that the calibration condition matches the inference condition. A query whose finest known rank is family is compared against calibration residuals computed at the same level of taxonomic resolution. (Because species was not used as a feature, genus-level residuals are the pooled residuals.) At inference time, the finest rank whose value occurs in the training vocabulary (i.e., the finest rank not mapped to `UNK`) is identified for each query taxon and the corresponding rank-specific q is used to construct the interval, producing narrower bands for genus-level queries and wider bands for order- or class-level queries.

Tool Description

Model performance

When evaluated on the held-out test set in $\log_{10}$ body-mass space, the model achieves a MAE of 0.32 $\log_{10}$ units which corresponds to a geometric-mean multiplicative error of $10^{0.32} \approx 2.11\times$, so typical predictions fall within roughly a factor of two of the true value (Fig. 1 and Table 3). The best cross-validated MAE from hyperparameter optimisation (0.335 $\log_{10}$ units, obtained with 80% of the training set per fold) is slightly larger than the held-out test MAE, as expected when fewer genera are represented in each fold's training partition, and indicates no overfitting of the Stage-2 trees. The Stage-1 network alone reaches an MAE of 0.39. The Stage-2 trees on its embeddings reduce it to 0.32. (The alternative single-stage XGBoost model reaches an MAE of 0.35 $\log_{10}$ units and $R^2 = 0.89$ on the same test set, see Supplementary Section S5.) At 90% coverage ($\alpha = 0.10$), the stratified interval half-width for genus-level queries is $q = 0.873 \log_{10}$ units, corresponding to a factor of ∼7.5× around the point estimate in grams. For example, a taxon predicted to weigh 10 g would have a 90% interval of approximately 1.3–75 g. A query whose genus is absent from the training vocabulary is treated as a family-level query (and so on for coarser ranks): of the 3,657 test species, 3,074 have a genus present in the training vocabulary, 502 fall back to the family stratum, 73 to the order stratum, and 3, 2 and 3 to the class, phylum and kingdom strata, respectively. The mean stratified half-width for genus-level queries reported in Supplementary Table S5, which averages over all test species, is therefore slightly larger than q.

Users should note that the stratified interval guarantee is conditional on taxonomic rank but otherwise *marginal*: within each rank level it holds on average across all taxa in the calibration set and does not ensure the same coverage within underrepresented subgroups (e.g. rare clades or extreme body-mass classes). For example, when test-set evaluation was restricted to species with mass > 0.1 g (3,369 species, ∼92% of the full test set), both RMSE and MAE improved (0.56 to 0.51 and 0.32 to 0.30, respectively; Fig. 1b and Table 3), indicating that very-small-mass species contribute disproportionately large errors in both squared and absolute terms. This is likely due to these species being under-represented in the training data by virtue of the more challenging measurement of their body mass. Users querying these clades should expect wider prediction intervals and higher prediction error than the aggregate test-set metrics suggest.

Because the calibration residuals are stratified by rank, nominal coverage is approximately maintained as the taxonomic resolution of a query coarsens. Re-predicting every test species with progressively coarser taxonomy, the 90% intervals covered 92.6% of true masses for genus-level queries, 91.4% for family-level queries, and 90.3% for order-level queries (Supplementary Section S4). At class and kingdom level, where the prediction itself is an extrapolation from almost entirely unknown features, the intervals fall short of nominal (88.1% and 86.3%). The same re-prediction experiment shows how accuracy degrades with taxonomic resolution (Supplementary Sections S2 and S3). Because species is not a feature, a query for an unmeasured species and a query for its genus give identical predictions; losing the genus raises the geometric-mean multiplicative error (10^{MAE}) from ∼ 2.11× to ∼ 2.86× (ΔMAE = +0.133 $\log_{10}$ units), losing the family as well raises it to ∼ 4.37× (ΔMAE = +0.317), queries resolved only to class or phylum are off by roughly an order of magnitude (MAE 1.006 and 0.926 $\log_{10}$ units, respectively), and queries resolved only to kingdom are off by many orders of magnitude (MAE 4.919).

Table 3: Performance of the two-stage entity-embedding model on the held-out test set (full) and on a subset restricted to species with body mass > 0.1 g. All metrics are in $\log_{10}$ space.

