Chapter 7 Combining messy phenological time series

Jörg Schaber[1], Franz Badeck[2], Daniel Doktor[3], Werner von Bloh[2]

[1]Max Planck Institute for Molecular Genetics, Computational Systems Biology, Berlin, Germany.

[2]Potsdam Institute of Climate Impact Research, Potsdam, Germany

[3] Imperial College, Department of Biology, London, UK

corresponding author: schaber@biologie.hu-berlin.de

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Abstract

We describe a method for combining phenological time series and outlier detection based on linear models as presented in Schaber and Badeck (2002). We extend the outlier detection method based on Gaussian Mixture Models as proposed by Doktor et al. (2005) in order to take into account year-location interactions. We quantify the effect of the extension of the outlier detection algorithm using Gaussian Mixture Models. The proposed methods are adequate for the analysis of messy time series with heterogeneous distribution in time and space as well as frequent gaps in the time series. We illustrate the use of combined time series for the generation of geographical maps of phenological phases using station effects. The algorithms discussed in the current paper are publicly available in the updated R - package 'pheno' (Schaber, 2007).

Key words: linear models, Gaussian mixtures, outliers, station effects, robust estimation

7.1 Introduction

Phenology, the science of 'the timing of recurrent biological events, the causes of their timing with regard to biotic and abiotic forces, and the interrelation among phases of the same or different species’ (Lieth 1974) has a long tradition embedded in biological sciences. Réaumur (1735) already proposed a temperature sum model as explanation for the variation in the onset of phenological phases, such as leaf bud break or initiation of flowering in the spring in temperate ecosystems. Linné described the purpose and methods of phenological observations as early as 1751. Phenological studies played a prominent role in the discovery of mechanisms with which organisms synchronise their development and behaviour with the environmental conditions. Spectacular changes in nature that are associated with the advancement of the seasons (greening of the vegetation, colourful flowering, indian summer or seasonal migration of animals) as well as their usefulness for the timing of human activities are at the origin of observational time series that date back as far as several centuries (see several chapters in Schwartz 2003 on the history of phenology in different countries). In recent years these data have been discovered and explored for studies in the context of climate change research. Since 1991, publications on phenology as one of the easily detectable biotic responses to climate change have experienced a rapid growth (for review see Parmesan 2006, Rosenzweig et al. 2007 and papers cited therein). The growth rate of papers was higher than in other rapidly growing research domains against a background of a slowly growing number of publications on phenology in general.

Phenological data have specific limitations that have to be considered, when inferences are to be made from their analysis. It must be realized that phenological data origin from observations rather than from exact measurements. To obtain the data phenological observers use instructions that leave room for interpretation. Additionally, the exact location of the observation and therefore the environmental conditions as well as the genotype of plant individuals are usually unknown. These various sources of uncertainty introduce an intrinsic variability to phenological observations that is difficult to quantify (Schaber 2002). Moreover, phenological time series are often incomplete and reveal large data gaps, further complicating their analysis. The problem of the uncertainty of individual time series and gaps is often reduced by averaging a set of phenological time series over a geographical area of interest or a time period of interest (e.g. Estrella and Menzel 2006, Menzel et al. 2006, Menzel et al. 2007). This way the resulting time series has less gaps and noise of individual time series is reduced at the cost of local information.

The principal problem associated with the use of average time series is often neglected, but can be demonstrated by a very simple consideration (Fig. 7.1): assume we have two phenological stations s_1 and s_2, and s_1 has observations in years y_1 and y_2, whereas s_2 has observations in years y_2 and y_3. Further assume that observations at s_1 are equal, say, c_1 and at s_2 we observe c_2 in both years and $c_1 > c_2$. Obviously, by averaging we obtain a monotonically decreasing time series $\{c_1, (c_1+c_2)/2, c_2\}$. Subsequent trend analysis, which is especially popular for phenological time series (see Schaber 2002 and references therein), would show a negative trend. However, neither station actually shows a trend and thus, the resulting combined time series should also not exhibit a trend. In this simple example the resulting trend is clearly due to the fact that the stations have different observation years and that one station happens to be earlier than the other.

In general terms, phenological time series are unequally distributed in time and space and simple averaging in order to obtain less noisy and longer time series can lead to artifacts as demonstrated in Schaber (2002) for trends of time series of the International Phenological Gardens as published in Chmielewski and Roetzer (2001). In the above example, a solution is simple; first, we take a general mean a, $a=(c_1+c_2)/2$ and correct the time series' observations according to their deviations from the general mean (i.e. c_1-(c_1-a) and c_2-(c_2-a)), and then take the average. Obviously, the resulting time series is now $\{a,a,a\}$, which shows no trend, as we expect from inspection of the single time series (Fig. 7.1).

