Manual for Bayesian Estimation of Depth-Integrated Lake Metabolism (BEDILM)

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Supplementary material for:

D.P. Giling, Staehr P.A., Grossart H.P., Andersen M.R., Boehrer B., Escot-Muñoz C., Evrendilek F., Gener L.G., Honti M., Jones I.D., Karakaya N., Laas A., Moreno Q., Rinke K., Scharfenberger U., Schmidt S.R., Weber M., Woolway R.I., Zwart J. & Obrador B. (in revision) Delving Deeper: Metabolic processes in the metalimnion of stratified lakes.

Introduction

This is a manual for the code 'BEDILM.R' to estimate daily rates of gross primary production (GPP) and ecosystem respiration (ER) from depth-specific measurements of dissolved oxygen (DO), water temperature and PAR in lakes. The code implements the depth-integrated framework of Staehr *et al.* (2012b) in a Bayesian framework as described by Grace *et al.* (2015) and Giling *et al.* (2016; in revision). This manual does not introduce the background or theory of the free-water diel oxygen technique (but see e.g. Staehr et al. 2012a). Using the model does not require experience with Bayesian techniques, but to gain a better understanding of the methods (e.g. providing informed prior distributions) and correctly interpret the outputs (e.g. checking model convergence), we recommend consulting introductory texts on Bayesian methods and the BUGS language (e.g. Kéry 2010; McCarthy 2007). It is crucial that model convergence and fit are considered when interpreting results (for discussion see Giling et al. in revision and references therein)

Briefly, the model partitions changes in depth-specific dissolved oxygen (DO) concentration between successive timesteps *t* into the contribution by biotic and physical processes (Staehr et al. 2012b and references therein). The sub-models describing the biological components (i.e. net ecosystem production [NEP], which is comprised of GPP and ER), are parameterized according to Grace *et al.*

(2015) and Song *et al.* (2016). The parameter estimation is performed by the JAGS software (Plummer 2003).

Getting started

Install or update both R (http://www.r-project.org/) and JAGS (http://mcmc-jags.sourceforge.net/). Download the zipped folder 'Depth-int_lake_metab' from https://github.com/dgiling/BEDILM and extract the files. The folder contains two subfolders and the model code:

- 'data' folder: Folder for input data (containing example data).
- 'results' folder: Location for writing of results tables and plots.
- BEDILM.R: This R code sets up the model, calculates the physical fluxes and calls JAGS to model the time series
- metab_model_jags_code.txt: JAGS code for the metabolism model. This does not need to be altered unless you want to change prior distributions or the method of Ds calculation (see 'calc.Ds.with.modDO' below).
- temperature_curve_jags_code.txt: JAGS code for the temperature curve model (Rimmer et al. 2005).

The JAGS code files are called automatically by JAGS, which runs in the background.

Input data

The 'data' folder contains example data series from Lake Stechlin, Germany, measured with automated profilers on the LakeLab research facility (Giling et al. 2016; www.lake-lab.de). We recommend first running the example data to ensure the model is working correctly on your system. The input data is structured so that each row is one vertical profile at a specific date and time (pr_dt; in hourly intervals for the Stechlin data). The column headers describe a single measure of wind speed (m s^{-1}), barometric pressure (mB), incoming surface PAR (μmol m^{-2} s^{-1}) and salinity (ppt; optional, provide a column of zeros if not available) per profile. The remaining columns provide the depth-specific measurements of DO,

water temperature and PAR_z, with one column for each layer (9 layers for the example data, at depths of 1 m to 17 m in 2-m intervals).

Description of 'BEDILM.R'

The following numbered sections refer to the corresponding numbers in 'BEDILM.R'

1. *Define inputs*

   The structure of the input data, measurement properties and lake physical characteristics are provided here. Some options are also selected:

   - `DO.in.mgL`: State whether DO measurements are in mgL (set to TRUE; default) or expressed in % saturation (set to FALSE).
   - `calc.Ds.with.modDO`: Select whether Ds (gas exchange with atmosphere; Staehr *et al.* 2012b) is calculated using the modelled DO data (TRUE; default) or the measured DO data (FALSE). Using the modelled DO can improve accuracy under some circumstances (Song et al. 2016). If you wish to change the default and use the measured DO, you must also alter the JAGS code 'metab_model_jags_code': comment out the line marked with 'calc.Ds.with.modDO = TRUE' (line 51) and uncomment the line marked with 'calc.Ds.with.modDO = FALSE' (line 52).
   - `meta.symmetrical`: Define how the bottom of the metalimnion zone is calculated. The default assumes the metalimnion is symmetrical around the thermocline (i.e. the depth of steepest temperature gradient; set to TRUE). Setting to FALSE will define the bottom of the metalimnion as the deepest point with the density gradient exceeding the threshold value defined for Z_{mix} ('p.gradient.threshold').