Test set	R^2	RMSE	MAE	n
Full test set	0.91	0.56	0.32	3,657
Reduced (mass > 0.1 g)	0.79	0.51	0.30	3,369

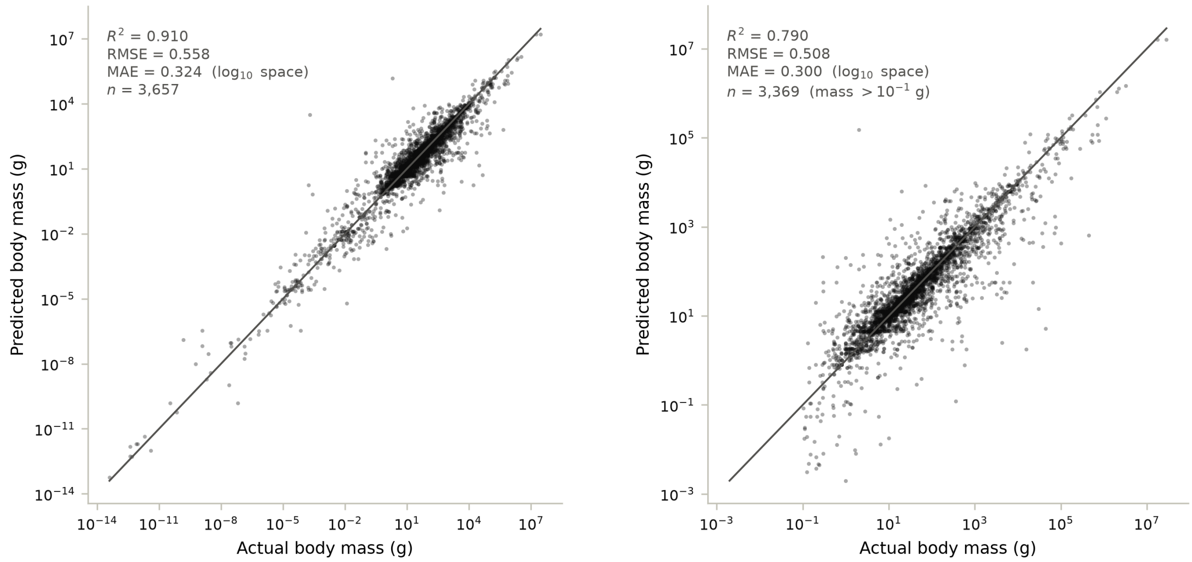

Figure 1: Predicted vs. actual body mass (g) for `TaxonBodyMassML` on the held-out test set. **(a)** Full test set. **(b)** Test set restricted to mass > 0.1 g.

Distribution and usage

`TaxonBodyMassML` is available through an online interface (no installation required) at `https://taxonbodymassml.github.io`, and as R and Python packages available on GitHub at `https://github.com/TaxonBodyMassML/TaxonBodyMassML` where installation instructions, usage examples (including an R vignette), and further documentation are provided. The web interface uses the default configuration only (the entity-embedding model, 90% rank-stratified intervals and database lookup, without fuzzy name matching); the full set of options described below is available through the packages. The taxonomically-enriched data are also available at `https://github.com/TaxonBodyMassML/TaxonBodyMass_DB`. The pre-trained models are distributed as 9 files (∼0.4 GB in total) hosted on Hugging Face (`https://huggingface.co/marknovak/TaxonBodyMassML`; release tags `r-v0.13.0` and `py-v0.13.0`). Both the R and Python packages download them automatically on first use. A species-to-mass lookup table (`lookup.json`) holding the recorded mass and data source of all 36,573 species in the database, including the test species, is also included. Both packages bundle a BibTeX bibliography of every data source in the database (returned by `get_citations()`) together with a table mapping each source identifier to its BibTeX key. The `create_bib()` function uses these to write a `.bib` file containing only the sources behind a given set of predictions (see Example 4). Inference requires `xgboost` ≥ 3.2 in Python and $\geq 3.1.2$ in R.

The primary entry point in both the R and Python packages is the `predict_mass()` function. Its key arguments in R are:

- `taxon` (character vector or `data.frame`): A vector containing one or more scientific names at any taxonomic rank (e.g., *Genus species*). Optionally passing a `data.frame` with the resolved taxonomy columns (kingdom through genus plus `species_resolved`) skips an online taxonomy lookup step.
- `confidence_interval` (`logical` or numeric; default `FALSE`): `FALSE` — point esti-

mate only. TRUE — 90% conformal interval. Any numeric in $(0, 1)$ — interval at desired coverage level. When active, output includes `lower_bound`, `upper_bound`, and `confidence` level.

