Gap-filling continuously-measured soil respiration data: A highlight of time-series-based methods

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A B S T R A C T

Soil respiration is an important ecosystem process that releases carbon dioxide into the atmosphere. While soil respiration can be measured continuously at high temporal resolutions, gaps in the dataset are inevitable, leading to uncertainties in carbon budget estimations. Therefore, robust methods used to fill the gaps are needed. The process-based non-linear least squares (NLS) regression is the most widely used gap-filling method, which utilizes the established relationship between the soil respiration and temperature. In addition to NLS, we also implemented three other methods based on: 1) artificial neural networks (ANN), driven by temperature and moisture measurements, 2) singular spectrum analysis (SSA), relying only on the time series itself, and 3) the expectation-maximization (EM) approach, referencing to parallel flux measurements in the spatial vicinity. Six soil respiration datasets (2017–2019) from two boreal forests were used for benchmarking. Artificial gaps were randomly introduced into the datasets and then filled using the four methods. The time-series-based methods, SSA and EM, showed higher accuracies than NLS and ANN in small gaps (<1 day). In larger gaps (15 days), the performance was similar among NLS, SSA and EM; however, ANN showed large errors in gaps that coincided with precipitation events. Compared to the observations, gap-filled data by SSA showed similar degree of variances and those filled by EM were associated with similar first-order autocorrelation coefficients. In contrast, data filled by both NLS and ANN exhibited lower variance and higher autocorrelation than the observations. For estimations of the annual soil respiration budget, NLS, SSA and EM resulted in errors between −3.7% and 5.8% given the budgets ranged from 463 to 1152 g C m−2 year−1, while ANN exhibited larger errors from −11.3 to 16.0%. Our study highlights the two time-series-based methods which showed great potential in gap-filling carbon flux data, especially when environmental variables are unavailable.

1. Introduction

The quantification of carbon (C) exchanges between natural ecosystems and the atmosphere, in the form of carbon dioxide (CO₂), has attracted great attention over the last few decades in the context of climate change (IPCC, 2013). With the development of automatic and continuous measurements at high temporal resolutions (e.g., eddy covariance), it is now possible to estimate the C budget of the ecosystems to a certain degree of accuracy and evaluate their contributions to climate change (e.g., Lu et al., 2017; Reichstein et al., 2007).

Among the key components of the C cycle in an ecosystem, soil respiration is the process that releases the CO₂ produced by roots, soil organisms and chemical oxidation into the atmosphere (Lloyd and Taylor, 1994). Soil respiration is usually measured using either static or dynamic chambers (Bekku et al., 1997; Jensen et al., 1996; Rochette et al., 1992). Automated soil respiration measurements have been performed in many studies at a temporal interval of 10–60 min (e.g., Suh et al., 2006; Wu et al., 2016). Among the approaches, the forced diffusion (FD) technique was developed based on the theory of dynamic chambers but has the advantage of low power consumption (see details in Risk et al., 2011). At the same time, FD chambers require no mechanical movement between or during measurements which allows them to operate even under snow cover (Lavoie et al., 2015). The FD chambers have been demonstrated to produce comparable results to conventional chambers under the same conditions (Risk et al., 2011). The FD technique, by producing data continuously throughout the year, provides a firm ground for estimating budgets of soil respiration in an ecosystem.

As with all automatic field measurements, missing data, due to e.g., power failure, instrumentation malfunction, disturbance during maintenance, data corruption, etc. are almost inevitable. Depending on the size and number of gaps, large uncertainties may be introduced to the
relationships (Zhang et al., 1998). ANNs have been successfully im-
put variable (soil respiration) based on the inputs (e.g., soil tem-
techniques (ANNs) use machine learning algorithms to simulate the
respiration gap-filling. As a data-driven alternative, artificial neural
et al., 2010; Mahecha et al., 2011; Schoeldammer, 2001; Shun and
mbers of squares with Satterthwaite approximation for the degrees of freedom. RMSE: root mean squared error.
Table 1
Summary of the 6 studied soil respiration datasets.

| Site     | Plot # | Period               | # of data points | Available | Missing |
|----------|--------|----------------------|------------------|-----------|---------|
| Hurdal   | H1     | 2017/7/27-2019/4/29  | 89,290           | 2972      |         |
|          | H2     | 2018/5/9-2019/3/20   | 39,974           | 5356      |         |
|          | H3     | 2017/9/18-2019/4/29  | 70,646           | 14,036    |         |
|          | H4     | 2017/9/8-2019/4/29   | 81,208           | 4905      |         |
| Løten    | L1     | 2018/6/1-2019/4/18   | 46,291           | 8         |         |
|          | L2     | 2018/3/14-2019/4/29  | 51,062           | 8148      |         |

The plot number is included in the models as random effects. SS: type III sums of squares with Satterthwaite approximation for the degrees of freedom. RMSE: root mean squared error.

Table 2
Summary of the analysis of variance (ANOVA) for the mixed effects models with RMSE as dependent variable and sampling window size, method, season, gap size and the two-way interactions between window size and the other three factors as independent variables.

| Independent variable | SS     | F-value | P-value |
|----------------------|--------|---------|---------|
| Window size          | 3.63   | 8.42    | <0.001  |
| Method               | 39.76  | 184.32  | <0.001  |
| Gap size             | 79.20  | 367.16  | <0.001  |
| Season               | 333.29 | 4636.62 | <0.001  |
| Window size*Method   | 2.44   | 1.89    | 0.013   |
| Window size*Gap size | 1.17   | 0.91    | 0.572   |
| Window size*Season   | 0.70   | 1.62    | 0.136   |

estimated C budget (Falge et al., 2001). Therefore, robust and suitable gap-filling methods are critical to ensure the accuracy of C budget esti-
respiration data gaps in six soil respiration datasets from two boreal forest sites in

In this study, we implemented the four gap-filling methods de-
scribed above, namely NLS, ANN, SSA, and EM, on artificially created data gaps in six soil respiration datasets from two boreal forest sites in Nor-

2. Material and methods

2.1. Datasets

The soil respiration datasets used in this study were collected at two forest sites in Hurdal (60°22′21″N, 11°04′41″E, 284 m a.s.l.) and Løten (60°51′33″N, 11°26′08″E, 262 m a.s.l.), southern Norway. Both sites are dominated by Norway spruce (Picea abies (L) Karst.). At Hurdal, the

Alternatively, methods using time series analysis can predict the

respiration is usually not significant in the winter (Alm et al., 1999; Liptzin et al., 2009; Merbold et al., 2012). As a result, gap-filling methods driven by environmental variables might perform poorly when being applied to winter time fluxes. This has not been investigated before.

