

Reaching the ideal weight?

Calibration of a Bayesian network weight-of-evidence model for supporting animal alternatives in ecotoxicity testing



Background

- A **Bayesian network (BN)** has been developed for predicting **acute fish toxicity (AFT)** from **fish embryo toxicity (FET)** in combination with other **lines of evidence (LoE)** (Moe et al. 2020)
- Data shortage** is a challenge for **model evaluation**
- Cross-validation** allows for efficient use of data for training and testing **independently**

BN model construction

- Acute toxicity data from 237 substances: juvenile fish (AFT), fish embryo (FET), algae, daphnids, gill cytotoxicity and/or QSAR (Fig. 1)
- Prior probability distributions are estimated by hierarchical Bayesian modelling (ANOVA) (Fig. 2)
- LoE weights are estimated by multiple linear regression of expected values from each LoE (Eq.1):
$$\text{AFT} \sim 0.326 * \text{FET} + 0.308 * \text{Algae \& daphnids} + 0.216 * \text{Gill cytotoxicity} + 0.149 * \text{QSAR}$$

Cross-validation

- The data are divided into $k = 10$ subsamples. For each k ,
 - 9 subsamples used for training (Eq. 1)
 - the 10th subsample is used for testing
- The resulting 10 sets of coefficients are averaged to obtain the calibrated LoE weights (Eq. 1)

Figure 1. BN model: main modules and functionality

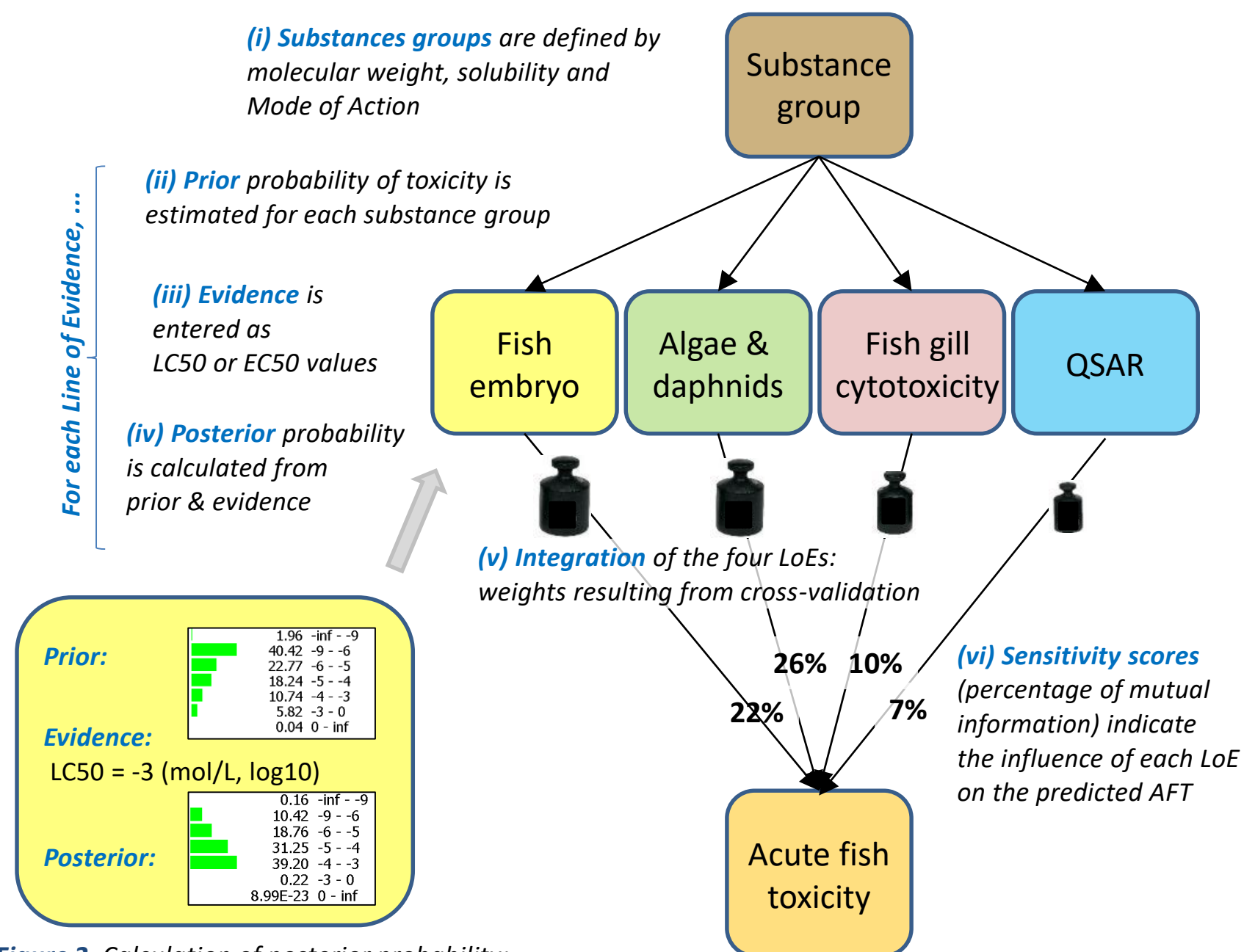


Figure 2. Calculation of posterior probability: example from one Line of Evidence

BN model evaluation

- Model accuracy is evaluated by the most probable AFT interval
- The BN is evaluated for 4x4 criteria (data availability and precision of prediction)
- The calibrated BN typically predicts a binary response (e.g. LC50 < 1 mg/L; Fig. 3) correctly for 75-80% of the cases

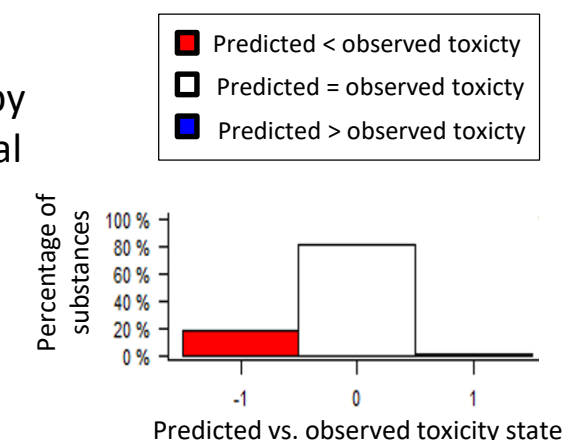


Figure 3. Example of BN predictive performance

- Sensitivity scores (Fig. 1) reflect the weights of LoEs, as well as uncertainties (conditional probabilities) within each LoE

Ongoing work and further improvements

- Expanded dataset for training and testing
- Refined definition of substance groups
- Update of the online model user interface & user guidance
- Include additional data to define the applicability domain
 - Touch-evoked response of fish embryos
 - Metabolic activity of embryo and juvenile fish

Acknowledgements

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Reference

Moe et al. 2020. Development of a hybrid Bayesian network model for predicting acute fish toxicity using multiple lines of evidence. *Env. Mod. Soft.*: 104655. <https://doi.org/10.1016/j.envsoft.2020.104655>