2. *Setup*

   This section contains the code for smoothing of DO, PAR_z and wind speed over the whole data series (4-h smoothing period by default). It also creates a vector called 'k.list' containing the Julian days

that contain no missing data over the 24-h period. Note that the model is currently only set up for modelling 24-h periods with evenly-spaced measurements. It could be altered to model for longer time periods with appropriate changes to the estimation of parameter R in the JAGS code (metab_model_jags_code.txt).

3. *Loop over days*

This section takes the parameters defined in code sections 1 and 2 and performs the calculations for each profile *i* and layer *j* iteratively for each day *k.* The remainder of the code is contained within this loop (i.e. metabolism on each day and layer is estimated sequentially).

3.1 Calculate mean daily light extinction coefficient (KD; m^{-1})

In the example data K_D is calculated from the relationship between depth and log(PAR), which was measured directly (K_D is not actually used in the example data, calculated only for later reference). An independent measure of K_D could be used to calculate PAR_z from surface PAR (PAR_0) prior to running the model, and providing this in the PAR columns.

3.2 Model temperature curve to define epi, meta and hypo

This section calls JAGS to model a higher resolution (0.1-m intervals) temperature curve from the measured data according to Rimmer *et al.* (2005). The surface temperature and Z_{max} temperature are used to calculate local buoyancy frequency (N^2) for the top and bottom layers. For this reason, Z_{max} should be set an appropriate depth below the deepest layer, not necessarily the maximum depth of the lake.

3.3 Calculate DO mg/L from % sat or mg/L at saturation as required

3.4 Calculate rates of diffusive DO fluxes (Ds, Dv, Dz)

3.4.1 Rate of exchange with atmosphere (Ds)

3.4.2 Vertical transfer among layers due to eddy diffusivity (Dv)

3.4.3 Fluxes due to mixed-layer deepening (Dz)

3.5 Model metabolism for each layer (index j) sequentially

This component takes the physical calculations made in 3.4 and calls JAGS to estimate the model parameters. JAGS will run in the background, estimating the metabolic parameters for each day and layer sequentially without further user input. The results table is written at each iteration, so that progress is saved in the case of an error. An error will occur if the results csv file is opened when R attempts to write it, but model progress can be observed by copying the csv to another location and opening the copied version. Note that the modelling can take some time for large datasets with frequent measures.

Description of metab_model_jags_code.txt

This JAGS code contains the actual metabolic model. By default, the Θ and p parameters have fixed values, as defined below comment "Option 1". Alternatively, Θ and/or p can be given an uninformed prior distribution within physically realistic bounds, and be simultaneously estimated by the model (Grace et al. 2015). To estimate Θ and/or p, comment and uncomment the appropriate lines of code below "Option 2". Note that either Θ, p or both may be estimated, but each can only be defined once, so make sure to comment out the fixed specification if providing a prior distribution. Allowing Θ and/or p to be estimated may improve model fit under some circumstances. However, estimating additional parameters penalizes DIC and may require a greater number of iterations to reach MCMC chain convergence.

The other option in the "metab_model_jags_code.txt" is defining whether to calculate Ds with measured or modelled DO concentration on lines 51 and 52.

Outputs

After running the code the following plots and table are written:

- *Plots of modelled temperature profiles*

  A plot of the modelled temperature curve is saved in the 'profile plots' folder. A good fit to measured temperature data is highly desirable because this high resolution (0.1-m resolution) curve defines the epi-, meta- and hypolimnetic depth zones. Different values for the density gradient defining Z_{max} can be tested by altering the 'p.gradient.threshold' in Section 1 of the R code. Poor fitting temperature curves may be improved by increasing the number of model iterations in Section 1.