Table 3

| Site     | Plot # | Period               | # of data points | Available | Missing |
|----------|--------|----------------------|------------------|-----------|---------|
|          |        |                      |                  |           |         |

Date format: year/month/day. Data temporal resolution: 10-min.
terrain is slightly sloping, and the soils are podzolic in the upper part and rather hydrogenic (partially waterlogged) in the lower part. The site at Løten is rather flat and contains a bog surrounded by mixed forests. The soils are loamy with a high water-holding capacity. Both sites are typically covered with snow for 4–5 months per year, with a long-term (1957–2018) annual mean air temperature of 3.9 °C for Hurdal and 3.1 °C for Løten, respectively according to the seNorge2018 database (Lussana et al., 2019). The soil respiration measurements were carried out automatically every 10-min using forced diffusion (FD) chambers (eosFDCO2, Eosense Inc., Dartmouth, NS, Canada). Specifically, each chamber is equipped with membranes allowing gases to freely diffuse into it. With different compartments, it separately measures the CO2 concentrations that represent the ambient air ($C_{\text{ambient}}$) and the air that mixes the ambient air with gases from the soil ($C_{\text{mix}}$). The soil respiration rate ($R_s$) is then calculated as (Risk et al., 2011):

$$R_s = G (C_{\text{mix}} - C_{\text{ambient}})$$

(1)

where $G$ is an empirical positive constant (a function of the gas diffusion rate through the membrane and measured soil surface area; unit: m s$^{-1}$) provided by the manufacturer. More details of the method are outlined in Risk et al. (2011). The $C_{\text{mix}}$ is larger than the $C_{\text{ambient}}$ under typical circumstances, implying a loss of CO2 from the soil (i.e., a positive flux). Since the FD chamber measures the fluxes with the same CO2 source from the soil (i.e., soil respiration) as static chambers and produces comparable soil respiration data (Risk et al., 2011), we suggest that the methods and results in this study can also be applied to the soil respiration measured by the widely used static chambers.

Along with the soil respiration, corresponding soil temperature and moisture (TMS-4, TOMST inc., Prague, Czech Republic) at 10, 20 and 50 cm depths were measured within <1 m from each chamber at the same temporal resolution (i.e., 10-min). In addition, the ambient temperatures were measured at ~5 cm above the soil surface, which represented either the temperature of the snowpack during winter time or air temperature when snow was absent. Data from a total of 6 plots (4 from Hurdal and 2 from Løten) were used for analysis. The datasets overall covered the period between July 2017 and April 2019 but varied among the plots (see details in Table 1). The soil respiration data were quality-checked before being analyzed and were rejected (marked as missing values): 1) during instrument malfunction or power failure, and 2) with implausible values (soil respiration rate < −2 or >10 µmol CO2 m$^{-2}$ s$^{-1}$). In total, 11% of the data were discarded (see Table 1 for the summary for each plot).

### 2.2. Artificial gaps

In order to compare the gap-filled data to the original observations, we created artificial gaps (flagged) in the soil respiration time series in all the 6 datasets. Specifically, we used each dataset to create four separate benchmark datasets: one with 80 one-hour gaps (6 observations per gap), a second one with 40 six-hour gaps (36 observations per gap), a third one with 30 one-day gaps (144 observations per gap), and the last one with 10 fifteen-day gaps (2160 observations per gap). The gaps
were added at random locations of the time series while avoiding overlapping with each other as well as with the original gaps in the dataset. These benchmark datasets were used to test the performance of the gap-filling methods in gaps of different sizes.

In addition, to evaluate the overall influences of different gap-filling methods on the estimations of annual soil respiration budget, we selected the datasets that were longer than 1 year (i.e., H1, H3 and H4 in Hurdal and L2 in Løten, Table 1) and extracted the data of a one-year period each from April 30, 2018 to April 29, 2019. Based on each of the extracted datasets, we created a random number of gaps with random lengths (uniformly distributed) up to 15 days (mixed gaps) that resulted in benchmark datasets with 5 levels of the gap proportion (10, 20, 30, 40 and 50%). For each of the 5 levels, 10 replicate datasets were created with different random gap arrangements (i.e., 200 benchmark datasets in total for the 4 plots, see Fig. A1 in the Appendices for an example of gap summary in the dataset). These mixed gap benchmark datasets were thereafter used for the estimation of the annual soil respiration sum after the artificial gaps have been filled.