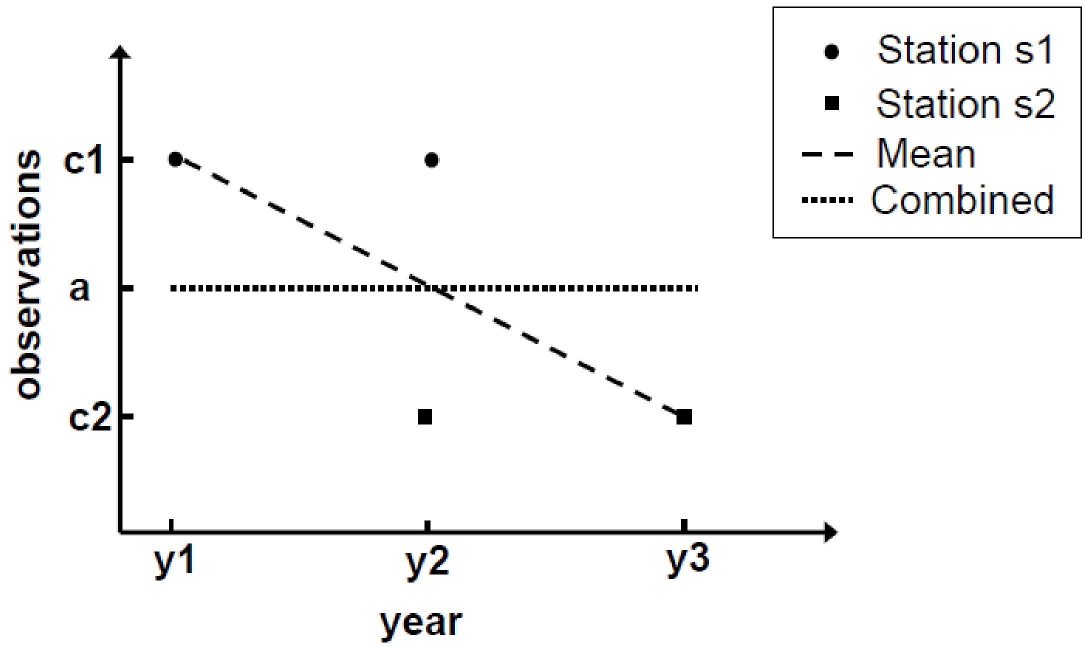

Fig. 7.1. Illustration how averaging time series for station s_1 and s_2 can lead to undesired results because of their unequal distribution of observations in time (arbitrary units).

In general, this process is called combination of time series and has been introduced to phenology by Häkkinen et al. (1995) and was put into the general framework of linear models by Schaber and Badeck (2002).

There are several areas of application where methods for combining phenological time series can be useful and where they have already been applied. One application is to obtain a reliable series out of several messy time series. In this application the focus would be on noise reduction (Häkkinen et al. 1995, Linkosalo et al. 1996, 2000, Linkosalo 1999, 2000, Schaber 2002). Another main application is to construct a long time series for trend analysis. In this application data gap filling is of primary interest (Schaber and Badeck 2005). Additionally, combined time series can also be used to find outliers in individual time series (Linkosalo et al. 2000, Schaber 2002, Schaber and Badeck 2002, Doktor et al. 2005). However, applying combined time series for outlier detection might lead to removal of correct observations, if the between station differences vary strongly at inter-annual time scales due to differences in the temperature trajectories, as already hypothesized by Schaber and Badeck (2002). Doktor et al. (2005) discussed some empirical evidence that cold spells that delay the transition to subsequent phenophases cause systematic deviations of the frequency distribution of dates of phase onset. They also introduced Gaussian mixtures as a tool for the quantification of the inter-annual variation in between station differences. This approach can potentially be integrated into the use of combined time series for outlier detection in order to avoid assignment of false outliers.

In the following, we will shortly introduce the method of combination of phenological times series by different types of linear models and discuss some practical issues. Moreover, we will discuss outlier analyses and show applications. We present the algorithms for integration of Gaussian normals (Fig. 7.2) into the outlier detection with combined time series and illustrate the effect of this model improvement (Fig. 7.3).

One useful result of the construction of combined time series is the extraction of station effects, (i.e. the characteristic deviation of the date of phase onset at a given observational station relative to the population of all stations). This result is less sensitive to gaps in the data series and different length of observation periods than the deviation from average values. It can be applied to producing maps of average geographical variation in the onset of a phenological phase. We illustrate this application for the bud break of beech in Germany (Figs. 7.4 – 7.6).

7.2 Linear Models of phenological time series

7.2.1 Linear Models

It is reasonable to assume that over a climatologically sufficiently homogeneous region, (e.g. middle Europe or Central North America), the phenological development of certain phases is consistent concerning years and stations. This means that a year, which is particularly late, should be late for all stations, and a station that is particularly late, because for example, it is situated on a top of a mountain, should be late in all years. Putting this in mathematical terms, we say that the effect of year y_i, i=1,…, n and the effect of station s_j, j=1,…, m are independent and additive, such that

$$o_{ij} = a + y_i + s_j + \varepsilon_{ij}, \qquad i = 1,...,n \text{ and } j = 1,...,m. \qquad (7.1)$$

where o_{ij} is the observation in year i at station j and a is the general mean. ε_{ij} is an error term that is usually assumed to be homoscedastically normally distributed around zero with some variance σ^2, i.e.

$$\varepsilon_{ij} \propto N(0,\sigma^2) \tag{7.2}$$

In statistics, (Eq. 7.1) is called a linear two-way crossed classification model. Usually, additional conditions are imposed that assure that a unique solution exists, such as setting

$$\tilde{y}_i = a + y_i \text{ and } \sum_{j=1}^{m} s_j = 0. \tag{7.3}$$

We call $\tilde{y}_i$, $i = 1,\ldots, n$ the combined time series.