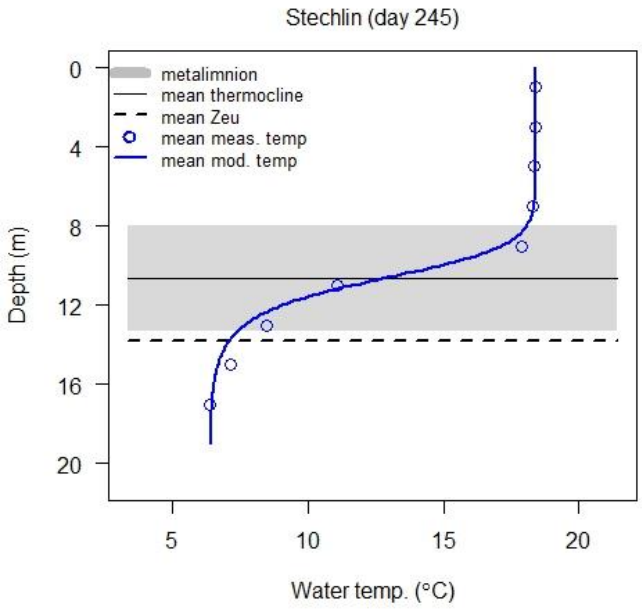

Figure 1. Example temperature curve plot

- *csv file of results and measures of model fit. Each row in output contains results for one layer.*

Column	Units	Description
Lake		
DOY		Julian day
layer.no		Index j, the layer number starting at 1 for the shallowest layer
Depth	m	Depth of layer
layer.thickness	m	Thickness
layer.zone.mean	m	Depth zone of layer based on mean daily temperature profile. 1 = epilimnion, 2 = metalimnion and 3 = hypolimnion.
TempC.mean	°C	Mean daily water temperature
TempC.sd	°C	SD of daily water temperature
PAR.max	μmol m^{-2} s^{-1}	Maximum PAR_z
PAR.mean	μmol m^{-2} s^{-1}	Mean PAR_z
Zmix.mean	m	Mean daily Z_{mix}
metalim.max.mean	m	Mean daily bottom of the metalimnion
thermocline.depth.mean	m	Mean daily depth of the thermocline (i.e. plane of steepest temperature gradient)
mean.K_D	m^{-1}	Mean daily coefficient of light attenuation
mean.Zeu	m	Mean daily photic depth ($\log(0.01)/K_D$)
Sc		Schmidt number
U10	m s^{-1}	Wind speed standardized to 10 m above lake surface
k600		Gas transfer velocity at a Schmidt number of 600
Ks	cm h^{-1}	Mean coefficient of oxygen exchange
Ds.sum	mg O_2 L^{-1} day^{-1}	Sum of the atmospheric fluxes into (negative) or out of (positive) the layer at each timestep
N^2	s^{-2}	Brunt-Väisälä buoyancy frequency (local)
Kv	m^2 h^{-1}	Mean vertical turbulent diffusivity
Dv.sum	mg O_2 L^{-1} day^{-1}	Sum of the vertical diffusive fluxes into (negative) or out of (positive) the layer at each timestep
Dz.sum	mg O_2 L^{-1} day^{-1}	Sum of the diffusive fluxes due to mixed-layer deepening fluxes into (negative) or out of (positive) the layer at each timestep
PPP		Posterior predictive p-value; see 'Assessing model fit'
R^2		Correlation between measured and modelled [O_2]
pD		Effective number of parameters; see 'Assessing model fit'
DIC		Deviance Information Criterion; see 'Assessing model fit'
Rhat.test		Logical test for convergence of all parameters (all R-hats < 1.1)
A.Rhat		R-hat for parameter *A*; see 'Assessing model fit'
R.Rhat		R-hat for parameter R; see 'Assessing model fit'
p.Rhat		R-hat for parameter p; see 'Assessing model fit'
theta.Rhat		R-hat for parameter Θ; see 'Assessing model fit'
A.auto.corr		Lag 1 autocorrelation in chains of parameter *A*
R.auto.corr		Lag 1 autocorrelation in chains of parameter *R*
p.auto.corr		Lag 1 autocorrelation in chains of parameter *p*
theta.auto.corr		Lag 1 autocorrelation in chains of parameter Θ
p.mean		Mean estimated *p* (exponent describing photosynthesis-irradiance curve)
p.sd		SD of estimated *p*
A.mean		Mean estimated *A* (primary production per unit light)
A.sd		SD of estimated *A*
R.mean		Mean estimated *R*
R.sd		SD of estimated *R*
theta.mean		Mean estimated Θ (temperature dependence of ER)
theta.sd		SD of estimated Θ
ER.mean	mg O_2 L^{-1} day^{-1}	Mean estimated ER (by default at TempC.mean)
ER.sd	mg O_2 L^{-1} day^{-1}	SD of estimated ER
GPP.mean	mg O_2 L^{-1} day^{-1}	Mean estimated GPP (by default at TempC.mean)
GPP.sd	mg O_2 L^{-1} day^{-1}	SD of estimated GPP
NEP.mean	mg O_2 L^{-1} day^{-1}	Mean estimated NEP (by default at TempC.mean)
NEP.sd	mg O_2 L^{-1} day^{-1}	SD of estimated NEP

