Supplementary materials for 'Unusually warm winter seasons may compromise the performance of current phenology models - Predicting bloom dates in young apple trees with PhenoFlex'

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# Introduction

Phenology models are crucial tools for assessing the impacts of climate change on forestry, ecology and agriculture. In the article 'Unusually warm winter seasons may compromise the performance of current phenology models - Predicting bloom dates in young apple trees with PhenoFlex,' we assessed the performance of the recently proposed PhenoFlex phenology modelling framework (Luedeling et al. 2021) in response to different characteristics of the calibration data. In this document, we provide supplementary materials to the main document. Among these, we highlight the specific set of parameters used in each of the ten model runs as well as the results of our supplementary validation of one of the versions of the framework used in the study (i.e. Phenoflex<sub>excluded</sub>).

# Parameters used in each model run

The phenologyFitter() function from the chill package (Luedeling 2021), which is needed to fit the 12 model parameters to data, requires an estimated set of parameters (i.e. par.guess) as well as the lower and upper bounds for these values. We initialized the model fitting procedure with a common set of parameters for both versions of the analysis (i.e. PhenoFlex<sub>all</sub> and PhenoFlex<sub>excluded</sub>).

## First model run

```
# Set the initial parameters (wide ranges)
# Parameter \leftarrow c(yc, zc, s1, Tu,
                                                                           Tf, Tc, Tb, slope)
                                                 E1,
                                                          AO.
            <- c(20, 100, 0.1, 0, 3000.0,
lower
                                             9000.0, 6000.0,
                                                                5.00e+13,
                                                                            0, 0, 0, 0.05)
            <- c(40, 190, 0.5, 25, 3372.8,
par.guess
                                             9900.3, 6319.5,
                                                                5.94e+13,
                                                                            4, 36, 4, 1.60)
            <- c(80, 500, 1.0, 30, 4000.0, 10000.0, 7000.0,
                                                                6.00e+13,
                                                                           10, 40, 10, 50.00)
upper
```

We introduced these parameters to the fitter function for each version of the analysis. Note that the specific values for the parameters and all scripts developed in this study are deposited in a public online repository (https://github.com/EduardoFernandezC/phenoflex\_exp\_data). The first fitting procedure resulted in RMSE values of 7.2 days for PhenoFlex<sub>all</sub> and 4.13 days for PhenoFlex<sub>excluded</sub>. In the second round of the fitting procedure, we adjusted the parameter inputs.

#### Second model run

```
# Set the parameters using the results from the previous run

# Version PhenoFlex_all (pheno_fit_v1_r1$model_fit$par)

# Parameter <- c(yc, zc, s1, Tu, E0, E1, A0, A1, Tf, Tc, Tb, slope)

lower_v1_r2 <- c(45, 290, 0.00, 18.0, 3000.0, 9000.0, 6000.0, 5.20e+13, 0.0, 29.0, 0.0, 0.05)
```

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```
par_v1_r2 <- c(59, 326, 0.16, 22.5, 3309.9, 9900.1, 6295.7, 5.94e+13, 6.1, 39.9, 8.6, 14.60)
upper_v1_r2 <- c(65, 380, 0.50, 30.0, 4000.0, 10000.0, 7000.0, 6.20e+13, 10.0, 44.0, 12.0, 30.00)

# Same for version PhenoFlex_excluded (pheno_fit_v2_r1$model_fit$par)
# Parameter <- c(yc, zc, s1, Tu, E0, E1, A0, A1, Tf, Tc, Tb, slope)
lower_v2_r2 <- c(25, 340, 0.00, 17.0, 3000.0, 9000.0, 6000.0, 5.20e+13, 0.0, 30.0, 0.0, 1.00)
par_v2_r2 <- c(35, 387, 0.03, 21.8, 3371.0, 9900.8, 6283.6, 5.94e+13, 5.1, 40.0, 6.3, 40.00)
upper_v2_r2 <- c(40, 420, 0.50, 32.0, 4000.0, 10000.0, 7000.0, 6.20e+13, 10.0, 42.0, 10.0, 50.00)</pre>
```

In the second round of the fitting procedure, PhenoFlex<sub>all</sub> reached an RMSE of 6.94 days, whereas PhenoFlex<sub>excluded</sub> reached an RMSE of 3.91 days. In the third round of the fitting procedure, we adjusted the parameter inputs as follow:

#### Third model run