Given observations o_{ij}, that may have missing data, (7.1) and the conditions (7.3) it is essentially straightforward to estimate the $\tilde{y}_i$ and s_j using least-square optimisation (i.e. minimizing the sum of squared residuals SSR),

$$SSR = \sum_{i,j} \varepsilon_{ij}^2 . \tag{7.4}$$

7.2.2 Fixed and mixed effects models

Depending on the type of analysis we are interested in, we can treat the year and station effects differently, which has consequences for the type of estimation procedure we apply. For instance, when we are mainly interested in the combined time series $\tilde{y}_i$, we can refrain from estimating the specific station effects but rather consider the stations to be randomly distributed. Thus, we treat the s_j as a random variable

$$s_j \propto N(0,\sigma_s^2) \tag{7.5}$$

and estimate the variance component σ_s^2, rather than station effects s_j. This is called the mixed model, because we have one fixed and one random effect. For this type of analysis special estimation and analysis procedures exist (Searle 1987, Milliken and Johnson 1992, Pinheiro & Bates 2000). Examples of the application of mixed models to obtain reliable phenological time series can be found in Schaber and Badeck (2002, 2005).

On other occasions, we might be interested in the year effects as well as in the specific station effects in order to identify stations that are particularly late, for instance. In this case, we would treat both effects as fixed. In section 7.3.2 we will give an example. For details on linear models and the large theoretical body that comes with it, please refer to Rencher (2000), Searle (1971, 1987) and Milliken and Johnson (1992) and the literature cited therein.

7.2.3 Practical issues and the R pheno-package

As already indicated, linear models constitute an entire field in statistics and calculations are far from being as easy as just calculating an average. The large theoretical body that comes with the theory of linear models can even be an obstacle rather than being helpful for phenological applications. Therefore, the authors wrote the software package 'pheno: auxiliary functions for phenological data analysis' (Schaber 2007) that was designed to make calculations of combined phenological time series and station effects as easy as possible. This software is freely available as a package for the free statistical computing environment R (R Development Core Team 2007). The user has just to provide a table with three columns (observation, year, station) to a function corresponding to the analysis of interest, without having to worry about the calculations. All subsequent examples were calculated using the pheno-package.

One especially useful feature of the pheno-package is that it automatically handles large data sets. To illustrate the problem, we refer to the example in the following section (Sect. 7.2.4). In order to calculate the average time series of beech and the station effects for Germany over the years 1951-2004, we considered 74,996 single data points from 2,318 stations. For calculation of the fixed year and station effects, this involves the inversion of a 74,996 x (2,319+53+1) matrix. With the usual 8-byte number coding the matrix itself occupies around 1.4 GB. With the extra storage needed for matrix inversion, even nowadays most personal computers would exceed their working storage capacity with this operation. Fortunately, the matrices involved mainly consist of zero-entries, such that the application of sparse matrix algorithms saves a great deal of computational and storage resources. Sparse matrix algorithms are provided in other R-packages such as SparseM and quantreg (Koenker and Ng, Koenker 2006) and are already integrated in the R-pheno package. This way, combined time series for whole Germany can be computed on a regular personal computer.

Another prerequisite for the application of linear models is that the time series be connected or overlapping. For many stations this is usually not a problem, but for few data (stations or years) it is recommendable to check (Schaber 2002). There are procedures within the R pheno-package that test for connectivity and automatically extract connected sets of time series.

7.2.4 Outlier detection

As already mentioned in the introduction, obtaining phenological data is often an error-prone process (Schaber 2002, Schaber and Badeck 2002). Therefore, a proper outlier detection method is indispensable. One of the few types of errors that can be detected is the so-called month mistake. Schaber and Badeck (2002) developed a method to detect month mistakes with combined time series. The usual least-square estimation of combined time series is sensitive to outliers. Therefore, Schaber and Badeck (2002) recommended applying a robust estimation procedure that minimizes least absolute deviations (LAD) (7.6),

$$LAD = \sum_{i,j} \left| \varepsilon_{ij} \right| , \tag{7.6}$$

before applying the classical least-square estimation. Residuals ε_{ij}, (i.e. the difference between observed and predicted values), that are estimated to be larger than 30 days are considered as month mistakes and are removed. The details of the procedure are described in Schaber and Badeck (2002) and are also implemented in the R pheno-package.

