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A Bayesian approach to estimating surface fluxes with the eddy covariance method

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Abstract. Eddy covariance is the state-of-the-art technique for measuring fluxes of energy and gases between the land surface and the atmosphere. However, many processing steps sit between the data that are actually measured and the calculated flux. In practice, the data processing constitutes a modelling exercise, requiring a model of the measurement system and of the surface layer of the atmosphere. In conventional data processing, we treat the parameters of this model as known constants, and this inevitably fails to propagate the true uncertainties. In a Bayesian approach, we treat the parameters of a model (representing the biological system, measurement system and atmosphere) as uncertain parameters, which we characterise with probability distributions. We use our knowledge of the system and previous data to specify prior probability distributions for these parameters. We then update these with the data we actually observe (a high-frequency time series of turbulence components, temperature, pressure, and mixing ratios) to yield the posterior distributions for these parameters. In this way, we can produce estimates of the fluxes of interest, such as the long-term net carbon balance of an ecosystem, in the form of posterior probability distributions, in which the uncertainty is correctly represented following the axioms of conditional probability.

1 Introduction

Eddy covariance is the state-of-the-art technique for measuring fluxes of energy and gases between the land surface and the atmosphere. The technique is now widely used to measure fluxes of greenhouse gases (GHGs, CO_2, CH_4, N_2O), and to determine whether ecosystems are a long-term net sink or source of these gases.

A typical system comprises a sonic anemometer for measuring the 3-D components of wind (u, v, and w), and a gas analyser which measures the molar density c of the gas of interest (this may have an open or closed path, and use infrared or laser-based spectroscopic analysis methods). These instruments are mounted on a mast so as to be within the surface layer above the vegetation canopy. The data are recorded on a computer or data logger at high frequency (10 or 20 Hz) to capture atmospheric transport by small-scale eddies near the surface. The basis of the method is that, if a number of assumptions are met (such as horizontal homogeneity), so that all the advective and horizontal eddy flux divergence terms are zero, then the mass balance equation simplifies to the change in storage below the measurement height and the eddy covariance:

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$$\bar{F}_t = \frac{\partial c}{\partial t} + \frac{\partial \overline{w'c'}}{\partial z} \quad (1)$$

In reality there is always some spatial heterogeneity, so the advective and divergence terms will not be zero, but these are very hard to measure in practice, and are generally ignored (Lee et al., 2006). Although Equation 1 appears simple, many processing steps sit between the data that are actually measured and the calculated flux for each time period (typically a half-hourly interval) (Aubinet et al., 2012). These include: estimating the orientation of the sonic anemometer and the wind flow in any given half-hour in relation to the plane of the mean wind flow at the site; estimating the true time lag between the vertical velocity component measured by the sonic anemometer and the mixing ratio measured by the gas analyser; estimating the background rate of change in mixing ratio associated with processes other than the local surface flux, as distinct from variance as part of the local eddy flux (the first and second terms on the RHS of Equation 1); estimating the high- and low-frequency components of the eddy flux which are outwith the range detectable by the measurement system; estimating whether outlying data points are true anomalies (e.g. spikes due to electronic noise) or genuine extreme values; estimating whether the extent of turbulence is large enough to warrant calculating an eddy flux, generally based on the friction velocity, u* (Papale et al., 2006); estimating whether other criteria (e.g. skewness, kurtosis, stationarity) are met so as to justify the assumptions of Equation 1 (Papale et al., 2006).

In practice, the data processing constitutes a modelling exercise, requiring a model of the measurement system and of the surface layer of the atmosphere. Several relatively complex software tools have been developed for this purpose. Of these, the EddyPro open-source software (hosted by LICOR Environment, USA) is the most widely used (Fratini and Mauder, 2014). In the usual data processing workflow, the parameters of the model of the measurement system and of the atmosphere implicit in this software are treated as known constants for each half-hour interval.