Table 3

| Gap size | Season | NLS Intercept | Slope | ANN Intercept | Slope | SSA Intercept | Slope | EM Intercept | Slope |
|----------|--------|---------------|-------|---------------|-------|---------------|-------|--------------|-------|
| 1-h      | Non-winter | 0.170 (0.017) | 0.919 (0.009) | 0.139 (0.016) | 0.936 (0.009) | 0.014 (0.013) | 0.998 (0.008) | 0.074 (0.016) | 0.960 (0.009) |
|          | Winter  | 0.043 (0.007) | 0.956 (0.010) | 0.038 (0.007) | 0.958 (0.010) | −0.003 (0.004) | 1.007 (0.005) | 0.014 (0.005) | 0.971 (0.007) |
| 6-h      | Non-winter | 0.012 (0.010) | 1.016 (0.006) | 0.059 (0.010) | 0.966 (0.006) | −0.023 (0.010) | 1.021 (0.006) | −0.033 (0.011) | 1.028 (0.009) |
|          | Winter  | 0.045 (0.004) | 0.935 (0.006) | 0.046 (0.004) | 0.942 (0.006) | −0.009 (0.003) | 1.010 (0.004) | 0.012 (0.009) | 0.978 (0.006) |
| 1-day    | Non-winter | 0.149 (0.007) | 0.923 (0.004) | 0.075 (0.006) | 0.966 (0.004) | 0.062 (0.008) | 0.949 (0.005) | 0.097 (0.003) | 0.948 (0.004) |
|          | Winter  | 0.051 (0.002) | 0.920 (0.005) | 0.045 (0.002) | 0.925 (0.005) | 0.006 (0.002) | 0.977 (0.004) | 0.025 (0.007) | 0.955 (0.004) |
| 15-day   | Non-winter | −0.055 (0.004) | 1.108 (0.003) | −0.297 (0.009) | 1.182 (0.005) | −0.236 (0.006) | 1.177 (0.004) | −0.130 (0.006) | 1.170 (0.004) |
|          | Winter  | 0.066 (0.002) | 0.914 (0.003) | 0.097 (0.002) | 0.920 (0.003) | 0.010 (0.002) | 0.979 (0.003) | 0.029 (0.002) | 0.977 (0.003) |

Standard errors of the coefficients are shown in the parentheses.

Fig. 2. Predicted values for the gaps of 1-h. (1 h, a–d), 6-h. (6 h, e–h), 1-day (1d, i–l) and 15-day (15d, m–p) by NLS (a, e, i, m), ANN (b, f, j, n), SSA (c, g, k, o) and EM (d, h, l, p) as a function of the corresponding observations. Non-winter and winter seasons are plotted in red and blue, respectively. Total least squares regression was used to accommodate the uncertainty of both dependent and independent variables. The black solid and dashed lines indicate the regressions for non-winter and winter seasons, respectively. The gray dashed lines indicate the 1:1 ratio. The coefficients of the regressions are presented in Table 3. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)
making the models (Lloyd and Taylor, 1994): compare other methods with. The Lloyd-Taylor function was used for Kunwor et al., 2017; Moffat et al., 2007), we took it as a reference to between soil temperature and soil respiration. Since NLS is the most gaps.

2.4. Gap-filling methods

includes the gap itself and may suffer from insufficient training data if the gap length. The shortest window length that a achieved best accuracy around the gap for training the models could have a significant influence on the accuracy of the gap-filled values, choosing a sampling window length that includes proper training data is important. In this study, we compared the performance of the gap-filling methods using sampling windows of 5, 10, 20, 30, 40, 50 and 60 days (i.e., 720, 1440, 2880, 4320, 5760, 7200, 8640 observations, respectively), arranged symmetrically around the gap. A sampling window of 10 days, for example, included data of 5 days before and after the gap, regardless of the gap length. The shortest window length that achieved best accuracy was chosen for each method. This sampling window is more flexible than the traditional fixed window (Moffat et al., 2007), which also includes the gap itself and may suffer from insufficient training data if the gap size approaches the sampling window size.

2.4. Gap-filling methods

Each of the gap-filling methods has its own algorithm to build models trained by available data around each gap, and the models were then used to predict the values in the gap. Since the data sampled around the gap for training the models could have a significant influence on the accuracy of the gap-filled values, choosing a sampling window length that includes proper training data is important. In this study, we compared the performance of the gap-filling methods using sampling windows of 5, 10, 20, 30, 40, 50 and 60 days (i.e., 720, 1440, 2880, 4320, 5760, 7200, 8640 observations, respectively), arranged symmetrically around the gap. A sampling window of 10 days, for example, included data of 5 days before and after the gap, regardless of the gap length. The shortest window length that achieved best accuracy was chosen for each method. This sampling window is more flexible than the traditional fixed window (Moffat et al., 2007), which also includes the gap itself and may suffer from insufficient training data if the gap size approaches the sampling window size.

2.5. Statistical analysis

The performance of the gap-filling methods was investigated separately in the winter and other periods of the year. Since the snow was not monitored at the sites, we defined the winter as the period with soil temperature <1.5 °C and the remaining period as non-winter. This criterion well separated each year into two seasons and characterized the winter by low soil temperature with a narrow variation range (<5% in total). Similarly, EM was not applied to gap-fill the mixed gap benchmark datasets from the plot L2 in Løten for determining the annual budget, due to the lack of a full year data at plot L1 as the reference. The EM gap-filling was performed using the R package “mtsdi” (Junger and Ponce de Leon, 2018).

Lastly, we implemented the method developed by Junger and Ponce de Leon (2015) based on the expectation-maximization (EM) algorithm (Dempster et al., 1977). This method takes multiple other parallelly measured soil respiration time series as references for the target gap-filling series and makes predictions accounting for both the correlation among the series and temporal structure of individual series. In this study, all the parallel soil respiration time series (no artificial gaps) that reached a certain degree of correlation with the target series (i.e., r > 0.75; see Table A1 for the correlations among the plots) from the same site (Hurdal or Løten) were used as references. We used the “spline” method to fit the time series at each iteration with a degree of freedom of 10 (chosen by cross validation). Due to the unequal data temporal range among the plots, the gaps located out of the temporal range of the references were not filled and excluded in further analyses (<5% in total). Similarly, EM was not applied to gap-fill the mixed gap benchmark datasets from the plot L2 in Løten for determining the annual budget, due to the lack of a full year data at plot L1 as the reference. The EM gap-filling was performed using the R package “mtsdi” (Junger and Ponce de Leon, 2018).

