COdos: CO2 Correction Tools

Installation

You can install the released version of codos from CRAN with:

```
install.packages("codos")
```

And the development version from GitHub with:

```
# install.packages("devtools")
devtools::install_github("special-uor/codos", "dev")
```

Background:

Vapour-pressure deficit (vpd)

vpd is given by mean daily growing season temperature, tmp [°C] and moisture index, mi [-]. Using the CRU TS 4.04 dataset (University of East Anglia Climatic Research Unit et al. 2020) we found the following relation:

$$\mathsf{vpd} = 4.589 \times \exp(0.0611 \times \mathsf{tmp} - 0.87 \times \mathsf{mi})$$

The steps performed were:

1. Generate a monthly climatology for the period between 1961 and 1990 (inclusive). Variables used: cld, pre, tmn, tmx, vap.

```
# Monthly climatology for `tmn`
codos::monthly_clim("cru_ts4.04.1901.2019.tmn.dat.nc", "tmn", 1961, 1990)
```

Output file:

```
"cru_ts4.04.1901.2019.tmn.dat-clim-1961-1990.nc"
```

2. Interpolate the monthly data to daily. Variables used: cld, pre, tmn, tmx, vap.

```
# Monthly to daily interpolation for `tmn`
codos::nc_int("cru_ts4.04.1901.2019.tmn.dat-clim-1961-1990.nc", "tmn")
```

Output file:

```
"cru_ts4.04.1901.2019.tmn.dat-clim-1961-1990-int.nc"
```

3. Calculate daily temperature, tmp. Variables used: tmn and tmx.

4. Calculate mean growing season for daily temperature

```
codos::nc_gs("cru_ts4.04-clim-1961-1990-daily.tmp.nc", "tmp", thr = 0)
```

Output file:

```
"cru_ts4.04-clim-1961-1990-daily.tmp-gs.nc"
```

5. Calculate potential evapotranspiration (pet)

Install SPLASH (unofficial R package) as follows:

```
remotes::install_github("villegar/splash", "dev")
```

Or, download from the official source: https://bitbucket.org/labprentice/splash.

Output file:

```
"cru_ts4.04-clim-1961-1990-pet.nc"
```

6. Calculate moisture index (mi)

$$MI_{i,j} = rac{ extsf{Total precipitation}}{ extsf{Total PET}}$$

Output file:

```
"cru_ts4.04-clim-1961-1990-mi.nc"
```

7. Approximate vpd

Output file:

```
"cru_ts4.04-clim-1961-1990-vpd-tmp.nc"
```

8. Find the coefficients for the following equation

```
\mathsf{vpd} = a \times \exp(\mathsf{kTmp} \times \mathsf{tmp} - \mathsf{kMI} \times \mathsf{mi})
```

```
mi <- codos:::nc_var_get("cru_ts4.04-clim-1961-1990-mi.nc", "mi")$data
Tmp <- codos:::nc_var_get("cru_ts4.04-clim-1961-1990-daily.tmp-gs.nc", "tmp")$data</pre>
vpd <- codos:::nc_var_get("cru_ts4.04-clim-1961-1990-vpd-tmp-gs.nc", "vpd")$data</pre>
# Apply ice mask
mi[codos:::ice_mask] <- NA
Tmp[codos:::ice_mask] <- NA</pre>
vpd[codos:::ice_mask] <- NA</pre>
# Filter low temperatures, Tmp < 5
mi[Tmp < 5] <- NA
Tmp[Tmp < 5] <- NA
# Create data frame
df <- tibble::tibble(Tmp = c(Tmp),</pre>
                      vpd = c(vpd),
                      MI = c(mi)
# Filter grid cells with missing Tmp, vpd, or MI
df <- df[!is.na(df$Tmp) & !is.na(df$vpd) & !is.na(df$MI), ]</pre>
# Linear approximation
lmod \leftarrow lm(log(vpd) \sim Tmp + MI, data = df)
# Non-linear model
exp_mod <- nls(vpd ~ a * exp(kTmp * Tmp - kMI * MI),
               df,
               start = list(a = exp(coef(lmod)[1]),
                             kTmp = coef(lmod)[2],
                             kMI = coef(lmod)[3]),
                control = list(maxiter = 200))
```