Although efforts have been made to quantify some of the uncertainties associated with the many unknowns involved in the calculation of fluxes (e.g. Burba et al., 2008), the widespread lack of closure of the energy balance indicates that systematic uncertainties are a serious issue.

In a Bayesian approach, we treat the parameters of the model (of the measurement system and atmosphere) as uncertain parameters, which we characterise with probability distributions. We use our knowledge of the physics of the system and previous data to specify prior probability distributions for these parameters. We then update these with the data we actually observe (a high-frequency time series of turbulence components, temperature, pressure, and mixing ratios) to yield the posterior distributions for these parameters. By a simple extension, we can include a model of the biological processes governing uptake and emissions of gases (e.g. in the case of carbon dioxide, photosynthesis and respiration). In this way, we can produce estimates of the fluxes of interest, such as the long-term net carbon balance of an ecosystem, in the form of posterior probability distributions, in which the uncertainty is correctly represented following the axioms of conditional probability.

Our aims here were to develop a Bayesian approach to quantify the uncertainty in estimates of ecosystem carbon balance derived from eddy covariance data. We compare estimates of the mean flux and its uncertainty with results from conventional processing methods. We apply this in the context of estimating CO_2 fluxes over ecosystems, but the princples apply generally.

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2 Methods

Firstly, we define the components of the model system that we attempt to estimate.

2.1 Biological processes

We represent the two key physiological processes which assimilate and emit CO_2 within an ecosystem, photosynthesis and respiration. Here, we use simple empirical models with a minimal number of parameters, but in principle the same procedure could be applied with a much more complex model. Photosynthesis is represented as a hyperbolic response to light, or more correctly, to the photosynthetic photon (or quantum) flux density, Q in units of μmol m^{-2} s^{-1}. This response has an initial slope α, reaching an asymptote $P_{\max}$. Respiration is represented as an exponential response to temperature T, with a reference rate at 10 °C and a sensitivity k_T.

$$P = \frac{P_{\max}\alpha Q}{P_{\max} + \alpha Q} \tag{2}$$

$$R = R_{10}\exp(k_T(T-10)) \tag{3}$$

$$F_{\mathrm{pred}} = \overline{w'c'}_{\mathrm{pred}} = R - P \tag{4}$$

2.2 Measurement system and atmospheric surface layer

2.2.1 Geometry of the sonic anemometer and the wind flow (coordinate rotation)

The long-term net flux is defined on a hypothetical plane, equivalent to that of the long-term mean wind flow. This deviates from the horizontal because of topographical effects distorting flow. The sonic anemometer is mounted so that the w wind component in its coordinate system is close to vertical but this is only approximate, and deviations occur because of sensor movement (in the short and long terms), as well as effects of the transducers themselves distorting flow across the measurement path (Nakai et al., 2006, Nakai2012). Consequently, in each measurement interval, we need to estimate the orientation of the wind flow (as recorded by the sonic anemometer) in relation to the plane of the mean wind flow at the site. A common approximation is to rotate the wind components such that the vertical component is minimised. However, this introduces a systematic error whenever this deviates from the true mean plane, over-estimating the calculated flux. A better approach is to calculate the plane of the mean wind flow at the site using long-term wind data. The half-hourly data are then rotated into this reference frame. We do this here using the implementation of Wilczak et al. (2001), but treat the rotation parameters du, dv, dw as random variables.

2.2.2 Time lag

A small number of open-path sensors combine the sonic anemometer and gas analyser in a single instrument so as to share the same path. However, in most set-ups, the instruments are physically separated by 10 to ~50 cm, and in the case of closed-path gas analysers, involve pulling ambient air down a sample inlet tube, which may be several metres long. This introduces a time

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lag between the vertical velocity component measured by the sonic anemometer and the mixing ratio measured by the gas analyser. This will vary with several factors, including wind speed, wind direction, attributes of the pump determining flow rate (e.g. supply voltage, diagphram state), and vagaries of the data acquisition system governing electronic signal delays. This time lag is often estimated from the cross-covariance function as the time lag which yields the maximum covariance. However, whenever there is noise in the data, this can result in an erroneous time lag being identified, with a concomitant effect on the calculated flux, and can result in serious systematic errors (Langford et al., 2015). A better approach is to estimate the time lag τ as a temporally-autocorrelated random variable.