- `interval_method` (character; default `"stratified"`): Controls the conformal interval computation when `confidence_interval` is not `FALSE`. `"stratified"` (default) uses rank-specific calibration residuals, providing approximate rank-conditional coverage. `"pooled"` applies a single quantile pooled across all calibration residuals, providing the standard marginal coverage guarantee for genus-level queries.

- `fuzzy_match_name` (`logical`; default `FALSE`): Pre-corrects names via GBIF before taxonomy lookup; adds `matched_name` to output.

- `include_taxonomy` (`logical`; default `FALSE`): Appends the resolved taxonomy columns to the output.

- `method` (character; default `"EntityEmbeddings"`): The entity-embedding model described above, or `"XGBoost"` for the single-stage alternative (Supplementary Section S5).

- `include_source` (`logical`; default `FALSE`): When `TRUE`, appends a `source` column identifying the provenance of each returned mass value. For species whose mass is recorded in the database, the value is the original source identifier. For model-inferred values, the value is `"tbmML_"` followed by the finest taxonomic rank present in the training data (e.g., `"tbmML_genus"` if the genus was seen during training but the species was not; `"tbmML_order"` if only the order was seen), or `"tbmML_UNK"` if no rank was. Unresolvable taxa receive `NA`.

- `lookup` (`logical`; default `TRUE`): When `TRUE` (the default), taxa whose species-level mass is recorded in the database are returned with their empirical measured value without invoking the model. Set to `FALSE` to route all resolved taxa through the model regardless of database membership.

The Python package uses identical names and defaults. The function always returns a data frame with at minimum `taxon` (the name as entered or, when `fuzzy_match_name = TRUE`, the GBIF-corrected name; `None`/`NA` when fuzzy matching finds no match) and `mass_g` (body mass in grams). By default (`lookup = TRUE`), for species whose mass is recorded in the database, the empirical measured value is returned without invoking the model; the conformal prediction interval columns (`lower_bound`, `upper_bound`, `confidence`) are `NA`/`NaN` for such rows. `mass_g` is `NA`/`NaN`, and a warning is issued, both for names that cannot be resolved and for resolved taxa whose kingdom-to-genus classification shares no value with the training data (since predicting such taxa would be an extrapolation from entirely unknown features). A warning is also issued, but a prediction still returned, for taxa whose only rank present in the training data is the kingdom, because such predictions are essentially uninformative (see *Discussion*).

When `fuzzy_match_name = TRUE`, provided taxon names are assessed for incorrect spelling and are corrected before taxonomy lookup by querying GBIF. A name is accepted if GBIF returns a match with confidence ≥ 75. For two-word names where GBIF recognises the genus but not the full binomial, a second lookup is attempted using the GBIF-corrected genus combined with the original species epithet. Single-word names that GBIF does not recognise as a species are retried at successively higher ranks (genus through kingdom), so misspelled genus, family, order, and class names are also corrected. In the resulting output of `predict_mass()`, `taxon` carries the canonical GBIF-resolved name (or `None`/`NA` for unresolvable inputs). `matched_name` carries the originally entered name when a correction was applied or the name could not be resolved, and carries `None`/`NA` when no correction was needed.

Examples

We illustrate the use of `TaxonBodyMassML` with four examples in R.

Example 1 (R): single-taxon queries. A species whose mass is recorded in the database returns that measurement; `lookup = FALSE` forces a model prediction, here with the default 90% conformal interval.

```
library(TaxonBodyMassML)
predict_mass("Nucella ostrina")
# Output:
#             taxon mass_g
# 1 Nucella ostrina    0.7

predict_mass("Nucella ostrina", lookup = FALSE, confidence_interval = TRUE)
# Output:
#             taxon   mass_g lower_bound upper_bound confidence
# 1 Nucella ostrina 1.570419   0.2103283    11.72555        0.9
```

Example 2 (R): batch query with fuzzy name matching and default prediction interval.

```
predict_mass(
  c("Haustrum haustorium",   # correctly spelled; mass recorded in the database
    "Nucela lima",           # misspelling; fuzzy-corrected, then model-inferred
    "Nutella haustrina"),    # unresolvable (not a true species); returns NA
  fuzzy_match_name = TRUE,
  confidence_interval = TRUE
)
# Output:
#                 taxon   mass_g lower_bound upper_bound confidence      matched_name
# 1 Haustrum haustorium 3.730000          NA          NA         NA              <NA>
# 2        Nucella lima 1.570419   0.2103283    11.72555        0.9       Nucela lima
# 3                <NA>       NA          NA          NA         NA Nutella haustrina
# Warning messages:
# 1: Fuzzy-matched 1 name(s): Nucela lima -> Nucella lima
# 2: Could not resolve taxonomy for: 'Nutella haustrina'. Predictions for these species
    will be NA.
```