7.2.5 Gaussian normals

The assumption that year effects and station effects are independent may not always hold true. This is the case when the inter-station differences vary due to the annual weather trajectories. Years with retarded phase onset in a subset of phenological observation stations due to a cold spell as compared to years without intermittent cold spells are an example of this class of interactions. As an extension to the outlier detection with LAD estimation, frequency distributions of observed budburst dates can be characterised and modelled using Gaussian Mixtures Models (*GMM*) (Fig. 7.2). In many years, observations of a single species can be approximated by a probability density function (*pdf*), which consists of one, two or more underlying distributions. These can be mainly attributed to changing weather situations within spring, which alter the phenological pace. *GMM* quantify the number and type of the underlying distributions and thereby allow distinguishing years with different temporal evolution of budburst dates in a quantitative manner. The models can describe distributions with unknown underlying patterns and have the property of being able to represent any distribution of natural observations (Gilardi et al. 2002). A mixture distribution with continuous components has a density of the form (Poland and Shachter 1994):

$$f(x) = p_1 f_1(x) + ... + p_n f_n(x) \qquad (7.7)$$

Where x is the probability to have an observation at a certain day, $p_1,..., p_n$ are positive numbers summing up to one and $f_1(x),..., f_n(x)$ are the component densities (7.7). To determine potential outliers one has firstly to analyse the uni- or multi-modal frequency distribution to identify the main underlying components (mixtures) and their describing parameters mean, standard deviation and weight (μ_k, σ_k, p_k).

For each year i, all observations o_{ij} are related to a component's mean μ_k. The component k_a an observation o_{ij} is most related to is determined based on the frequencies f_{ijk} of component k at the observation day o_{ij}:

$$f_{ijk} = \frac{np_k}{\sigma_k \sqrt{2\pi}} e^{-\frac{(o_{ij}-\mu_k)^2}{2\sigma_k^2}}, \qquad (7.8)$$

where n is the total number of observations of the analysed year i. Then,

$$k_a = \arg\max_k f_{ijk} . \qquad (7.9)$$

An observation is declared to be an outlier if

$$\left| o_{ij} - \mu_{k_a} \right| \geq 30 . \qquad (7.10)$$

An optimisation algorithm is applied on the minimisation of several (here maximum four) Gaussian Mixture functions. Due to the authors' experience from phenological data analysis it is very unlikely that changes in temperature regimes with a sustained impact on the phenological evolution happen more than three times within the period the plant population is experiencing budburst, at least in Central Europe. Akaike's Information criterion (Akaike 1974) is applied to choose the most appropriate model, balancing between model complexity (number of components) and model fit. The parameterised mixture components are used for outlier detection in order to reduce the number of falsely detected outliers in years showing bi- or multi-modal distributions (i.e. in years with a high variability of observed phenological events).

Obviously, this method is more conservative as the one based on LAD estimates. LAD estimation assumes that observations are distributed around one general mean per year (i.e. the station effect) whereas applying Gaussian mixtures we assume that there might be several means. We detect only outliers at the margins of the whole Gaussian mixture and consequently less than before (Fig. 7.3).

Interestingly, even a unimodal distribution could be more accurately defined by a Gaussian mixture (Fig. 7.2). In fact, there was not year between 1951 and 2004 where the distribution of observations could be described by a normal distribution ($P < 0.01$, Shapiro-Wilk test).