2.2.3 Background change in mixing ratio

Variation in the measured mixing ratio comes both from (i) the effects of local uptake and emissions at the surface within the footprint of the measurement tower, and (ii) the effects of surface fluxes in the wider region, advected in horizontally,as well as entrainment fluxes at the top of the boundary layer. To isolate the local flux, we need to identify the effects of the latter terms, and remove this from the total variance in the measured mixing ratio. That is, in order to correctly specify the second term on the RHS of Equation 1 (the eddy covariance), we need to estimate the background rate of change in the mixing ratio associated with processes other than the local surface flux. Common methods for doing this in conventional processing are block averaging (removing the mean within a moving window) and using linear regression to remove the linear trend in mixing ratio across the half hour. However, it is not obvious what time scale this should be applied on, nor whether the trend will be constant and linear over a half hour, and this results in uncertainty. Although we do not know the advective and entrainment fluxes, they are associated with systematic change over time, and it is the residual variation around this from which we calculate the eddy covariance. To represent this, we can apply smoothing to the time series of mixing ratio data, allowing for a greater or lesser extent of smoothness. This recognises the fact that we do not know for certain the time scale and magnitude of the signal in the background change. We represent this with a general additive model (GAM) with a variable number of knots n_k which dictate the degree of smoothness (Wood, 2006).

2.3 High- and low-frequency components

Scalars are transported by eddies with a range of time and length scales. The measurement system is limited in the range of eddies it can detect, by the frequency of data acquisition and instrument response times at the high frequency end, and by the length of the measurement interval at the low frequency end. The contribution from the unmeasured eddies is generally estimated and added on to that in the measured range. High frequency losses are often estimated with the method of Moncrieff et al. (1997). There is little consensus in accounting for low frequency losses. Here, we take the approach that the high- and low-frequency losses represent an unknown term, proportional to the measured flux, but dependent upon the relative contributions from different eddy sizes in any given half hour. This can be represented as a fractional parameter λ with prior mean as calculated by eddypro, but with uncertainty specified by a probabilty distribution.

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2.4 Implementation of Bayesian parameter estimation

We limited the analysis to a subset of data at a single field site, the UK-AMo ICOS site Auchencorth Moss in central Scotland (https://meta.icos-cp.eu/resources/stations/ES_UK-AMo), and we only show results here for 12 days (1-12th June 2012). We used the `BayesianTools` package (Hartig et al., 2017) in the R software environment to perform the Bayesian parameter estimation using the DREAM Markov Chain Monte Carlo (MCMC) algorithm (ter Braak and Vrugt, 2008). Eleven parameters were estimated, from the model of the system described above: $P_{\mathrm{max}}, \alpha, R_{10}, k_T, d_u, d_v, d_w, \tau, n_k, \lambda_{\mathrm{high}}$ and λ_{low}. The prior distributions for these were defined as truncated normal distributions. The likelihood is often calculated as the probability of the observed data given the model, assuming deviations are normally distributed, with measurement uncertainty σ. Here, the model of the biological process predicts a flux F_{pred} which gives our expectation of the covariance $\overline{w'c'}_{\mathrm{pred}}$. The observations feed into the model of the measurement system and the atmospheric surface layer, to give a calculated flux based on the observations and the model parameters (ususally referred to as an "observed" flux), $\overline{w'c'}_{\mathrm{obs}}$. The likelihood was calculated as the probability of the difference in $\overline{w'c'}_{\mathrm{pred}}$ and $\overline{w'c'}_{\mathrm{obs}}$, assuming deviations are normally distributed, with measurement uncertainty σ from the method of Finkelstein and Sims (2001). The posterior distributions for the parameters were obtained for each half hour by running 4000 iterations of the MCMC algorithm on three chains, after excluding a burn-in phase. Because of the computational expense, each half hour of data was run in parallel, so produce independent estimates of the posterior distribution, which can then be combined. Future work will include the temporal dependence among adjacent time periods, which requires running in series, but will provide better constraints on the parameters.