Example 3 (R): show the provenance of each returned mass value.

```
predict_mass(
  c("Haustrum haustorium",  # mass recorded in the database; returns the measurement
    "Nucella lima"),    # not in the database; model infers from genus
  include_source = TRUE
)
# Output:
#                 taxon   mass_g      source
# 1 Haustrum haustorium 3.730000  Novak_2013
# 2        Nucella lima 1.570419 tbmML_genus
```

Example 4 (R): export the data sources behind a set of predictions as a BibTeX file. Only recorded (database) values contribute; model-inferred rows (`tbmML_*`) have no source to cite and are skipped.

```
res <- predict_mass(c("Haustrum haustorium", "Nucella lima"), include_source = TRUE)
create_bib(res, file = "my_sources.bib")
readLines("my_sources.bib")
# Output:
# [1] "%% TaxonBodyMassML create_bib(): 1 data-source citation(s) for 2 taxa"
# [2] ""
```

```
# [3] "@article{Novak:2013qg,"
# [4] "\tauthor = {Novak, Mark},"
# [5] "\tdate-added = {2026-09-22 13:09:03 -0700},"
# [6] "\tdate-modified = {2026-09-22 13:09:03 -0700},"
# [7] "\tdoi = {10.1098/rspb.2013.1415},"
# [8] "\tjournal = {Proceedings of the Royal Society B: Biological Sciences},"
# ...
```

Discussion

TaxonBodyMassML targets analyses that require a body mass estimate for every taxon in a dataset but for which direct measurements are unavailable. Applications include food web model parameterisation, functional diversity assessments, metabolic-rate scaling calculations, and the FracFeed database (Novak et al., 2026) which motivated the development of the tool because it contains many records for species for which body mass information could not be found in the literature. Although the tool will be most reliable for taxonomic groups well-represented in the training dataset (Tables 1 and 2), and prediction uncertainty for underrepresented groups will be higher than the aggregate test metrics suggest, the estimates of uncertainty that TaxonBodyMassML provides will also allow users to conduct sensitivity analyses to assess the robustness of their conclusions to the uncertainty of the body mass estimates.

Linnaean taxonomy was chosen as the sole predictor because it should be available for every scientifically described species, whereas fully-resolved, branch-length-calibrated phylogenetic trees exist for only a small fraction of taxa. The embedding model learns dense representations in which taxonomic groupings (genera, families, orders) with similar body-mass distributions lie close together, and the gradient-boosted trees then exploit these representations, capturing much of the phylogenetic signal embedded in the Linnaean hierarchy without requiring an explicit tree. The rank-resolution analysis (Supplementary Section S3) showed that prediction accuracy degrades steadily as ranks are lost. Predictions remain largely useful to the order level (geometric-mean multiplicative error of $\sim 4.37\times$), but queries resolved only to class or phylum are off by roughly an order of magnitude, and kingdom-only queries by far more. When a high-quality resolved phylogeny is available, phylogenetic methods (e.g., Goolsby et al., 2017; Thorson and van der Bijl, 2023; Sanchez-Martinez et al., 2024) are likely to achieve lower per-species prediction error (Richard-Bollans and Silvestro, 2026). TaxonBodyMassML therefore offers broader taxonomic coverage and simpler deployment at the cost of not exploiting fine-grained evolutionary relationships within resolved clades.