Table 4. Summary of the analysis of variance (ANOVA) for the mixed effects models with RMSE, relative error, AR (1) and variance as dependent variables and method, season, gap size and their two-way interactions as independent variables.

| Dependent variable | Independent variable | SS  | F-value | P-value |
|--------------------|---------------------|-----|---------|---------|
| RMSE               | Method              | 0.27| 1.72    | 0.161   |
|                    | Season              | 41.81| 791.66 | <0.001  |
|                    | Gap size            | 15.43| 97.411 | <0.001  |
|                    | Method*Season       | 0.30| 1.90    | 0.128   |
|                    | Method*Gap size     | 1.57| 3.29    | <0.001  |
| Relative error     | Method              | 0.40| 1.95    | 0.119   |
|                    | Season              | 14.98| 217.81 | <0.001  |
|                    | Gap size            | 6.35| 30.75   | <0.001  |
|                    | Method*Season       | 0.21| 1.00    | 0.394   |
|                    | Method*Gap size     | 1.14| 1.83    | 0.057   |
| Variance           | Method              | 3.37| 25.99   | <0.001  |
|                    | Season              | 3.89| 119.77  | <0.001  |
|                    | Gap size            | 11.12| 114.28 | <0.001  |
|                    | Method*Season       | 1.61| 12.37   | <0.001  |
|                    | Method*Gap size     | 4.28| 10.98   | <0.001  |
| AR (1)             | Method              | 25.62| 47.32  | <0.001  |
|                    | Season              | 39.06| 288.60 | <0.001  |
|                    | Gap size            | 271.34| 668.25 | <0.001  |
|                    | Method*Season       | 18.56| 34.28  | <0.001  |
|                    | Method*Gap size     | 18.33| 11.28  | <0.001  |

The plot number is included in the models as random effects. SS: type III sums of squares with Satterthwaite approximation for degrees of freedom. RMSE: root mean squared error. AR (1): first order autocorrelation coefficient. The sampling window length of 5 days was used.

The Lloyd-Taylor function was used for making the models (Lloyd and Taylor, 1994):

\[ R_s = R_{10}e^{\left(\frac{1}{T_{ref} - T_0} - \frac{1}{T - T_0}\right)} \]  

(2)

where \( R_{10} \) and \( E_0 \) are parameters to be estimated, \( T_{ref} \) and \( T_0 \) take the values of 283.15 and 227.13 K, respectively, following Lloyd and Taylor (1994), and \( T_s \) is the soil temperature measured at 10 cm depth (K). The NLS regression was performed by applying the Levenberg-Marquardt algorithm using the “minpack.lm” package (Elzhov et al., 2016) in the program R 3.5.2 (R Development Core Team, 2018). In cases when the variance of soil temperature in the winter was too low for the NLS function to fit with, the mean value of the soil respiration rate within the sampling window was taken to fill the gap (71% of the gaps in the winter).

Secondly, to include environmental variables other than the soil temperature, artificial neural network (ANN) models similar to Moffat et al. (2010) were implemented to fill the gaps. The inputs of the ANN models were soil temperature, soil moisture and ambient temperature (i.e., either snow temperature in the winter or air temperature in non-winter periods), and the output was soil respiration rate. The input variables were normalized to be centered around 0 with a standard deviation of 1 before used to train the models. We included one hidden layer with two neurons in the models and a back-propagation algorithm was performed using the R package “neuralnet” (Fritsch et al., 2019).

Thirdly, being independent of the variations of other environmental variables, the singular spectrum analysis (SSA) method analyzes the structure of the soil respiration time series and predicts the missing values in the gap. In this study, we used the iterative approach suggested by Kondrashov and Ghil (2006) to determine the major periodic component of the time series in the sampling windows and projected this periodic component into the gaps. In addition to the major periodic (i.e., low frequency) component, we also extracted the high frequency component (i.e., the eigentriples with periodicity band < 10, unit: 10-min) of the time series in the sampling window and added its average diurnal variations to the projected low frequency values in the gap at the corresponding time of the day. This approach takes both low and high frequency components derived from the time series into account for the gap-filled data. The SSA was conducted using the R packages “spectral.methods” (Buttlar, 2015) and “Rssa” (Golyandina et al., 2015).

Lastly, we implemented the method developed by Junger and Ponce de Leon (2015) based on the expectation-maximization (EM) algorithm (Dempster et al., 1977). This method takes multiple other parallelly measured soil respiration time series as references for the target gap-filling series and makes predictions accounting for both the correlation among the series and temporal structure of individual series. In this study, all the parallel soil respiration time series (no artificial gaps) that reached a certain degree of correlation with the target series (i.e., \( r > 0.75 \); see Table A1 for the correlations among the plots) from the same site (Hurdal or Løten) were used as references. We used the “spline” method to fit the time series at each iteration with a degree of freedom of 10 (chosen by cross validation). Due to the unequal data temporal range among the plots, the gaps located out of the temporal range of the references were not filled and excluded in further analyses (<5% in total). Similarly, EM was not applied to gap-fill the mixed gap benchmark datasets from the plot L2 in Løten for determining the annual budget, due to the lack of a full year data at plot L1 as the reference. The EM gap-filling was performed using the R package “mtsdi” (Junger and Ponce de Leon, 2018).

2.5. Statistical analysis

The performance of the gap-filling methods was investigated separately in the winter and other periods of the year. Since the snow was not monitored at the sites, we defined the winter as the period with soil temperature <1.5 °C and the remaining period as non-winter. This criterion well separated each year into two seasons and characterized the winter by low soil temperature with a narrow variation range (mostly 0–1 °C).
calculated as:

$$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^{n} (P_i - O_i)^2}$$  \hspace{1cm} (3)$$

where $n$ is the number of data points in the gap, and $P_i$ and $O_i$ are the predicted (gap-filled) and observed soil respiration rates ($\mu$mol CO$_2$ m$^{-2}$ s$^{-1}$), respectively. A linear mixed-effects model was used to investigate the effects of sampling window size, gap-filling method, season, gap size and the interactions between window size and each of the other three factors on RMSE. Plot ID was included as random effect in the model. Normality and homoscedasticity of the model were evaluated visually by plotting residuals. The post-hoc Tukey HSD test was used to further investigate the differences among the groups of the significant effects. The smallest window size associated with the lowest RMSE was chosen for each method for further analyses.