```
# Set the parameters using the results from the previous run
# Version PhenoFlex_all (pheno_fit_v1_r2$model_fit$par)
# Parameter <- c(yc, zc,
                          s1,
                                Tu,
                                         E0,
                                                  E1,
                                                          A0,
                                                                    A1,
                                                                          Tf,
                                                                                Tc,
lower_v1_r3 <- c(48, 290, 0.00, 15.0, 3000.0, 9000.0, 6000.0, 5.20e+13, 0.0, 24.0, 0.0, 0.05)
          <- c(58, 332, 0.39, 22.1, 3310.5, 9900.3, 6344.8, 5.94e+13, 7.2, 35.0, 8.8, 18.20)</p>
upper_v1_r3 <- c(68, 370, 0.65, 32.0, 4000.0, 10500.0, 7000.0, 6.20e+13, 11.0, 44.0, 11.0, 35.00)
# Same for PhenoFlex_excluded (pheno_fit_v2_r2$model_fit$par)
# Parameter <- c(yc, zc,
                          s1,
                                Tu,
                                         E0,
                                                  E1,
                                                          A0,
                                                                    A1,
lower_v2_r3 <- c(20, 350, 0.00, 18.0, 3000.0, 9000.0, 6000.0, 5.20e+13, 0.0, 30.0, 0.0, 1.00)
          <- c(34, 406, 0.20, 21.4, 3371.4, 9901.3, 6214.0, 5.94e+13, 1.5, 42.0, 6.1, 10.70)</pre>
upper_v2_r3 <- c(50, 450, 0.55, 35.0, 4000.0, 10500.0, 7000.0, 6.20e+13, 10.0, 46.0, 10.0, 35.00)
```

After the third round of the fitting procedure, RMSE values decreased to 6.63 days for PhenoFlex<sub>all</sub> and 3.91 days for PhenoFlex<sub>excluded</sub>. In the fourth round of the fitting procedure, we used the following set of parameters:

## Fourth model run

```
# Set the parameters using the results from the previous run
# Version PhenoFlex_all (pheno_fit_v1_r3$model_fit$par)
\# Parameter <- c(yc, zc,
                           s1,
                                Tu,
                                         E0,
                                                  E1,
                                                          A0,
                                                                    A1,
                                                                           Tf,
                                                                                 Tc.
lower_v1_r4 <- c(45, 290, 0.00, 15.0, 3000.0, 9000.0, 5500.0, 5.20e+13, 0.0, 20.0, 0.0, 1.00)
par_v1_r4 <- c(60, 339, 0.54, 23.0, 3310.3, 9901.5, 6346.3, 5.94e+13, 7.2, 30.7, 7.6, 7.30)
upper_v1_r4 <- c(70, 370, 0.75, 32.0, 4000.0, 10300.0, 7000.0, 6.20e+13, 12.0, 40.0, 12.0, 20.00)
# Same for version 2 (pheno_fit_v2_r3$model_fit$par)
# Parameter <- c(yc, zc,
                                         E0,
                                                  E1,
                                                                           Tf,
                                                                                 Tc,
                           s1,
                                Tu,
                                                           A0,
                                                                     A1,
lower_v2_r4 <- c(28, 360, 0.00, 17.0, 3000.0, 9300.0, 5800.0, 5.30e+13, 0.0, 35.0, 0.0, 10.00)
par_v2_r4 <- c(34, 396, 0.20, 21.6, 3371.0, 9901.3, 6214.0, 5.94e+13, 1.5, 46.0, 5.9, 11.12)
upper v2 r4 \leftarrow c(44, 440, 0.45, 30.0, 4000.0, 10500.0, 6800.0, 6.50e+13, 10.0, 48.0, 12.0, 40.00)
```

In this round of the fitting procedure, PhenoFlex<sub>all</sub> reached an RMSE of 6.59 days, whereas PhenoFlex<sub>excluded</sub> reached an RMSE of 3.65 days.

#### Fifth model run