BHPMF (Schrodt et al., 2015) employs hierarchical Bayesian probabilistic matrix factorisation using taxonomic hierarchy as a structured prior for multi-trait gap-filling for plants. It therefore shares with TaxonBodyMassML the use of taxonomy as the core predictor. *Rphylopars* (Goolsby et al., 2017) fits a multivariate Brownian motion or Ornstein-Uhlenbeck model on an ultrametric phylogenetic tree: principled when a tree is available but inapplicable when it is not. Random forest imputation (e.g., Penone et al., 2014) treats body mass as one of many correlated traits and outperforms simpler approaches but requires a partially observed multi-trait matrix — often not possible in food webs or ecological communities having species that share few trait types in common. Most recently, Moura et al. (2024) applied XGBoost-based phylogenetic multiple imputation on a global tetrapod supertree, producing high-quality predictions for amphibians, reptiles, birds, and mammals. This resource is the preferred choice for tetrapods when a resolved phylogeny is available. For users focused on mammals specifically, PHYLACINE (Faurby et al., 2018) provides curated and imputed body-mass estimates for all known mammal species alongside integrated phylogenies and should be consulted as a first-resort resource for that clade. `TaxonBodyMassML` therefore occupies a distinct niche: rapid, taxonomy-only, query-based prediction across all scientifically named animal-like life, requiring no phylogeny and no trait matrix.

Predictions from `TaxonBodyMassML` represent a central tendency for a taxon based on its taxonomic identity and the masses reported for the species in the training data. Within-species variation due to factors such as sex, age, ontogenetic stage, or geographic location is not captured. Moreover, the model is static: taxonomic revisions and newly described taxa will necessitate retraining. Future versions of the tool aim to provide versioned models as taxonomic changes occur and more body mass data become available, as well as additional model frameworks as these are developed and validated. Promising avenues for future development include integration with continuously updated trait databases and retraining pipelines targeting underrepresented clades.

Data, Software, and Code Availability

- **Source code and packages** (R v0.13.0; Python v0.13.0; MIT licence): `https://github.com/TaxonBodyMassML/TaxonBodyMassML`
- **Pre-trained models** (`r-v0.13.0`, `py-v0.13.0`): `https://huggingface.co/marknovak/TaxonBodyMassML`
- **Web interface**: `https://taxonbodymassml.github.io`
- **Training data** (`TaxonBodyMass_DB` v6.0.0; CC BY 4.0 licence): `https://github.com/TaxonBodyMassML/TaxonBodyMass_DB`

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Author Contributions

Conceptualization: MN. **Data curation:** MN. **Methodology:** GP, HP, ACP. **Software:** GP, HP, ACP, MN. **Formal analysis:** GP, MN. **Website design:** HP. **Visualization:** GP, HP. **Writing – original draft:** MN. **Writing – review:** GP, HP, ACP.

AI Use Statement

MN used Anthropic's Claude Sonnet 4.6 to audit the taxon names of the database (see *Training data*), to convert the web-based version of the tool produced by GP, HP, and ACP into R and Python packages, and to assist with drafting the manuscript, and Claude Fable 5.1 to refactor the training pipeline and packages and to incorporate the entity-embedding model.

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Supplementary Materials

TaxonBodyMassML: Taxonomy-informed prediction of body mass using gradient-boosted trees

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Contents

S1. Model architecture and hyperparameters

Table S1 summarises the Stage-1 embedding network and Table S2 the Stage-2 XGBoost hyperparameters of the entity-embedding model. "Tuned" parameters were selected by Optuna (100 trials, 5-fold cross-validation within the training set, with the Stage-1 network refit inside each fold).

Table S1: Stage 1 of the entity-embedding model: embedding dimensions per rank and the network that learns them.

Rank	Training vocabulary (excl. UNK)	Embedding dimensions
`kingdom`	5	4
`phylum`	39	8
`class`	115	8
`order`	458	16
`family`	2,148	16
`genus`	9,431	32
Concatenated input		84
Stage 1 network and training		
Hidden layers		84 → 64 → 32 → 1, ReLU
Loss		L1 (MAE in $\log_{10}$ g)
Optimiser		Adam, learning rate 0.001, OneCycleLR schedule
Epochs / batch size		100 / 256
Seeds		PyTorch and NumPy 42
UNK vector		mean of the rank's learned embeddings
Stage 1 test MAE		0.392 $\log_{10}$ g

Table S2: Stage 2 XGBoost hyperparameters of the entity-embedding model. *Tuned value lies at the upper bound of its search range.