2.5 Implementation of standard data processing

Fluxes were also calculated by the commonly-used EddyPro software, version v7.0.9. Settings were prescribed to specify double coordinate rotation, time lag estimation by covariance maximisation, detrending by block averaging, and frequency loss correction by the method of Moncrieff et al. (1997). Random uncertainty was estimated by the method of Finkelstein and Sims (2001).

3 Results

Figure 1 shows the time series of estimated CO_2 fluxes for the 12 days. The prior distribution shows the expected diurnal pattern purely from the prescribed response to Q and T, but with a relatively wide range of possible values. Fluxes based purely on the observed data, as calculated by the EddyPro software, generally show smaller absolute fluxes (less negative and less positive) with a rather narrow range of ostensible uncertainty. The posterior distribution is intermediate between the prior values and those calculated by EddyPro, with a narrower range of uncertainty than the prior, but wider than that calculated by EddyPro. The posterior values generally agree closely with EddyPro estimates during the daytime, but deviate systematically on some days and at night.

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Figure 2 shows the posterior distribution of the cumulative net sum of the fluxes over the same 12-day period. The data provide a strong constraint, so as to narrow the distribution compared to the prior. This distribution is somewhat wider than the uncertainty estimated by EddyPro, and systematically shifted to be less negative, around 40 % of the EddyPro value.

4 Discussion

The results suggest that the biological model parameter values which are most plausible, given their agreement with the daytime observations, when fluxes are most reliable, are less consistent with the nighttime observations. Because the biological parameters do not change over short time scales, the nighttime data are better explained by variation in the parameters of the measurement system and atmospheric surface layer. The Bayesian approach can reflect this in the choice of priors. The standard processing approach takes no account of what is plausible biologically, and calculates the flux taking the data at face value, and this may deviate systematically from the true value, particularly in conditions where the assumptions for the method are poorly met. Various issues have been identified with the interpretation of nighttime eddy covariance fluxes, when turbulence may be poorly developed and topography-driven drainage flows may dominate (Yi et al., 2008). The Bayesian approach may deal with such issues better than the standard approach since it gives less weight to the observations when they are less informative.

The cumulative effect of the systematic difference, mainly at nighttime, adds up to a substantial difference in the longer-term net flux. The results remind us that eddy covariance data may contain more systematic uncertainty than we generally acknowledge; similar issues which result in the energy balance closure may affect gas fluxes, although demonstrating closure of the mass balance is much more difficult. Random uncertainties will cancel out over time, and these systematic uncertainties dominate in long-term data sets. The Bayesian method provides one means to quantify these.

The method used here is relatively simplistic, but one could add complexity to this basic model as needed for different ecosystems and over different time scales. Where the leaf area index L varies substantially, we can represent this effect by making P_{max} proportional to L. L itself is difficult to measure, but can be estimated with uncertainty from sampling on the ground, or with remotely-sensed products such as NDVI. To introduce the process of plant growth so as to make a dynamic model, we can introduce the dependence of the growth in L on the net carbon gain. This provides a physical constraint on how much L can increase in successive time steps. Senescence and leaf fall are potentially more complex, but can be approximated in the same way. Computationally, running a dynamic model makes parallelisation much more difficult, so innovative methods may be needed to make this quicker for long data sets, and this is an area of current research.