```
# Set the parameters using the results from the previous run
# Version PhenoFlex_all (pheno_fit_v1_r4$model_fit$par)
# Parameter <- c(yc, zc, s1, Tu, E0, E1, A0, A1, Tf, Tc, Tb, slope)</pre>
```

```
lower_v1_r5 <- c(50, 330, 0.00, 18.0, 3000.0, 9600.0, 6000.0, 5.50e+13, 2.0, 30.0, 2.0, 0.50)

par_v1_r5 <- c(60, 354, 0.47, 22.8, 3310.3, 9901.5, 6344.3, 5.94e+13, 7.2, 36.0, 7.6, 7.63)

upper_v1_r5 <- c(75, 370, 0.55, 28.0, 4000.0, 10300.0, 7000.0, 6.50e+13, 10.0, 42.0, 12.0, 15.00)

# Same for version PhenoFlex (pheno_fit_v2_r4$model_fit$par)

# Parameter <- c(yc, zc, s1, Tu, E0, E1, A0, A1, Tf, Tc, Tb, slope)

lower_v2_r5 <- c(27, 360, 0.00, 18.0, 3000.0, 9500.0, 5800.0, 5.50e+13, 0.0, 35.0, 1.0, 1.00)

par_v2_r5 <- c(34, 383, 0.21, 22.5, 3371.0, 9901.3, 6213.9, 5.94e+13, 1.5, 45.6, 5.9, 1.08)

upper_v2_r5 <- c(37, 400, 0.55, 32.0, 4000.0, 10300.0, 6800.0, 6.30e+13, 8.0, 48.0, 10.0, 25.00)
```

In this round of the fitting procedure, PhenoFlex<sub>all</sub> reached an RMSE of 6.57 days, whereas PhenoFlex<sub>excluded</sub> reached an RMSE of 3.56 days.

#### Sixth model run

```
# Set the parameters using the results from the previous run
# Version PhenoFlex_all (pheno_fit_v1_r5$model_fit$par)
# Parameter \leftarrow c(yc, zc, s1,
                                Tu,
                                         EO,
                                                   E1,
                                                          A0,
                                                                    A1,
                                                                           Tf,
lower_v1_r6 <- c(40, 290, 0.00, 18.0, 2900.0, 9000.0, 5700.0, 5.30e+13, 0.0, 20.0, 0.0)
par v1 r6 < c(60, 343, 0.32, 25.1, 3310.3, 9901.6, 6342.9, 5.94e+13, 5.6, 33.6, 7.0, 2.24)
upper_v1_r6 \leftarrow c(80, 390, 0.55, 32.0, 3900.0, 10500.0, 6900.0, 6.80e+13, 12.0, 48.0, 12.0, 20.00)
\# Same for version PhenoFlex_excluded (pheno_fit_v2_r5model_fitpar)
# Parameter \leftarrow c(yc, zc, s1, Tu,
                                                                   A1,
                                         E0,
                                                   E1,
                                                          AO,
                                                                          Tf,
lower_v2_r6 <- c(25, 330, 0.00, 18.0, 3000.0, 9200.0, 5700.0, 5.40e+13, 0.05, 40.0, 0.0, 0.50)
          <- c(35, 361, 0.15, 22.4, 3371.0, 9901.3, 6213.8, 5.94e+13, 1.45, 48.0, 5.9, 1.10)</pre>
upper_v2_r6 <- c(40, 390, 0.35, 30.0, 4000.0, 10800.0, 6900.0, 6.60e+13, 10.00, 50.0, 10.0, 20.00)
```

In this round of the fitting procedure, PhenoFlex<sub>all</sub> reached an RMSE of 6.41 days, whereas PhenoFlex<sub>excluded</sub> reached an RMSE of 3.55 days.

## Seventh model run