Parameter	Value	Search range	Description
`objective`	`reg:absoluteerror`	fixed	MAE loss, $\log_{10}$ space
`random_state`	42	fixed	Reproducibility seed
`n_estimators`	1,500	200–1,500 (step 50)*	Trees in ensemble
`max_depth`	17	4–25	Maximum tree depth
`learning_rate`	0.01534	0.003–0.3 (log)	Step size per tree
`subsample`	0.6695	0.5–1	Row sampling fraction per tree
`colsample_bytree`	0.5225	0.5–1	Feature sampling fraction per tree
`min_child_weight`	2	1–30	Minimum sum of instance weight in a leaf
`reg_alpha`	0	default	L1 regularisation on leaf weights
`reg_lambda`	1	default	L2 regularisation on leaf weights

S2. Feature importance

Gain-based feature importances were extracted from the Stage-2 trees. Each tree splits on individual embedding dimensions, so gains were summed over the dimensions belonging to each rank and normalised to 100% (Table S3). This aggregation is biased toward ranks with more embedding dimensions (4 for kingdom up to 32 for genus) and toward ranks whose embeddings vary most between records, so it should be read alongside the rank-resolution analysis of Section S3, which measures directly how much predictive accuracy each rank contributes, and alongside the importances of the single-stage XGBoost model, whose features are the ranks themselves (Section S5, Table S11).

Table S3: Gain-based feature importance of the entity-embedding model by taxonomic rank, normalised to 100%. Gain measures the average improvement in loss per split, summed over the embedding dimensions of each rank.

Taxonomy rank	Relative importance (%)
`kingdom`	3.8
`phylum`	38.4
`class`	4.6
`order`	16.5
`family`	12.8
`genus`	23.9

S3. Prediction error vs. taxonomic rank resolution

To quantify the accuracy penalty when only partial taxonomy is available, all 3,657 test-set species were re-predicted with progressively coarser taxonomy by setting finer ranks to `UNK`. Species is never a feature, so the genus level is the ordinary prediction for an unmeasured species and serves as the baseline. Each rank removed adds error (Table S4): ΔMAE = +0.133 $\log_{10}$ units when the genus is unknown (geometric-mean multiplicative error 10^{MAE} of 2.11× to 2.86×), +0.317 when the family is also unknown (4.37×), and +0.682 when the order is also unknown (10.14×).

Table S4: Mean absolute error (MAE, $\log_{10}$ g) of the entity-embedding model on the 3,657 test species when the finest known rank is progressively coarsened by setting finer ranks to `UNK`. ΔMAE is the penalty relative to the genus-level baseline; 10^{MAE} is the geometric-mean multiplicative error.

Finest known rank	MAE ($\log_{10}$ g)	ΔMAE	10^{MAE}
`genus` (species unseen; baseline)	0.324	—	2.11×
`family` (genus = UNK)	0.456	+0.133	2.86×
`order`	0.641	+0.317	4.37×
`class`	1.006	+0.682	10.14×
`phylum`	0.926	+0.603	8.44×
`kingdom`	4.919	+4.595	82967.02×

S4. Empirical coverage of the conformal prediction intervals

For each level of taxonomic resolution of Section S3, the 3,657 test species were re-predicted with 80%, 90% and 95% conformal intervals under both `interval_method` settings, and the fraction of true masses falling inside the interval was recorded (Tables S5 and S6). For queries resolved to genus, family or order, the stratified intervals stay close to their nominal coverage (92.6%, 91.4% and 90.3% at a nominal 90%) because their half-width grows with the rank-specific calibration residuals (from 0.87 $\log_{10}$ units for genus-level queries to 6.30 for kingdom-level queries), whereas the pooled intervals, calibrated for genus-level queries only, under-cover increasingly at coarser ranks (86.0% at family, 74.4% at order and 46.2% at class level).

Table S5: Empirical coverage of the entity-embedding model's 90% prediction intervals on the 3,657 test species by finest known rank, for the default rank-stratified calibration and for pooled calibration. Half-width is the mean half-width of the stratified interval in $\log_{10}$ g. Rows are defined by the coarsest rank retained in the query; a test species whose retained ranks are absent from the training vocabulary falls into a coarser stratum, so the mean half-width of a row can exceed that row's rank-specific q.

Finest known rank	n	half-width ($\log_{10}$ g)	coverage at nominal 90%	
		stratified	stratified	pooled
`genus` (species unseen; baseline)	3,657	0.92	92.6%	91.1%
`family` (genus = UNK)	3,657	1.08	91.4%	86.0%
`order`	3,657	1.42	90.3%	74.4%
`class`	3,657	1.75	88.1%	46.2%
`phylum`	3,657	2.46	93.3%	61.0%
`kingdom`	3,657	6.30	86.3%	2.4%

Table S6: As Table S5, for nominal 80% and 95% intervals (coverage in %).