With the gaps filled using the optimal sampling windows, we further calculated relative error, variance and first order autocorrelation coefficient (AR (1)), in addition to RMSE (Eq. (3)), for each gap to evaluate the performance of the gap-filling methods. They are given as follows:

$$Relative \ error = \frac{\sum_{i=1}^{n} |P_i - O_i|}{\sum_{i=1}^{n} |P_i|}$$ \hspace{1cm} (4)$$

$$Variance = \frac{1}{n} \sum_{i=1}^{n} (PO_i - \overline{PO})^2$$ \hspace{1cm} (5)$$

$$AR(1) = r(PO_t, PO_{t+1})$$ \hspace{1cm} (6)$$

where $PO_i$ is either the predicted (gap-filled) or observed soil respiration rate ($\mu$mol CO$_2$ m$^{-2}$ s$^{-1}$) and $\overline{PO}$ is the mean of the rates in each gap. AR (1) is the Pearson Correlation Coefficient ($r$) between the time series in the gap ($OP_i$) and the series itself with a lag of one-time step (i.e., 10-min) ($PO_{i+1}$). Variance and AR (1) were calculated separately for the gap-filled and observed values. The gaps that were filled with the mean value of the sampling window in the winter were excluded in the AR (1) calculations for NLS. Linear mixed-effects models were established to determine the effects of the method, season, gap size and their two-way interactions on RMSE, relative error, variance and AR (1) with the random effect of plot ID.

The relationships between the observations and the gap-filled values were fitted by linear regressions using the total-least-squares approach to account for variances of both the dependent and independent variables. We assumed that the residue variance of the gap-filled values was the same as the observations (i.e., the variance ratio was set to 1). The regression slopes were used to indicate systematic bias of each method in different gap sizes and seasons. The standard errors of the regression coefficients were estimated by bootstraps (1000 random replicates).

In addition, we also calculated the Nash-Sutcliffe Efficiency (NSE)

$$Fig. 3.$ The RMSE for the gap-filled values of different gap sizes (1 h: 1-h, 6h: 6-h, 1d: 1-day, 15d: 15-days) predicted by different methods. The boxplots are plotted as in Fig. 1. Different lowercase letters indicate significant differences in RMSE among the different methods in (a–d) and among different gap sizes in (e–h) ($P < 0.05$).
The relative error was significantly different among seasons (P < 0.01) and gap sizes (P < 0.01) (Fig. 3b–d). The difference was present in the 1-h gap where the relative error was the greatest RMSE being present in the window of 30, 50 and 60 days, respectively, compared to the 5-day window (P < 0.05) (Fig. 3a). While the RMSE of SSA was also significantly lower than that of NLS (P > 0.05) for the other 3 methods (P < 0.01) (Fig. 3b–d). Therefore, the 5-day window, which is the smallest window size associated with the lowest RMSE for all the four gap-filling methods, was chosen in this study for further analysis.

3.2. Performance of the gap-filling methods

The relative error was significantly different among seasons (P < 0.01) and gap sizes (P < 0.01) but not among different methods in general (P = 0.16). However, differences of the RMSE were present among the methods when considering the interaction with the gap size (P < 0.01) but not when considering the season (P = 0.13). The difference was present in the 1-h gap where the results from SSA showed significantly lower RMSE than those from the other 3 methods (P < 0.01) (Fig. 3a). While the RMSE of EM was also significantly lower than that of NLS (P < 0.05), ANN resulted in similar RMSE as NLS (P > 0.05). For the gap sizes of 6-h, 1- and 15-day, the RMSE from ANN, SSA and EM were not significantly different from NLS (P > 0.05) (Fig. 3b–d).

All the four methods generally showed significantly greater RMSE as gap size increased from 1 h to 15 days (Fig. 3e–h). For NLS and ANN, the RMSE remained similar in gaps ≤ 1 day (P > 0.05) while the RMSE became significantly higher in the 15-day gaps (P < 0.01) (Fig. 3e and f). The RMSE of SSA showed much higher sensitivity to gap size changes with a significant RMSE increase with every step of gap enlarging from 1-h to 15-day (P < 0.01) (Fig. 3g). The RMSE of EM showed a similar pattern with significantly lower values exhibited in 1-h gaps than in 15-day gaps (P < 0.01) while 15-day gaps had the greatest RMSE (P < 0.01) (Fig. 3h).

The relative error was significantly different among seasons (P < 0.01) and gap sizes (P < 0.01), but not among the methods (P = 0.12) (Table 4). The interactions of method with season

program R 3.5.2 (R Development Core Team, 2018). In addition, the packages “lme4” (Bates et al., 2015) and “lmerTest” (Kuznetsova et al., 2016) were used to estimate linear mixed-effects models, the “emmeans” package was used for the post-hoc Tukey HSD test (Lenth, 2019), the “MethComp” package was used to perform regressions with the total-least-squares approach (Carstensen, 2015), and “ggplot2” package was used for plotting graphs (Wickham, 2016). The R code to perform the gap-filling with the four methods in this study is incorporated into the R package “FluxGapsR” freely available at https://github.com/junbinzhao/FluxGapsR/.

3. Results

3.1. Effect of sampling window size

According to the mixed-effects model (Table 2), the sampling window size showed a significant effect on the RMSE of the gap-filling results (P < 0.01). This window size effect differed among the methods (P = 0.01), but not among the gap sizes (P = 0.57) or the seasons (P = 0.14). Of the four methods, NLS, ANN and EM showed slight increases in RMSE along the window size gradient from 5 to 60 days with significantly higher values of RMSE being present in the window of ≥30, 50 and 60 days, respectively, compared to the 5-day window (P < 0.05) (Fig. 1a, b and d). In contrast, SSA showed no significant changes in RMSE with different sampling window sizes (P > 0.05) (Fig. 1c).