```
# Set the parameters using the results from the previous run
# Version PhenoFlex all (pheno fit v1 r6$model fit$par)
# Parameter <- c(yc, zc,
                                                          A0,
                                                                                     Tb, slope)
                          s1,
                                Tu,
                                         E0,
                                                   E1,
                                                                    A1,
                                                                           Tf,
                                                                                 Tc,
lower_v1_r7 \leftarrow c(55, 325, 0.00, 20.0, 3000.0, 9000.0, 5500.0, 5.50e+13, 0.0, 30.0, 2.0, 0.00)
par_v1_r7 <- c(61, 334, 0.53, 25.0, 3310.3, 9901.6, 6342.7, 5.94e+13, 6.4, 33.9, 7.0, 1.57)
upper_v1_r7 \leftarrow c(65, 345, 0.65, 30.0, 4000.0, 10500.0, 6600.0, 6.50e+13, 10.0, 40.0, 10.0, 10.00)
# Same for version PhenoFlex_excluded (pheno_fit_v2_r6$model_fit$par)
# Parameter \leftarrow c(yc, zc, s1,
                                                                                       Tb, slope)
                                Tu,
                                         E0,
                                                  E1 .
                                                          AO.
                                                                    A1,
                                                                           Tf,
                                                                                Tc,
lower_v2_r7 <- c(30, 365, 0.000, 20.0, 3000.0, 9500.0, 5800.0, 5.50e+13, 0.0, 35.0, 0.0, 1.00)
par_v2_r7 <- c(34, 380, 0.160, 26.4, 3371.0, 9901.3, 6214.2, 5.94e+13, 1.3, 41.2, 3.3, 1.12)
upper_v2_r7 <- c(40, 385, 0.225, 30.0, 4000.0, 10500.0, 6800.0, 6.40e+13, 6.0, 45.0, 8.0, 20.00)
```

In this round of the fitting procedure, PhenoFlex<sub>all</sub> reached an RMSE of 6.05 days, whereas PhenoFlex<sub>excluded</sub> reached an RMSE of 3.46 days.

# Eigth model run

```
# Set the parameters using the results from the previous run

# Version PhenoFlex_all (pheno_fit_v1_r7$model_fit$par)

# Parameter <- c(yc, zc, s1, Tu, E0, E1, A0, A1, Tf, Tc, Tb, slope)

lower_v1_r8 <- c(55, 315, 0.30, 22.0, 2800.0, 9500.0, 5900.0, 5.60e+13, 2.0, 26.0, 2.0, 0.00)
```

```
par_v1_r8 < -c(62, 336, 0.52, 27.1, 3310.3, 9901.7, 6395.4, 5.94e+13, 6.5, 30.2, 5.6, 1.39)
upper_v1_r8 <- c(70, 355, 0.70, 32.0, 3800.0, 10200.0, 6700.0, 6.40e+13, 9.0, 36.0, 8.0, 15.00)
# Same for version PhenoFlex_excluded (pheno_fit_v2_r7$model_fit$par)
\# Parameter <- c(yc, zc,
                            s1,
                                  Tu,
                                          E0,
                                                    E1,
                                                            A0,
                                                                            Tf,
                                                                                   Tc,
                                                                                         Tb, slope)
lower_v2_r8 <- c(28, 345, 0.01, 20.0, 2800.0, 9600.0, 5800.0, 5.60e+13,
                                                                           0.0, 38.0,
                                                                                       0.0, 7.00)
           <- c(35, 375, 0.13, 26.4, 3371.0, 9901.3, 6214.4, 5.94e+13,</pre>
                                                                           1.3, 44.7,
                                                                                       3.0,
upper_v2_r8 \leftarrow c(40, 405, 0.30, 30.2, 3700.0, 10300.0, 6800.0, 6.30e+13, 8.0, 52.0,
                                                                                       8.0, 30.00)
```

In this round of the fitting procedure, PhenoFlex<sub>all</sub> reached an RMSE of 5.96 days, whereas PhenoFlex<sub>excluded</sub> reached an RMSE of 3.45 days.

#### Ninth model run