- *Validation plots*

Section 3.5 of the code saves a multi-panel plot to the 'validation plots' folder for every layer in each day to aid in visually assessing model fit (Fig. 2).

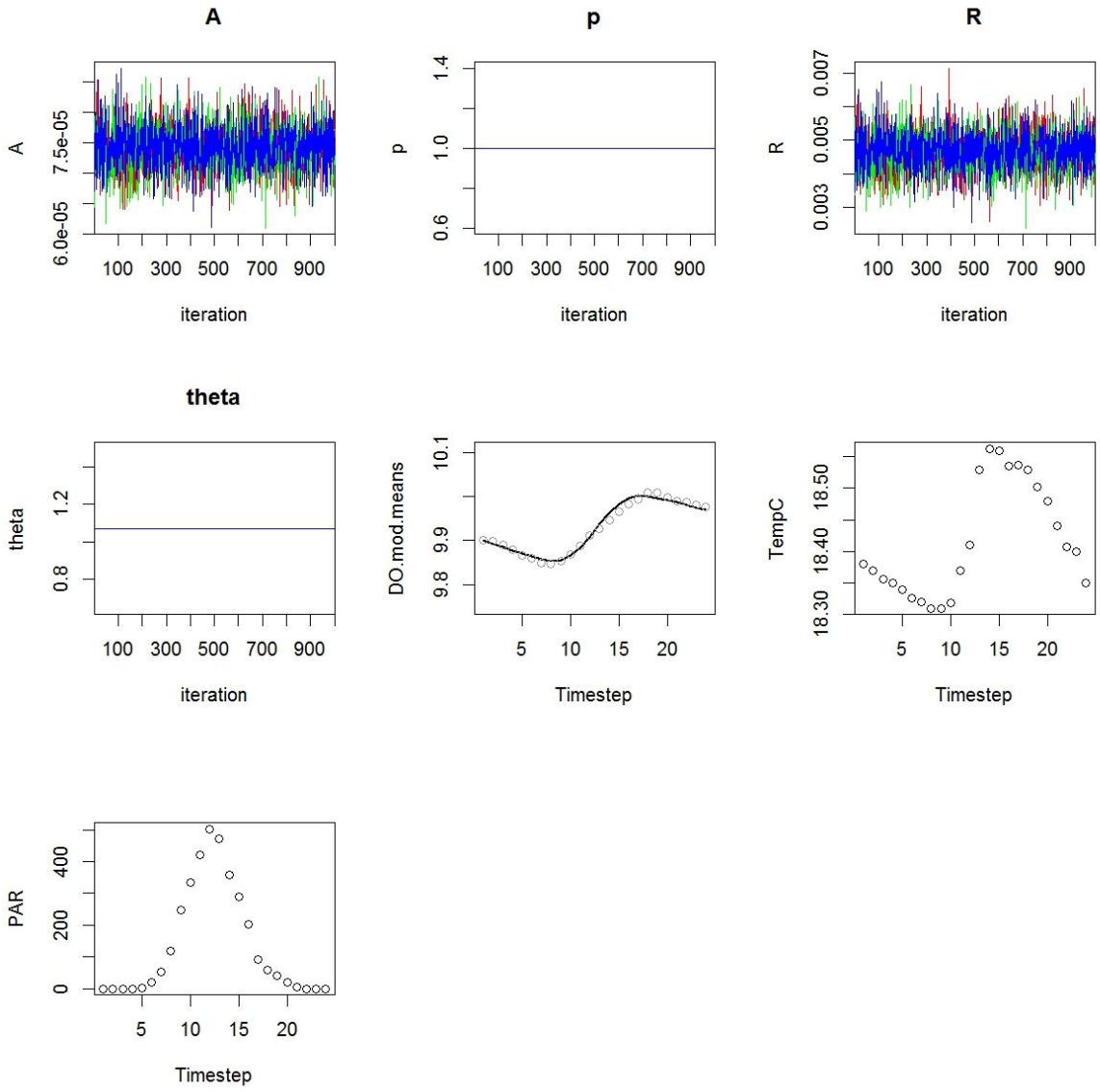

Figure 2. Example validation plot. The first four panels show the MCMC chains for *A*, *p*, *R* and *Θ*. The other panels show the measured [O_2], water temperature and PAR (open circles), with the mean modelled [O_2] shown as a solid line. When set as fixed values the trace plots for p and Θ show a horizontal lines with no variation.