3.2. Performance of the gap-filling methods

The scatterplots of the gap-filled (predicted) soil respiration values versus the original observations generally followed the 1:1 line in the gaps ≥ 1 day (Fig. 2). While the corresponding regression slopes for SSA and EM were between 0.95 and 1.03, the slopes for NLS and ANN occasionally dropped down to 0.92 (Table 3), indicating a slight underestimation. For the 15-day gaps, all the methods generally overestimated the values in the non-winter gaps (i.e., regression slope > 1.1, Fig. 2m–p and Table 3). For the winter gaps, SSA and EM exhibited slopes of 0.98 but NLS and ANN slightly underestimated the flux values in the gaps (i.e., slopes were 0.91 and 0.92, respectively).
Furthermore, even though the RMSE was generally lower in the winter gaps compared to those in the non-winter \( (P < 0.01) \) (Fig. 4a), the relative errors were significantly higher in the winter than in the non-winter for the 1-h, 1- and 15-day gaps \( (P < 0.05) \) (Fig. 4b). The greatest relative error was present in the winter 15-day gaps.

The mixed-effects model for the variance showed significant effects of method, season, gap size as well as the two-way interactions of method with season and gap size \( (P < 0.01) \) (Table 4). Among the four methods, only SSA resulted in similar variance in the gap-filled values compared to the original observations across the seasons and the gap sizes \( (P > 0.05) \) (Fig. 5). The variances of the values filled by other 3 methods were overall much lower than those of the observations \( (P < 0.05) \), particularly for the winter gaps \( (P < 0.05) \) (Fig. 5e–h). Exceptions are the non-winter 15-day gaps filled by ANN, which also showed similar level of variance as the observations \( (P > 0.05) \) (Fig. 5d).

The AR (1) were affected by method, season, gap size as well as the two-way interactions of method with season and gap size \( (P < 0.01) \) (Table 4). Of the four methods, EM outputted data series with similar AR (1) to the original observations \( (P > 0.05) \), except for the 6-h and 1-day gaps in the winter (Fig. 6). NLS also resulted in similar AR (1) structure as the observations in the winter gaps of \( \leq 1 \) day \( (P > 0.05) \) when excluding those filled using the mean values in the sampling windows (Fig. 6e–g). AR (1) of the data series generated by SSA were similar to the observations only in 1-h gaps (Fig. 6a and e) and the winter 6-h gaps (Fig. 6f). ANN produced data series with significantly higher AR (1) than the observations in all cases \( (P < 0.01) \) (Fig. 6).

The NSE were \( >0.85 \) in the gaps of \( \leq 1 \) day for all the methods, among which the NSE values of SSA and EM were \( >0.95 \) in the 1-h gaps (Table 5). The NSE values dropped below 0.8 in the 15-day gaps for all the methods with the values being \( <0.7 \) for ANN in the winter and EM in the non-winter periods and being even \( <0.6 \) for ANN in the non-winter periods. The more comprehensive index KGE, which considers accuracy, bias and variance of the gap-filled data, showed a similar pattern as the NSE (Table 5). Specifically, KGE values were \( >0.9 \) for gaps \( \leq 1 \) day for all the methods and the values were even \( \geq 0.95 \) for SSA and EM in the 1- and 6-h gaps. In the 15-day gaps, lower KGE values were present, which ranged between 0.8 and 0.9.
3.3. Annual budget estimation

The annual soil respiration budget was estimated to be 1152, 463, 627 and 865 g C m\(^{-2}\) year\(^{-1}\), respectively, at the plot H1, H3, H4 in Hurdal and L2 in Løten during April 30, 2018–April 29, 2019 based on the observations (Fig. 7). By filling the mixed artificial gaps in the datasets, the corresponding annual soil respiration budget estimations ranged 1108–1136, 449–475, 598–646 and 767–955 g C m\(^{-2}\) year\(^{-1}\), respectively, for the four plots. Overall, the errors of budget estimations tended to be larger as the proportion of gaps increased. For different gap-filling methods, the overall budget errors were −3.7 to 3.6%, −11.3 to 16.0%, −3.7 to 5.8% and −3.2 to 5.3%, respectively, for NLS, ANN, SSA and EM. Significant biases only occurred in the H3 and L2 datasets with 50% gaps (Fig. 7b and d). Specifically, NLS and ANN overestimated the budget in the L2 dataset (\(P < 0.05\)), while NLS and SSA underestimated the budget in the H3 dataset (\(P < 0.05\)).

![Fig. 6. The AR (1) coefficient of the gap-filled values predicted by different methods in gaps of different sizes (1 h: 1-h, 6 h: 6-h, 1d: 1-day, 15d: 15-days) as compared to variance of the observations. The AR (1) coefficients are shown separately for the winter (a–d) and the non-winter (e–h) with different scales. The boxplots are plotted as in Fig. 1. Different lowercase letters indicate significant differences in AR (1) coefficient among different methods (\(P < 0.05\)). Note that the gaps failed to be filled with NLS (but filled with the average of the sampling window) in the winter are not included in the AR (1) calculations (e–h).](#)

### Table 5
Nash-Sutcliffe efficiency (NSE) and Kling-Gupta Efficiency (KGE) for the gap-filled values predicted using different methods.

