WOMBAT: A fully Bayesian global flux-inversion framework

The WOllongong Methodology for Bayesian Assimilation of Trace-gases

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WOMBAT extends the standard Bayesian synthesis flux-inversion setup (e.g., Enting, 2002) to a Bayesian hierarchical framework, allowing full uncertainty quantification of all unknowns, including fluxes.

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Key features of WOMBAT

WOMBAT is a framework that combines key features that have individually been found to be important:

- **Correlated errors** (Chevallier, 2007), with length scales estimated online
- **Online bias correction** (Worden et al., 2017)
- **Online measurement-error scaling** (Worden et al., 2017)
- **Online estimation of prior variances and length scales of fluxes** (e.g., Michalak et al., 2005)
- **Full uncertainty quantification** using Markov chain Monte Carlo (MCMC) (e.g., Ganesan et al., 2014)

WOMBAT’s hierarchical Bayesian framework

Data model (mole-fraction observations): 
\[ Z_{2,i} = Y_{2,i} + x'_i \beta + \xi_i + \epsilon_i \]

Process model (mole fraction): 
\[ Y_2(s, h, t) = \mathcal{H}(Y_1(\cdot, \cdot); s, h, t) + \nu_2(s, h, t) \]

Process model (flux): 
\[ Y_1(s, t) = Y_1^0(s, t) + \sum_{i=1}^{n_s} \sum_{j=1}^{n_t} \varphi_{i,j}(s, t) \alpha_{i,j} \]

Parameter model (flux): 
\[ \alpha_{i,j} = \kappa_i \alpha_{i,j-1} + \eta_{i,j}, \quad \eta_{i,j} \sim N(0, \sigma_i^2) \]

Parameter model (errors): Length scale of \( \xi_i \) is \( \ell \), variance of \( \xi_i \) is \( \rho \nu_i \), and variance of \( \epsilon_i \) is \( (1 - \rho) \nu_i \)

Unknown parameters, estimated online using MCMC

OSSEs stress the importance of bias correction and correlated error

OSSEs using simulated OCO-2 column-average CO₂ retrievals (from the LN and LG modes) show the importance of accounting for biases and correlated errors if they are present.

Flux estimation is severely impacted otherwise, especially at the regional level.

Model performance in an OSSE experiment when estimating fluxes at the TransCom3 level when the data are biased and have correlated errors:

<table>
<thead>
<tr>
<th>Inversion configuration</th>
<th>RMSE [PgC/mo]</th>
<th>CRPS</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>LG</td>
<td>LN</td>
</tr>
<tr>
<td>Bias correction/correlated</td>
<td>0.023</td>
<td>0.021</td>
</tr>
<tr>
<td>Bias correction/uncorrelated</td>
<td>0.038</td>
<td>0.038</td>
</tr>
<tr>
<td>No bias correction/correlated</td>
<td>0.045</td>
<td>0.026</td>
</tr>
<tr>
<td>No bias correction/uncorrelated</td>
<td>0.092</td>
<td>0.063</td>
</tr>
</tbody>
</table>

Lower is better

Estimated fluxes for two TransCom3 regions, with 95% credible regions, under four inversion configurations.

Comparison to the OCO-2 MIPv7 ensemble

We performed CO₂ flux inversions using WOMBAT following the OCO-2 MIPv7 protocol (Crowell et al., 2019).

This used OCO-2 data from version 7, and fluxes were estimated for 2015–2016. Inversions were run separately for LN and LG data.

Mean-squared error [ppm²] averaged across TCCON stations for MIP participants + WOMBAT for inversions using LG data (first row) and LN data (second row)

<table>
<thead>
<tr>
<th></th>
<th>TMS-4D VAR</th>
<th>CT-NRT</th>
<th>OU</th>
<th>CAMS</th>
<th>Baker-mean</th>
<th>Schuh</th>
<th>UT</th>
<th>CMS-Flux</th>
<th>UoE</th>
<th>WOMBAT Post.</th>
<th>WOMBAT Prior</th>
</tr>
</thead>
<tbody>
<tr>
<td>LG</td>
<td>1.33</td>
<td>1.63</td>
<td>1.31</td>
<td>1.31</td>
<td>1.88</td>
<td>1.41</td>
<td>1.85</td>
<td>1.78</td>
<td>1.71</td>
<td><strong>1.19</strong></td>
<td><strong>3.56</strong></td>
</tr>
<tr>
<td>LN</td>
<td>1.36</td>
<td>2.09</td>
<td>1.74</td>
<td>1.24</td>
<td>2.12</td>
<td>1.58</td>
<td>1.71</td>
<td>2.72</td>
<td>1.37</td>
<td>1.57</td>
<td>3.56</td>
</tr>
</tbody>
</table>

Lower is better

WOMBAT’s estimates corroborate the MIP, and compare favourably on the TCCON data used to validate the MIP results.

The future of WOMBAT

- We plan to submit to the next round of the OCO-2 MIP, which will use OCO-2 version 10 data

- We also plan to investigate the properties of transport model error further by using multiple transport models

- With New Zealand’s NIWA, we plan to investigate the use of WOMBAT’s posterior fluxes as boundary conditions for a regional CO$_2$ inversion over parts of Oceania


(Photo taken on the Eyre Highway in the remote Nullarbor region of Australia)