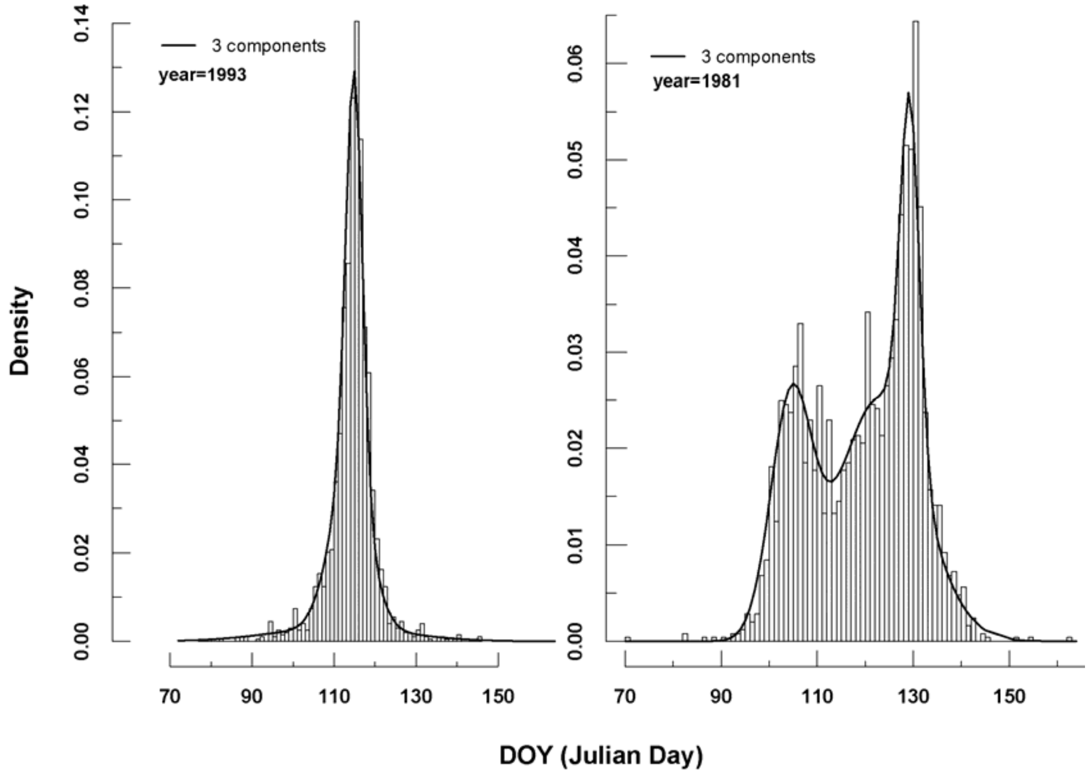

Fig. 7.2: The density function of observed budburst dates of Beech (grey bars) modelled for 1993 and for 1981 each with 3 components (curves). A large scale and consistent warming up in spring time usually produces unimodal distributions, as in 1993. In contrast, strong changes in temperature regimes as experienced in 1981 result in multimodal distributions. Still, even unimodal distributions might not be normally distributed but can be more accurately be described by a Gaussian mixture.

7.3 Applications

7.3.1 Gaussian Normals

The two outlier detection methods are compared with respect to the number of observations declared as outliers in each year, respectively. As expected *GMM* identifies, in general, fewer outliers (Fig. 7.3). This, however, comes at a cost of false negatives (declaring an observation not to be an outlier when it actually is).

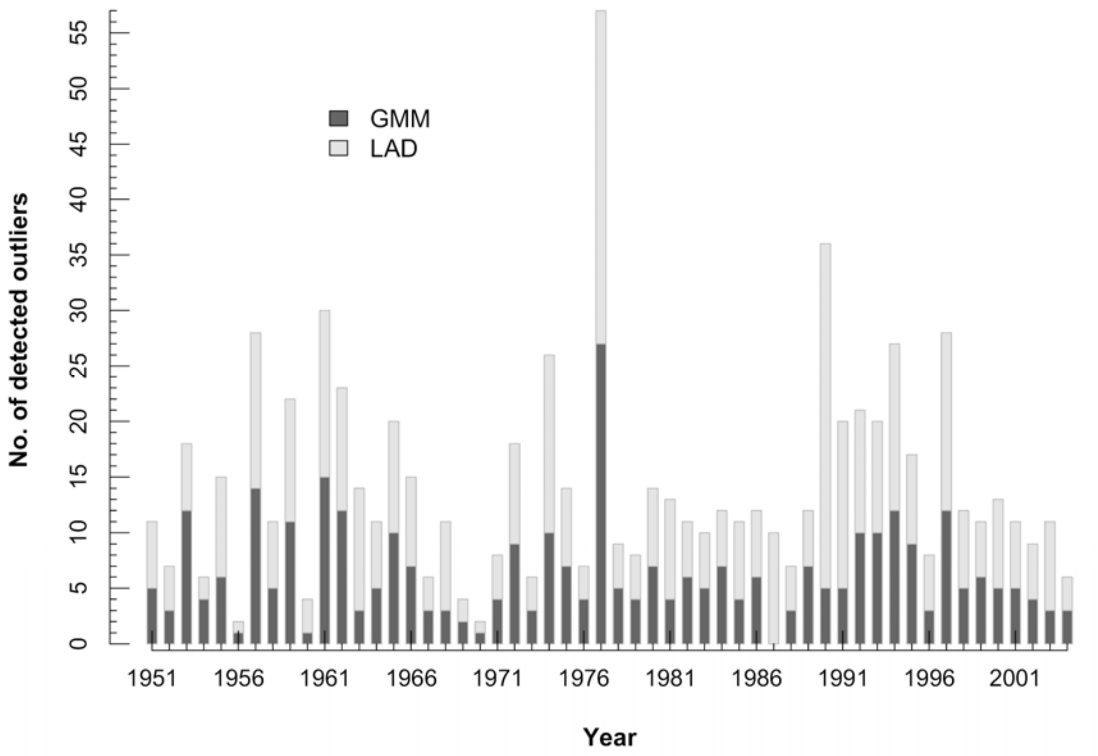

Fig. 7.3. Number of detected outliers per year for Beech using the outlier detection algorithm of Schaber and Badeck (2002) (LAD) and using Gaussian Mixture Models (GMM). The mixture components are determined and parameterised by an optimisation algorithm.

7.3.2 Station effects

We calculated the fixed effect model (1) with constraints (2) for whole Germany for the years 1951–2004 for beech budburst without month-mistakes. We considered only stations that had at least 20 observations. After the removal of 433 outliers according to the robust estimation method based we considered 74562 observations from 2318 stations. In Fig. 7.4 we present a map of the calculated station effects plus the general mean *m*=120 (30th of April in non-leap years) in day of the year (DOY). To our knowledge, this is the first time that a consistent map for the characteristic timing of a specific phenological phase for such a large region is presented. Note that for this application the underlying trends (see Schaber and Badeck, 2005) have not been removed.