| Gap size | Season | NSE | KGE |
|----------|--------|-----|-----|
|          |        | NLS | ANN | SSA | EM | NLS | ANN | SSA | EM |
| 1-h      | Winter | 0.89 | 0.90 | 0.97 | 0.96 | 0.92 | 0.93 | 0.98 | 0.97 |
|          | Non-winter | 0.93 | 0.94 | 0.97 | 0.96 | 0.91 | 0.93 | 0.99 | 0.95 |
| 6-h      | Winter | 0.89 | 0.90 | 0.94 | 0.96 | 0.92 | 0.92 | 0.97 | 0.97 |
|          | Non-winter | 0.91 | 0.92 | 0.94 | 0.93 | 0.95 | 0.95 | 0.97 | 0.96 |
| 1-day    | Winter | 0.89 | 0.89 | 0.88 | 0.91 | 0.91 | 0.92 | 0.94 | 0.94 |
|          | Non-winter | 0.90 | 0.92 | 0.89 | 0.91 | 0.92 | 0.95 | 0.93 | 0.94 |
| 15-day   | Winter | 0.76 | 0.69 | 0.76 | 0.79 | 0.85 | 0.83 | 0.88 | 0.89 |
|          | Non-winter | 0.78 | 0.58 | 0.72 | 0.69 | 0.88 | 0.85 | 0.80 | 0.84 |
advantage and their accurate annual budget estimations, we suggest SSA and EM to be considered as alternatives to the more conventional methods (e.g., NLS) for gap-filling in soil respiration data and possibly in other carbon flux data (e.g., net ecosystem CO$_2$ exchange measured by eddy covariance, methane fluxes, etc.), especially when the controlling environmental variables are unavailable, missing or unknown.

4.1. The accuracy of the gap-filling methods

In our study, we selected the sampling window size of 5 days, because this window size already achieved the most accurate results for all the methods. Previous studies commonly use sampling windows ranging from half a month up to a full year depending on the method used (e.g., Kunwor et al., 2017; Moffat et al., 2007; Zhao and Huang, 2015), which might not be necessary according to our result. Our result implies that a smaller sampling window that captures the local data structures or relationships around the gap can be more representative for the gap than one that includes data of longer periods. Using a smaller sampling window also significantly reduces the computing time for the methods involving iterations (e.g., ANN). However, we do not recommend windows that are smaller than 5 days, because they may simply underrepresent the diurnal variation of the variables in the gap if e.g., only 1 day before and 1 day after the gaps are considered. In addition, it is worth to note that our datasets have a temporal resolution of 10 min, which is three times as many as the commonly used 30-min interval flux datasets in a 5-day window. Thus, we further aggregated the 10-min-interval data by averaging data within each half hour and generated datasets with 30-min intervals. The gap-filling results on the aggregated datasets also indicated that the 5-day sampling window had the lowest RMSE among the window sizes for all the methods (see Fig. A2 in the Appendices). Therefore, we suggest a 5-day sampling window could be suitable for most gap-filling procedures on carbon flux data.

Among the four methods, NLS is the most widely accepted method for carbon flux gap-filling since it is usually supported by well-acknowledged relationships between the flux and environmental factors, such as the one between soil respiration and temperature used in this study (Gomez-Casanovas et al., 2013; Lloyd and Taylor, 1994). This method provides the basis to evaluate the other methods. Compared to NLS, ANN models were trained against more environmental variables (i.e., soil moisture and ambient temperature); however, it showed no improvement over NLS in terms of the RMSE (Fig. 3a–d). A previous study that included soil moisture in soil respiration gap-fillings also reached the same conclusion (Gomez-Casanovas et al., 2013). This is mainly because the controls of soil moisture over soil respiration are complicated and depend on many other factors (e.g., time, microbial communities, etc.) (Cook and Orchard, 2008). Particularly in this study, we found large prediction errors by ANN associated with the pulse in soil moisture induced by precipitation events that occurred in the gaps or the sampling windows (see Fig. 8 for examples). Depending on when those pulses occurred as well as their magnitude, gap-filled values predicted by ANN could greatly over- or under-estimate the fluxes in the gaps due to a mismatch of the soil moisture magnitudes in the gaps to those in the sampling windows. These large errors were also reflected in the lower NSE values in the 15-day gaps (Table 5) and the large uncertainties in soil respiration budget estimations by ANN (Fig. 7). Yet, models that better represent soil moisture in soil respiration gap-filling are still needed.

The SSA yielded the smallest errors among the methods in the small gaps (i.e., 1-hour) and outcompeted NLS (Fig. 3a), suggesting that SSA is a highly robust method for filling small gaps. In larger gaps, SSA could also capture the diurnal pattern and well construct the data series in the gap close to the observations if the variation pattern persisted throughout the gap (see Fig. 9a for an example). However, drifts in the diurnal patterns and magnitudes of soil respiration, which are driven by environmental factors, often occur in larger gaps (e.g., Fig. 9b). Without
referring to environmental variables, these drifts in the gap could be hardly predicted by SSA (but could be predicted by NLS and ANN), and, thus, introduced large errors in the gap-filled values. In addition to the gap size, the completeness of the data in the sampling windows also plays a big role in the SSA predictions. Without sufficient data to construct the diurnal pattern, a “blind guess” by SSA can deviate well away from the observations (e.g., Fig. 9c). A high gap proportion (e.g., 50%) significantly increases the chances of incomplete data in the sampling window. This can increase the errors of the budget estimation with SSA, as shown, for example, in the H3 mixed-gap dataset (Fig. 7b). Therefore, caution needs to be taken when applying SSA for large gaps or highly fragmented datasets.

EM is a method whose performance relies on the relationship between the target time series and the references (Junger and Ponce de Leon, 2015). For our datasets, the accuracy of EM was higher than that of NLS in the 1-hour gaps but not in larger gaps (Fig. 3a–d). This may be partly due to the heterogeneity of our sites where time series considerably deviated from each other ($r < 0.85$, Table A1). A better accuracy from EM is expected in cases when more closely related time series are available to be used as references. Nevertheless, EM provides a practical approach to gap-fill missing data when parallel measurements are available, which is common for measurements such as soil respiration when multiple replicates are needed.