Finest known rank	n	nominal 80%		nominal 95%	
		stratified	pooled	stratified	pooled
`genus` (species unseen; baseline)	3,657	83.8	81.8	96.5	95.7
`family` (genus = UNK)	3,657	81.3	69.5	95.5	93.7
`order`	3,657	80.7	54.2	95.3	87.2
`class`	3,657	73.4	27.2	95.3	67.7
`phylum`	3,657	86.3	42.6	96.1	74.4
`kingdom`	3,657	73.2	1.1	92.8	3.3

S5. Alternative method: single-stage XGBoost

`TaxonBodyMassML` retains a single-stage XGBoost regressor fitted directly to the six categorical ranks, using XGBoost's native categorical splits (no one-hot encoding), the same MAE objective, the same training, test and calibration splits and the same conformal procedure as the entity-embedding model. Tuning was performed with Optuna (100 trials, 5 folds; best cross-validated MAE 0.348 $\log_{10}$ units; Table S7). It is available as `method = "XGBoost"`.

We provide it because (i) it serves as a useful reference model that operates on the taxonomy directly so that the comparison in Tables S8–S10 shows what the embedding stage adds, and (ii) its gain-based importances refer to the ranks themselves and are therefore directly interpretable (Table S11, Fig. S2).

Table S7: Hyperparameters of the single-stage XGBoost model.

Parameter	Value	Search range	Description
`objective`	`reg:absoluteerror`	fixed	MAE loss, $\log_{10}$ space
`enable_categorical`	`True`	fixed	Native categorical splits
`random_state`	42	fixed	Reproducibility seed
`n_estimators`	350	200–900 (step 50)	Trees in ensemble
`max_depth`	32	5–50	Maximum tree depth
`learning_rate`	0.08801	0.01–0.3 (log)	Step size per tree
`subsample`	0.5782	0.5–1	Row sampling fraction per tree
`colsample_bytree`	0.7948	0.5–1	Feature sampling fraction per tree
`gamma`	0.2004	0–1	Min. loss reduction to split a node
`min_child_weight`	2	1–10	Minimum sum of instance weight in a leaf
`reg_alpha`	0	default	L1 regularisation on leaf weights
`reg_lambda`	1	default	L2 regularisation on leaf weights

Table S8: Performance of both models on the held-out test set (full) and on the subset restricted to species with body mass $> 0.1\,\mathrm{g}$. All metrics are in $\log_{10}$ space.

Model	Test set	R^2	RMSE	MAE	n
Entity Embeddings	Full test set	0.91	0.56	0.32	3,657
Entity Embeddings	Reduced (mass $> 0.1\,\mathrm{g}$)	0.79	0.51	0.30	3,369
XGBoost	Full test set	0.89	0.61	0.35	3,657
XGBoost	Reduced (mass $> 0.1\,\mathrm{g}$)	0.75	0.56	0.33	3,369