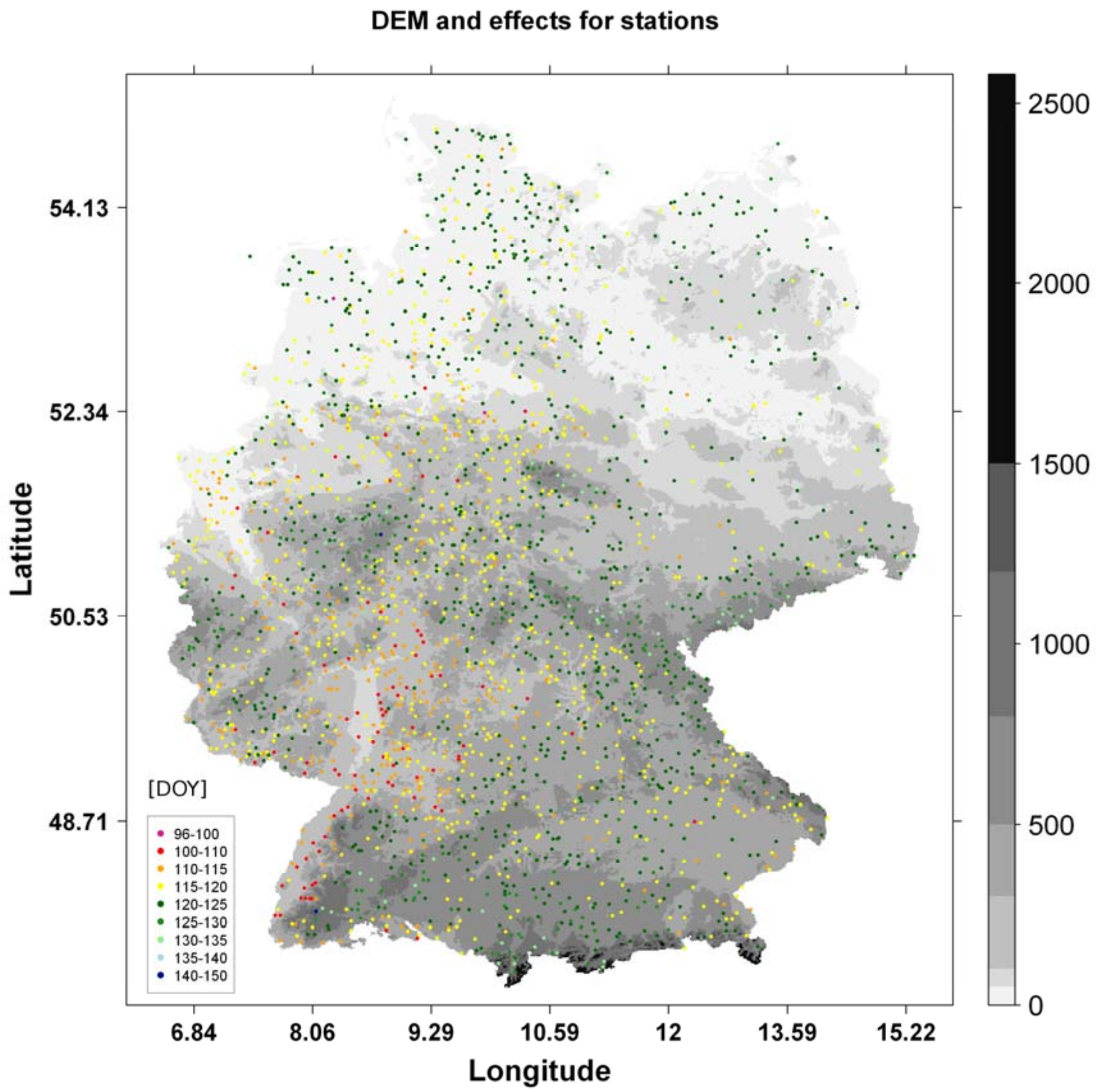

Fig. 7.4. Computed station effects + the general mean (day of year) based on observed budburst dates of Beech from 1951-2004 over Germany. A Digital Elevation Model (DEM) (1*1 km in meters) represents the topography, which considerably influences the timing of phenological phases in spring time. Observation stations are indicated as coloured points.

The underlying assumption that the observations within the relatively large geographic space of Germany (357,092 km^2) are elements of a unimodal population is illustrated with Fig. 7.2 (curve for year 1993). In many cases a station net well distributed over a geographical space with continuous gradients of environmental conditions will result in such a distribution. However, the distribution may be different from unimodal, if a geographical domain is made up by two sub-domains with very different environmental conditions (Fig. 7.2, year 1981).

The maps of the station effects (Fig 7.4) and the interpolated station effects by external drift krigging (EDK) (Fig. 7.5) illustrate phenological responses to

a) climatological differences between regions at similar elevation (e.g. 50 to 100 [m] asl): the northern lowlands of Saxony are phenologically later than the Muensteraner Becken and the Northern Upper Rhine valley. The average March and April temperatures (1951-2003) are 3.94 and 8.27 °C, respectively in Saxony at 15 stations at 12.4 to 13.9 longitude and 51.4 to 51.9 latitude. They are 5.19 and 8.62 °C, respectively in the vicinity of Muenster at 11 stations at 7.0 to 7.9 longitude and 51.7 to 52.2 latitude. They are 6.26 and 9.91 °C, respectively in the Northern Upper Rhine valley at 7 stations at 8.3 to 8.45 longitude and 49.3 to 49.9 latitude,

b) the lapse rate across elevational gradients (the higher, the later),

c) the combined influence of the inverse lapse rate of early spring (see Table 1 and Fig. 2 in Doktor et al. (2005)) and general climatological gradients between east and west Germany (northern lowlands: the closer to the sea the later at similar elevation).