Due to the limited variations under the snow cover, soil temperature and soil respiration usually decouple from each other during the winter (Alm et al., 1999; Liptzin et al., 2009; Merbold et al., 2012). As expected, the NLS could not be applied to up to 71% of the small winter gaps in this study because of the low variance of the soil temperature. Compared to NLS, the time-series-analysis-based methods (i.e., SSA and EM), which were implemented independent of the soil temperature, achieved a better accuracy in gaps ≤ 6 h and less biased predictions in the 15-day gaps in the winter. Even though the RMSE in the winter was generally much lower than in the non-winter season, larger relative errors were present in the winter gaps. This suggests that the errors introduced by filling winter gaps can account for a large fraction of the annual budget in higher latitude ecosystems when the winter contribution is a significant component (Alm et al., 1999; Aurela et al., 2002; Groffman et al., 2006; Zhao et al., 2016). According to our results, gap-filling methods that are based on time series analysis (i.e., SSA and EM), rather than the more conventional NLS approach, are recommended in ecosystems with substantial winter contributions.

4.2. Data structure restoration

The time series analyses are useful tools in ecology studies; however, they are usually very sensitive to gaps in the data (Barnea et al., 2008). In addition to achieving low errors, gap-filled data that restore the original structure of the time series can potentially be further used in time series analysis for, e.g., forecasting (Kohn and Ansley, 1986). Variance and AR (1) are two important structural properties of time series data (Box et al., 2015). In our study, the conventional method NLS as well as ANN largely underestimated the variances, especially during the winter time (Fig. 5). This is because the structures of their predicted data series closely followed the corresponding environmental variables, which usually have much lower variances than the flux data (Kunwori et al., 2017). The data series produced by EM were also low in variances and this is mainly due to the relatively low degrees of freedom (i.e., 10) we chose for spline constructions to achieve better
accuracy. In contrast, only SSA, which considered the high frequency signal of the data in the sampling window, restored the variance to the same level as the observations.

For AR(1), we found the gap size showed a significant effect, which was mainly due to the systematic errors introduced to the auto-correlation coefficient estimations when sample size was small, known as finite size effects. The finite size effect is most evident in the observations of 1-hour gaps ($n = 5$) which had large variances that covered the full range from $-1$ to $1$, and, thus, hardly represented the AR(1) structure of the original time series. Apart from the 1-h gaps, only EM attained the same level as the observations in most cases (Fig. 6) mainly because of the similar AR(1) structures between the target series and the references. In contrast, the other 3 methods all over-estimated the AR(1). It is worth to note that even though the predictions from NLS showed lower AR(1) in the winter time to roughly the same degree as the observations, this low AR(1) was largely caused by the low winter soil temperature variances and, also, that 71% of the gaps with extremely low temperature variances were excluded in AR(1) calculations for NLS. Given that the AR(1) became much larger than the observations in the non-winter season, we suggest the capability of NLS to reproduce the AR(1) is limited, which agrees with Kunwor et al. (2017).

Overall, SSA and EM can restore the original structure of the data in certain respects. Nevertheless, to restore the full structural properties of the data is challenging and new methods are still needed.

5. Conclusions

All the four studied methods achieved good accuracy in estimating the annual soil respiration budget. However, they all have different strengths and weaknesses which need to be considered when used for gap-filling in different situations. NLS is a widely used method; however, due to its poor performance in the winter (i.e., failing to fit the equation and lack of variance), ecosystems with substantial winter contributions should consider other alternatives for gap-filling, at least during the winter. In contrast, SSA has great advantages (i.e., good accuracy, variance and less bias) for winter gaps, especially the small ones. Also, because SSA is independent from environmental variables, it can be implemented even when the driving variables are unavailable, missing or even unknown. Compared to SSA, implementation of EM is more limited by the availability of the corresponding reference data. With a highly related reference dataset, EM is also a reliable option to be used without involving environmental variables. ANN is a flexible approach to include other potential driving factors in the gap-filling models without specifying the exact mathematical formulation. However, its performance may suffer under certain conditions (e.g., a precipitation event). At the same time, the long computing time of ANN compared to its (usually disproportional) improvement in the accuracy over NLS must also be considered.

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Appendices

Figs. A1-A2 and Table A1.
Fig. A1. Summary of the gap number and their sizes in the benchmark mixed gap datasets at the plot H1 in Hurdal. Columns indicate gap proportion from 10% to 50% and rows indicate 10 replicate datasets (R1–R10) for each gap proportion level. See Method and Materials Section 2.2 for details.
Fig. A2. The RMSE for the gap-filled values as a function of the sampling window size using different methods for the datasets that were aggregated to achieve a temporal resolution of 30-min. The bottom and top of a box indicate the lower and upper quartiles, respectively, and the horizontal line within the box is the median. The lower and upper whiskers are the 10th and 90th percentiles, respectively. Different lowercase letters indicate significant differences in the RMSE among different sampling window sizes (P < 0.05).

Table A1
Correlation matrix of the soil respiration time series.

| Site     | Plot ID | Hurdal | | | | | Løten |
|----------|---------|--------|---|---|---|---|---|---|
|          |         | H1     | H2 | H3 | H4 | L1 | L2 |
| Hurdal   | H1      | –      | 0.57| 0.81| 0.78| –  | –  | –  |
|          | H2      | 0.57   | –   | 0.84| 0.65| –  | –  | –  |
|          | H3      | 0.81   | 0.84| –   | 0.83| –  | –  | –  |
|          | H4      | 0.78   | 0.65| 0.83| –   | –  | –  | –  |
| Løten    | L1      | –      | –   | –  | –  | 0.83| –  | –  |
|          | L2      | –      | –   | –  | –  | –  | –  | –  |

Pearson correlation coefficients (r) are shown among plots from the same site. Only those relationships with r > 0.75 (in bold) were taken for gap-filling the in the expectation-maximization (EM) method (see details in the Method and Materials Section 2.4).

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