5 Figures

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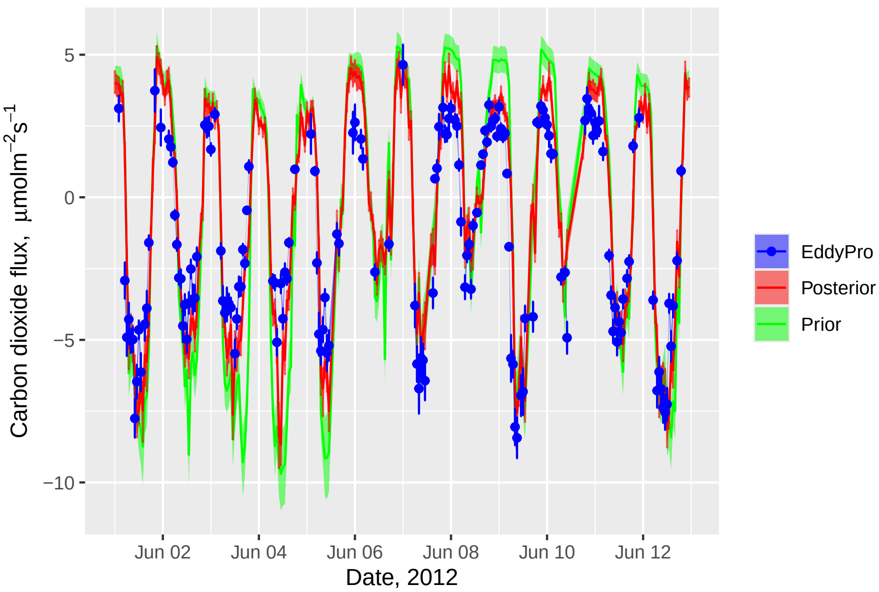

Figure 1. Time series of estimated CO_2 fluxes for the 12 days. Blue points show the estimates produced based purely on the observed time series of u, v, w and c, as calculated by the EddyPro software. The green interval shows the distribution of estimated fluxes solely on the prior distribution of the parameters in Equations 2-4. The red interval shows the posterior distribution of estimated fluxes, updated by the observed time series data.

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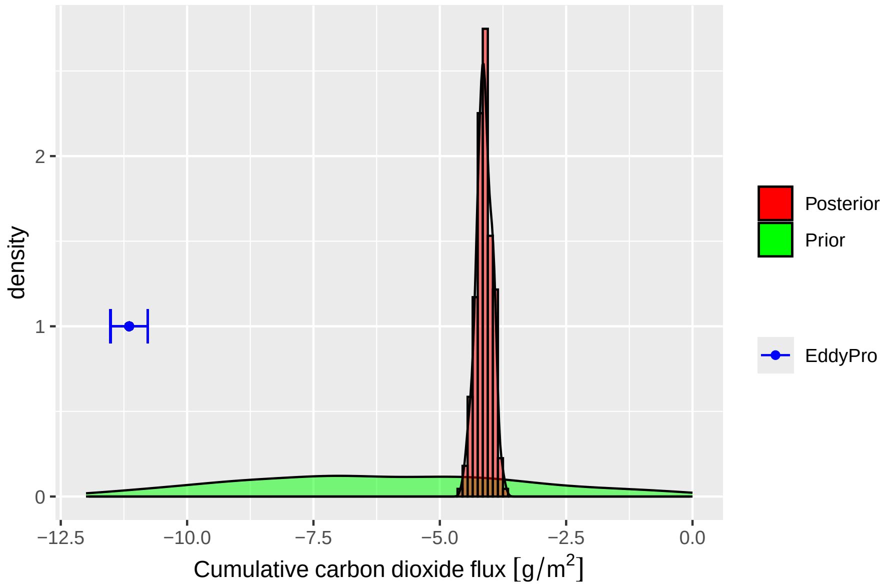

Figure 2. Distribution of the cumulative sum of the CO_2 flux over the 12-day period, estimated by the Bayesian approach and by standard data processing using the EddyPro software (blue, with error bars showing the 95% uncertainty interval from the method of Finkelstein and Sims (2001). The prior distribution (green) is largely uninformative, and is wider than the x-axis range shown here. The posterior distribution (red) is strongly constrained by the data.

. The authors declare no competing interests.

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