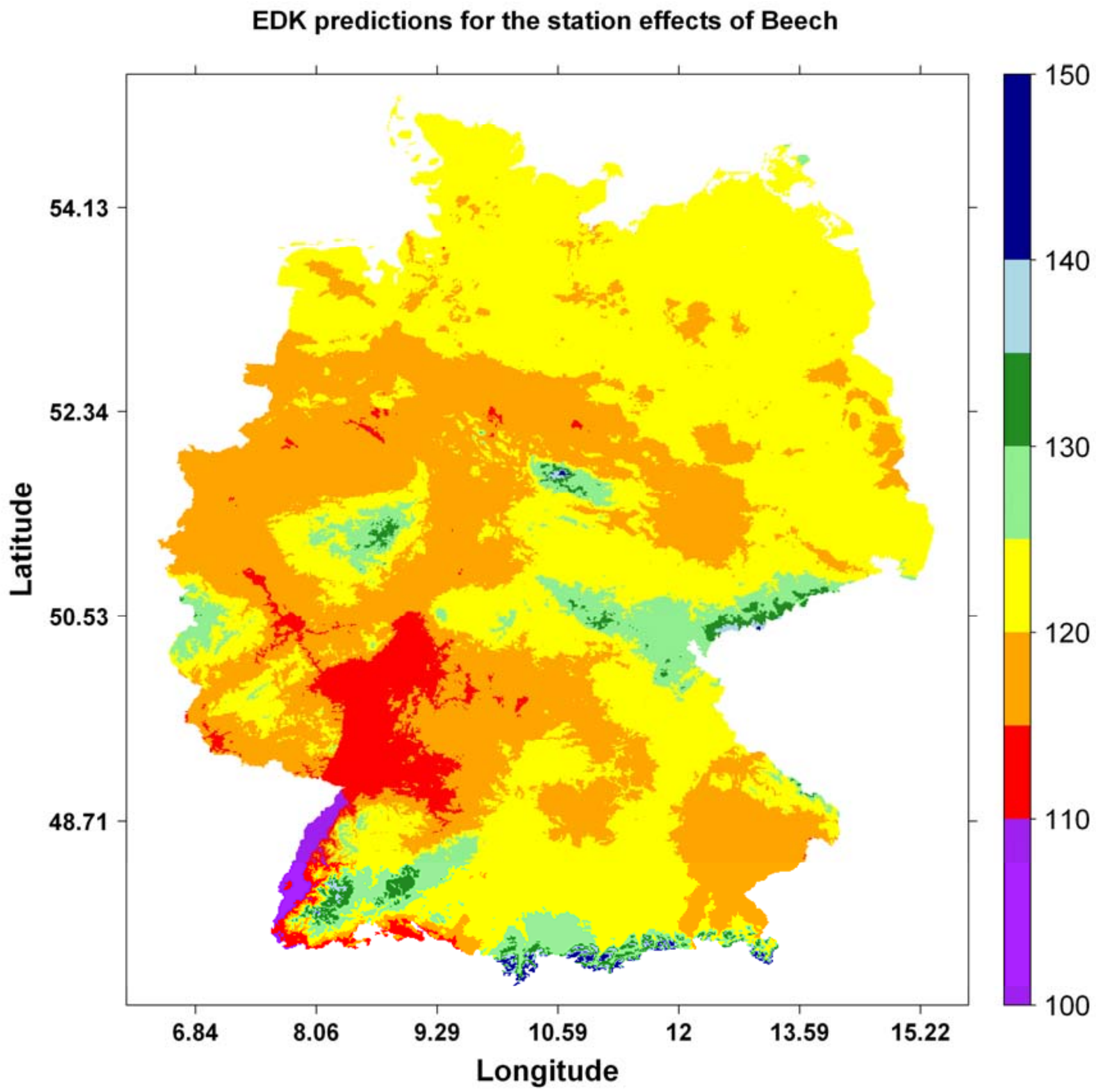

Fig. 7.5. Computed station effects + general mean (day of year) based on observed budburst dates of Beech interpolated using External Drift Kriging (EDK). The DEM of Germany (1*1 km) provides the external variable. Coordinates are based on the Gauss-Krueger system (4th stripe).