Assessing model convergence and fit

Visual assessment of convergence and fit

The first four panels of the validation plots show trace plots of the MCMC chains. These chains must be converged and stationary, as shown in Fig. 3. Unconverged chains render parameter estimates unreliable. The three chains should be converged (overlapping) and stationary (centered) (Fig. 3).

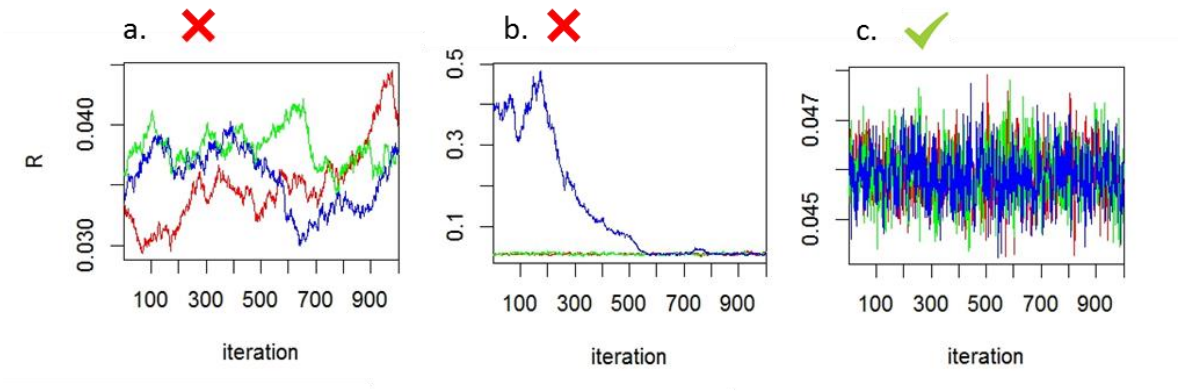

Figure 3. Example trace plots showing (a) three chains with poor mixing, (b) an example where a longer burn-in period is required, and (c) converged and stationary chains.

The model fit also can be confirmed visually using the validation plots, which show the measured (empty circles) and predicted (black line) DO curve for each diel period and the measured temperature and PAR data. It may be possible to see if there are any inconsistencies in the data that may indicate a violation in the assumption of the free-water DO method. For example, a sharp increase or decrease in temperature or DO may indicate the influence of physical processes that are unaccounted for by the model.

Quantitative assessment of convergence

The 'R-hat' statistic is an assessment of model convergence. Values close to 1 indicate good convergence, while values >1.1 indicate poor mixing of the chains. R-hat for model parameters (*A*, *R*, *K*, *theta*, *p* and *GPP*) are included in the results table. Poor mixing can (but not always) be improved by increasing the

number of iterations, increasing the thinning rate, or providing better initials. The output csv contains a column titled 'Rhat.check', which tests whether all the R-hat values are < 1.1 and can be used to quickly assess convergence (returns 'fine' when all R-hats < 1.1).

Assessing model fit quantitatively

There are two measures of model fit included in the results table: (1) the posterior predictive p-value (PPP), and (2) the R^2 value. The PPP compares lack of fit of the model to the actual data against lack to fit to a distribution of possible model discrepancies by using data simulated from the parameterized model (Gelman et al. 1996). A PPP value close to 0.5 indicates a very plausible model, while values <0.1 or >0.9 indicate that the parameterized model is not a plausible explanation of the observed data. The correlation (R^2) between the observed and modelled DO data is reported in the results table.

Model selection

The results table returns the Deviance Information Criterion (DIC), an assessment of how well the model will predict a replicate dataset. DIC takes into account the complexity of the model and can be used for model selection (for example to choose between models with Θ and/or p fixed or estimated). Lower DIC is desirable, and DIC may be negative. There is no hard rule, but a difference of ≥ 5 between models may be considered evidence that the model with lower DIC best predicts the data because values exceeding 5 correspond to 10-fold or greater support for the model with the lower DIC.

References

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