```
# Set the parameters using the results from the previous run
# Version PhenoFlex_all (pheno_fit_v1_r8$model_fit$par)
# Parameter <- c(yc, zc,
                            s1,
                                   Tu,
                                           E0,
                                                    E1,
                                                            A0,
                                                                       A1,
                                                                             Tf,
                                                                                   Tc,
                                                                                          Tb, slope)
lower_v1_r9 <- c(55, 300, 0.50, 20.0, 3000.0, 9500.0, 5500.0, 5.00e+13,
                                                                           1.0, 20.0,
                                                                                        2.0, 0.00)
          <- c(63, 315, 0.70, 27.9, 3310.3, 9901.7, 6396.2, 5.94e+13, 6.5, 27.9, 5.7, 1.39)</pre>
upper_v1_r9 \leftarrow c(75, 325, 0.85, 35.0, 4000.0, 10500.0, 6900.0, 7.00e+13, 11.0, 37.0, 10.0, 25.00)
# Same for version PhenoFlex_excluded (pheno_fit_v2_r8$model_fit$par)
\# Parameter <- c(yc, zc,
                            s1,
                                   Tu,
                                           E0,
                                                            A0,
                                                                       A1,
                                                                             Tf,
                                                    E1,
                                                                                   Tc,
lower_v2_r9 <- c(23, 325, 0.00, 16.0, 3000.0,
                                                9500.0, 5700.0, 5.60e+13,
                                                                           0.0, 40.0,
                                                                                        0.0, 1.00)
          <- c(34, 357, 0.14, 26.8, 3371.0, 9901.2, 6214.1, 5.94e+13, 1.4, 51.3, 3.6, 8.45)</pre>
upper_v2_r9 \leftarrow c(43, 375, 0.50, 36.0, 3800.0, 10500.0, 6700.0, 6.30e+13, 10.0, 55.0, 10.0, 20.00)
```

In this round of the fitting procedure, PhenoFlex<sub>all</sub> reached an RMSE of 5.94 days, whereas PhenoFlex<sub>excluded</sub> reached an RMSE of 3.37 days.

### Tenth model run