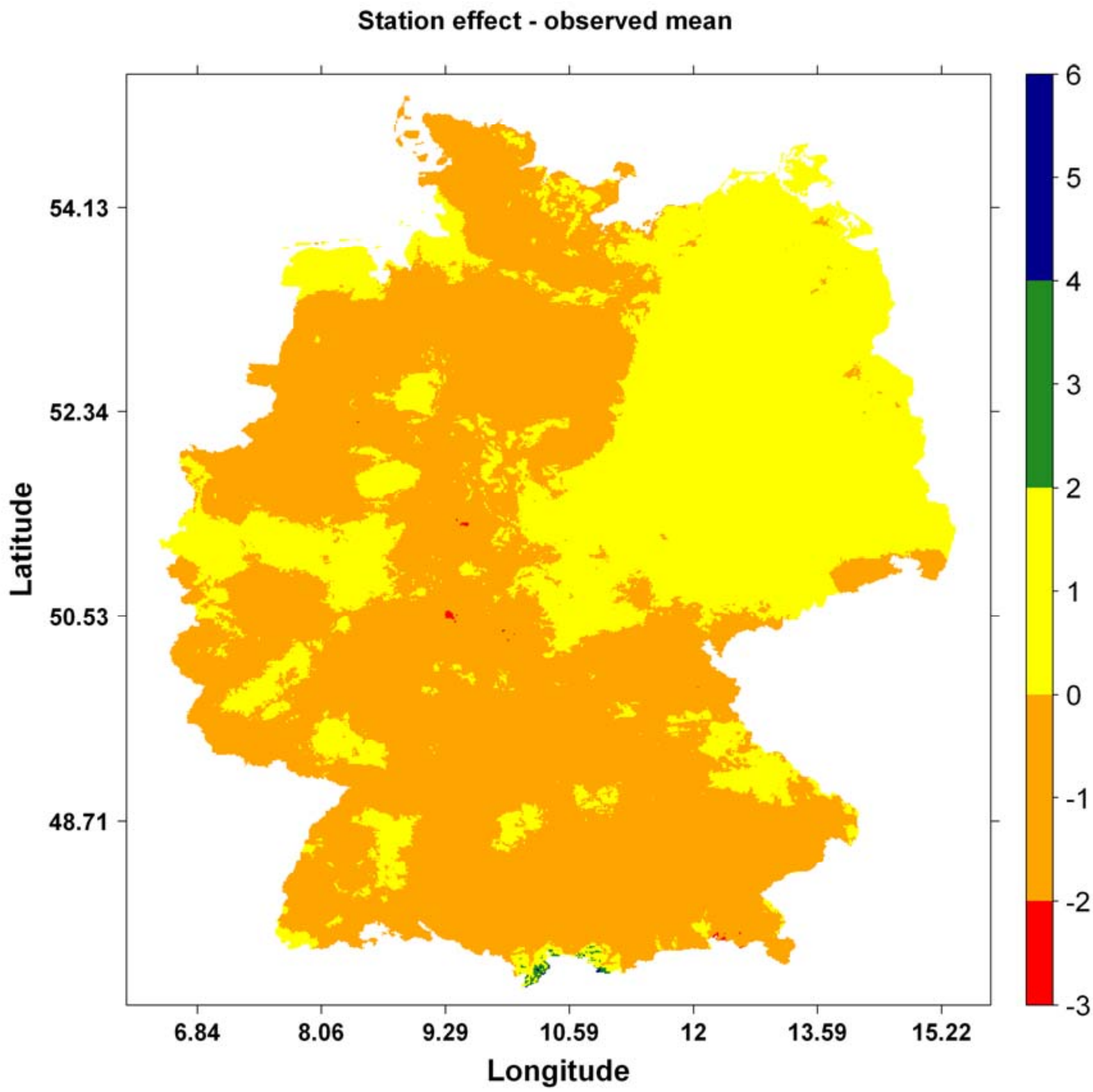

Fig. 7.6. Difference of the interpolated maps: the computed station effects **-** observed mean budburst dates of the respective stations.

The difference map (Fig. 7.6) between station effects and station averages shows a slight general bias towards later combined station effects especially in the eastern part of Germany. These differences might be due to gaps in the time series, which are particularly common in this part of Germany. An indication that this is indeed the case is the fact there is a slight negative tendency between difference and number of observations per station ($P<0.07$).

7.4 Summary

Phenological data are messy data. Their analysis calls for appropriate methods that can deal with their inherent uncertainties as well as correct for effects due to their heterogeneous distribution in time and space. Simple averaging as a method to accommodate noise and gaps is likely to lead to erroneous results especially when the ratio of gaps to total number of observations is high or when a low number of observation series is averaged. The application of linear models to obtain combined time series constitutes an adequate method to handle gaps and noise in individual time series.

The application of Bayes statistics is an alternative way of analysing messy phenological datasets (see e.g. Dose and Menzel 2004). Future work should compare Bayes statistics to the methods discussed in the current paper and address the respective sensitivity to assumptions about priors and underlying distributions as well as to the types of errors and data gaps.

The approach of Gaussian mixtures to consider station x year effects can be further developed by assigning stations to tentative mixture components before checking for outliers or including mixed terms in the linear model (1).

With ongoing efforts to expand the databases of phenological observations by data mining it is very likely that more data sets with sparse data and data gaps will become available in the near future. For example, see the instructive account of the spatial and temporal coverage of the Japanese cherry flowering time series and the step-wise expansion of the data base (Aono and Kazui 2007). The methods described with the current paper are available as an R-package. The routines within this R pheno-package allow for the construction of combined time series that can serve for time series analyses. They can be applied for outlier detection. The calculation of station and year effects facilitates geo-statistical analyses of geographic patterns in the onset of phenological phases as well as their relation to weather pattern in specific years.

7.5 Acknowledgements

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