Summary statistics:

```
summary(exp_mod)
#>
\# Formula: vpd \sim a * exp(kTmp * Tmp - kMI * MI)
#>
#> Parameters:
       Estimate Std. Error t value Pr(>|t|)
       4.589148 0.019843 231.3 <2e-16 ***
#> kTmp 0.061108 0.000174
                             351.2 <2e-16 ***
                             336.7 <2e-16 ***
#> kMI 0.870229 0.002585
#> ---
#> Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
#> Residual standard error: 2.241 on 60291 degrees of freedom
#> Number of iterations to convergence: 8
#> Achieved convergence tolerance: 7.419e-06
coefficients(exp_mod)
           \boldsymbol{a}
                   kTmp
#> 4.58914835 0.06110768 0.87022950
```

Corrected mi from reconstructed mi

The following equations were used:

$$f = e/1.6 = D/[c_a(1-\chi)]$$

OLD:

$$\chi = [\xi/(\xi + vpd^{1/2})][1 - \Gamma^*/c_a] + \Gamma^*/c_a$$

NEW:

$$\chi = \frac{[\xi \times \text{vpd} + \text{vpd}]}{[\text{c}_{\text{a}}/(c_a + 9.7)]}$$

$$\xi = [\beta(K + \Gamma^*)/(1.6\eta^*)]^{1/2}$$

where:

- e ratio of water lost to carbon fixed [-]
- vpd vapour pressure deficit [Pa]
- ca ambient CO2 partial pressure [Pa]
- χ ratio of leaf-internal to ambient CO2 partial pressures [–]
- *ξ* stomatal sensitivity factor [Pa1/2]
- Γ^* photorespiratory compensation point [Pa]: a function of temperature and elevation
- β ratio of cost factors for carboxylation and transpiration = 146 [-]
- ullet K effective Michaelis constant of Rubisco [Pa]: a function of temperature and elevation
- η^* viscosity of water relative to its value at 25°C [-]

And the equilibrium relation:

$$f(T_{c1}, MI_1, C_{a,1}) = f(T_{c0}, MI_0, C_{a,0})$$

where:

- T_{c1} past temperature (assume equal to reconstructed value) [K]
- MI₁ past MI (unknown) [-]
- c_{a.1} past ambient CO2 partial pressure [Pa], adjusted for elevation
- T_{c0} present temperature [K]
- MI₀ reconstructed MI [-]
- c_{a,1} 'recent' ambient CO2 partial pressure [Pa], adjusted for elevation

Steps in the solution:

- 1. Evaluate $f(T_{c0}, MI_0, c_{a,0})$
- 2. Equate this to:

OLD:

$$[\xi(\mathsf{T}_{\mathsf{c1}},z)\mathsf{vpd}_1^{1/2}+\mathsf{vpd}_1]/[\mathsf{c_{\mathsf{a,1}}}(z)-\Gamma^*(\mathsf{T}_{\mathsf{c1}},z)]$$

NEW:

$$[\xi({\rm T_{c1}},z){\rm vpd}_1+{\rm vpd}_1]/[{\rm c_{a,1}}(z)/({\rm c_{a,1}}(z)+9.7)]$$

where:

• z is elevation

• vpd_1 is past vapour pressure deficit

And solve for vpd_1 .

3. Convert vpd_1 back to MI (at temperature T_{c1}), to yield an estimate of MI₁.

Using codos, all the steps translate to a simple function call

Note that this function takes temperatures in [°C] and ambient CO_2 partial pressures in [μ mol/mol] (unless, scale_factor is overwritten, e.g. scale_factor = 1 to use ambient CO_2 partial pressures in [Pa]).

More details:

```
?codos::corrected_mi
```

References

University of East Anglia Climatic Research Unit, Ian C. Harris, Philip D. Jones, and Tim Osborn. 2020. *CRU TS4.04: Climatic Research Unit (CRU) Time-Series (TS) Version 4.04 of High-Resolution Gridded Data of Month-by-Month Variation in Climate (Jan. 1901- Dec. 2019)*. Centre for Environmental Data Analysis. https://catalogue.ceda.ac.uk/uuid/89e1e34ec3554dc98594a5732622bce9.