```
# Set the parameters using the results from the previous run
# Version PhenoFlex_all (pheno_fit_v1_r9$model_fit$par)
\# Parameter \leftarrow c(yc, zc,
                             s1,
                                   Tu,
                                           E0,
                                                    E1,
                                                            A0,
                                                                       A1,
                                                                             Tf,
                                                                                   Tc,
lower_v1_r10 <- c(58, 305, 0.15, 20.0, 2800.0,
                                                9500.0, 5800.0, 5.70e+13, 0.0, 20.0,
                                                                                        0.0, 0.00)
           <- c(63, 319, 0.85, 27.9, 3310.4, 9901.6, 6396.2, 5.94e+13, 6.5, 27.9, 5.6, 1.39)</pre>
upper_v1_r10 <- c(68, 335, 1.05, 35.0, 3700.0, 10400.0, 6600.0, 6.20e+13, 12.0, 34.0, 10.0, 15.00)
# Same for version PhenoFlex_excluded (pheno_fit_v2_r9$model_fit$par)
# Parameter <- c(yc, zc,
                              s1,
                                    Tu,
                                            E0,
                                                                        A1,
                                                                              Tf,
                                                     E1,
                                                              A0,
                                                                                    Tc,
                                                                                          Tb, slope)
lower_v2_r10 <- c(28, 360, 0.050, 20.0, 2900.0,
                                                 9500.0, 5800.0, 5.70e+13,
                                                                             0.0, 45.0,
                                                                                         0.0, 0.00
par_v2_r10 <- c(34, 371, 0.130, 25.0, 3371.0, 9901.3, 6214.6, 5.94e+13, 1.7, 53.3,
upper_v2_r10 <- c(38, 380, 0.325, 30.0, 3700.0, 10400.0, 6600.0, 6.20e+13, 10.0, 58.0, 10.0, 15.00)
```

In this round of the fitting procedure, PhenoFlex<sub>all</sub> reached an RMSE of 5.94 days, whereas PhenoFlex<sub>excluded</sub> reached an RMSE of 3.37 days. Note that the RMSE values obtained in this run did not improve compared to the results of run number 9. For this reason, we used the parameters estimated in the ninth run as final values.

# Supplementary validation of $PhenoFlex_{excluded}$

As mentioned in the main text, we assessed the performance of the PhenoFlex<sub>excluded</sub> version when used to predict bloom dates in the marginal seasons. Following this approach, we aimed to test the viability of extrapolating the modelling framework to conditions outside the calibration data set. The results of this analysis demonstrated the importance of explicitly testing the predictive accuracy of the model under environmental conditions outside the range of the calibration

data. When comparable temperature conditions are used for calibration and validation, the model is – despite potentially incorrect assumptions – sufficiently flexible to be well fitted to data and shows good projection quality. However, when validation data contain conditions outside the calibration range, the conceivably inaccurate model structure cannot be compensated by parameter fitting and finds expression in high residual errors (Fig. S1). In this validation, RMSE and RPIQ reached values of 61.2 days and 0.3, respectively. It should be noted, however, that these results are greatly influenced by one outlier showing 127 days of error (observed versus predicted). When removing the outlier from the marginal seasons, the prediction error ranged between 9.3 and 44.4 days (Fig. S1).

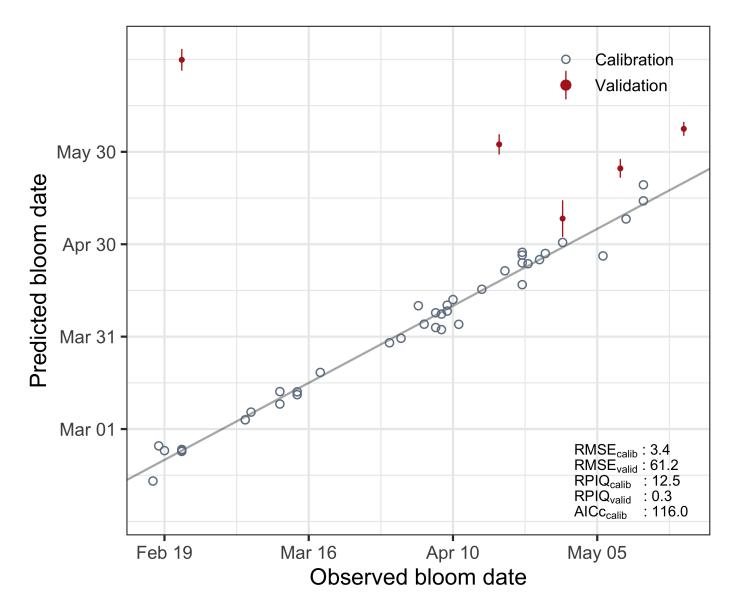


Figure S1: Validation of the PhenoFlex<sub>excluded</sub> version using the five marginal seasons excluded from the calibration data set. Whereas the open blue circles represent the experimental seasons used for calibration, the filled red circles represent the five marginal seasons used for validating the framework. The vertical lines in the marginal season dots represent the uncertainty estimated by bootstrapping.

### References

Luedeling, Eike, Katja Schiffers, Till Fohrmann, and Carsten Urbach. 2021. "PhenoFlex - an Integrated Model to Predict Spring Phenology in Temperate Fruit Trees." Agricultural and Forest Meteorology 307: 108491. https://doi.org/10.1016/j.agrformet.2021.108491.