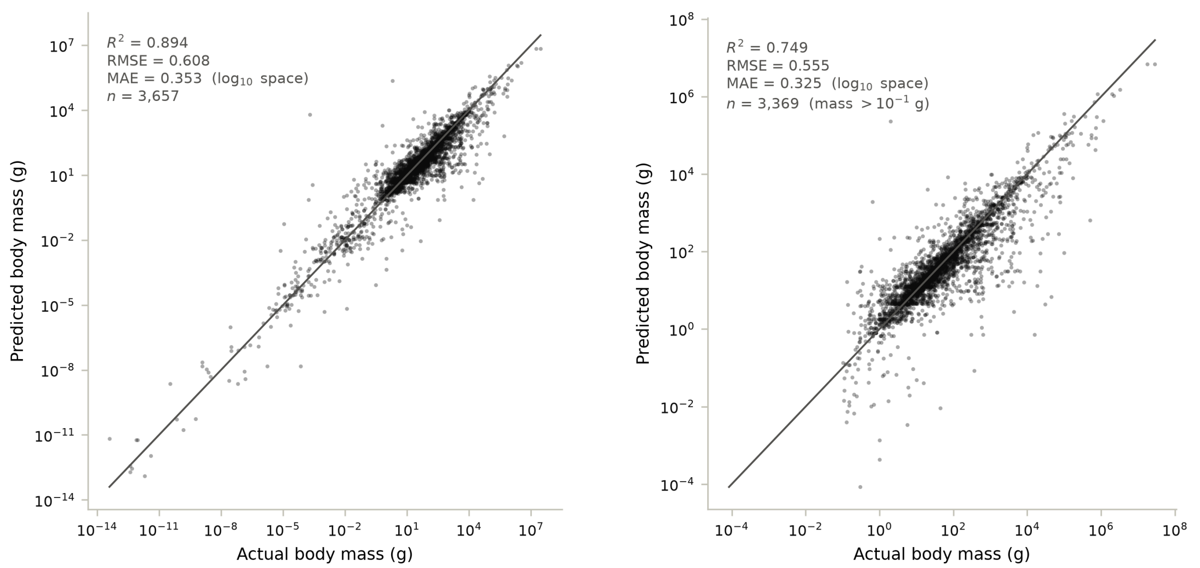

Figure S1: Predicted vs. actual body mass (g) of the single-stage XGBoost model on the held-out test set. **(a)** Full test set. **(b)** Test set restricted to mass $> 0.1\,\mathrm{g}$. Compare Fig. 1.

Table S9: Mean absolute error ($\log_{10}$ g) of both models when the finest known rank is progressively coarsened (cf. Table S4).

Finest known rank	Entity Embeddings		XGBoost	
	MAE	ΔMAE	MAE	ΔMAE
`genus` (species unseen; baseline)	0.324	—	0.353	—
`family` (genus = UNK)	0.456	+0.133	0.492	+0.139
`order`	0.641	+0.317	0.752	+0.399
`class`	1.006	+0.682	0.920	+0.566
`phylum`	0.926	+0.603	2.135	+1.782
`kingdom`	4.919	+4.595	3.942	+3.589

Table S10: Empirical coverage (%) of the 90% prediction intervals of both models by finest known rank, stratified vs. pooled calibration (cf. Table S5).

Finest known rank	n	EE nominal 90%		XGB nominal 90%	
		stratified	pooled	stratified	pooled
`genus` (species unseen; baseline)	3,657	92.6	91.1	91.3	89.7
`family` (genus = UNK)	3,657	91.4	86.0	90.2	83.7
`order`	3,657	90.3	74.4	89.9	67.0
`class`	3,657	88.1	46.2	89.1	59.6
`phylum`	3,657	93.3	61.0	78.8	10.3
`kingdom`	3,657	86.3	2.4	90.4	3.4

Table S11: Gain-based feature importance by taxonomic rank for both models, normalised to 100%. For the single-stage XGBoost model the features are the ranks themselves; for the entity-embedding model gains are summed over each rank's embedding dimensions.

Taxonomy rank	Entity Embeddings (%)	XGBoost (%)
`kingdom`	3.8	1.8
`phylum`	38.4	5.1
`class`	4.6	5.4
`order`	16.5	17.9
`family`	12.8	25.8
`genus`	23.9	44.1

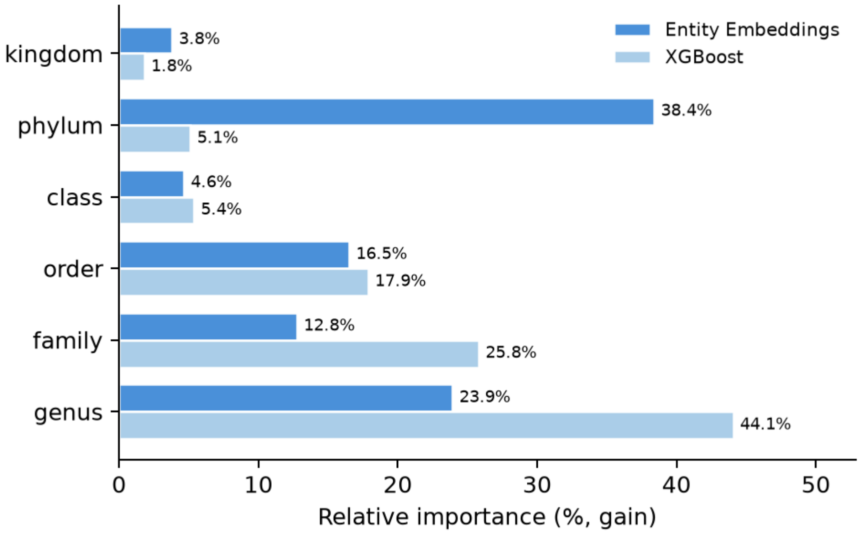

Figure S2: Gain-based feature importance by taxonomic rank (Table S11).

S6. Training data sources

The following primary literature sources and databases contributed to the full dataset.

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